Logical Expressiveness of Graph Neural Networks

DIG seminar

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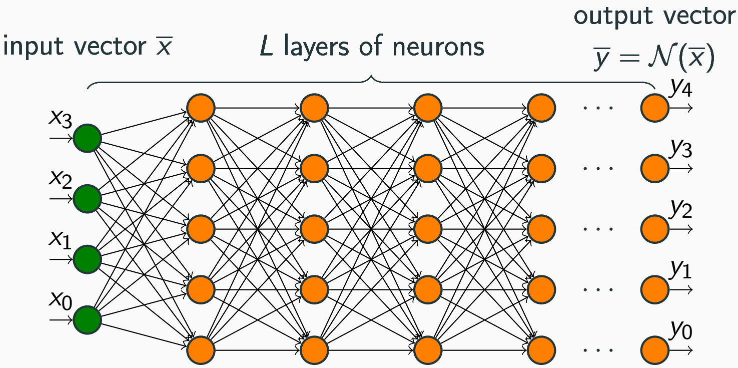
Millennium Institute for Foundational Research on Data, Chile

Graph Neural Networks (GNNs)

- **With:** Pablo Barceló, Egor Kostylev, Jorge Pérez, Juan Reutter, Juan Pablo Silva
- Graph Neural Networks (GNNs) [Merkwirth and Lengauer, 2005, Scarselli et al., 2009]: a class of NN architectures that has recently become popular to deal with structured data
  - → Goal: understand what they are, and their theoretical properties

Neural Networks (NNs)



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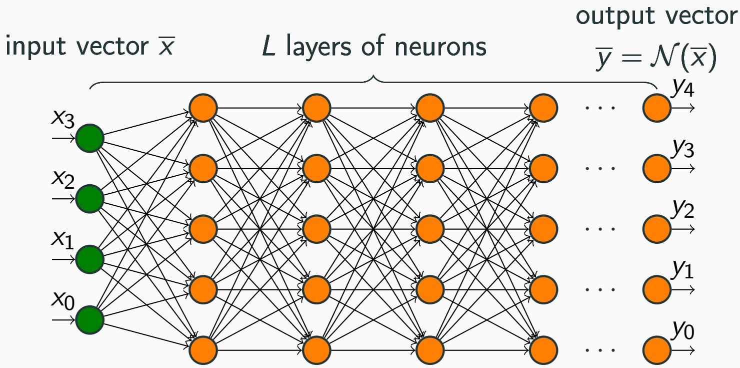

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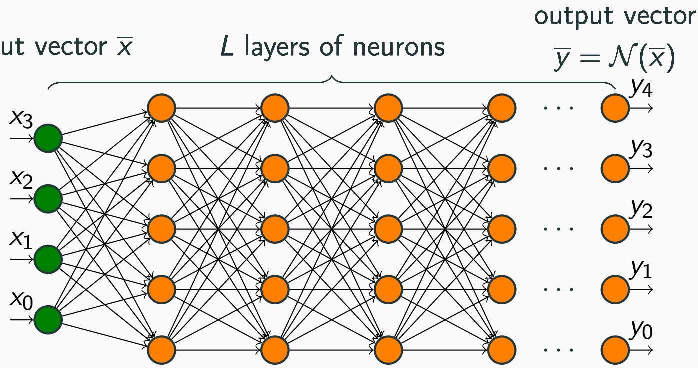

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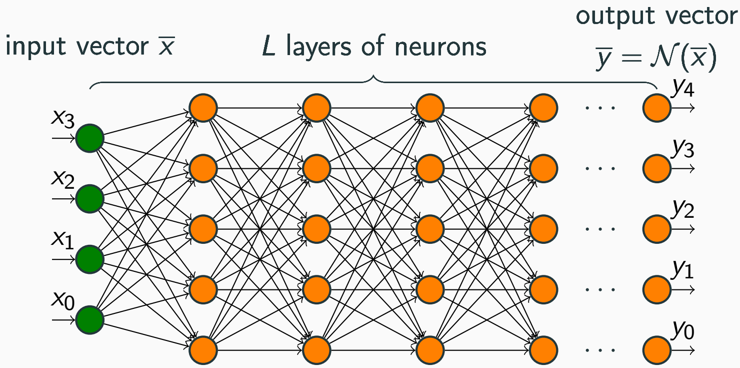

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- Goal: find the weights that "solve" your problem (classification, clustering, regression, etc.)

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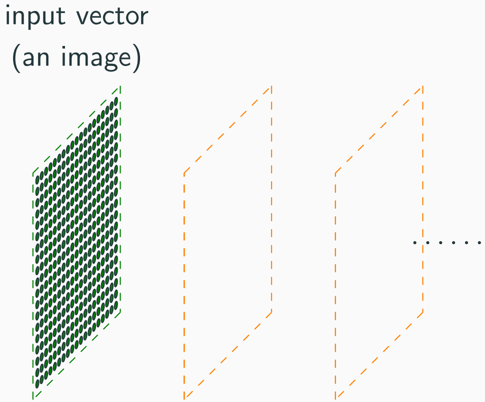
$\rightarrow$ example: input is a 250×250 pixels image, and we want to build a fully connected NN with 500 neurons per layer

$\rightarrow$ between the first two layers we have $250 \times 250 \times 500 = \mathbf{31,250,000}$ weights

Convolutional Neural Networks



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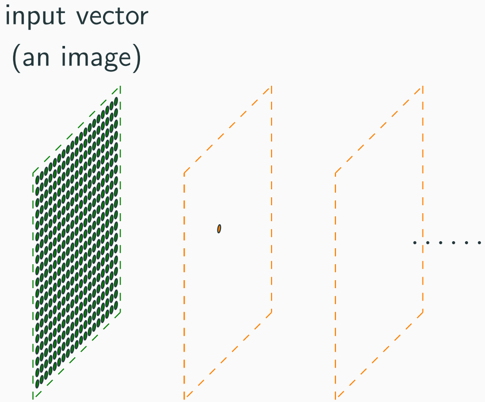

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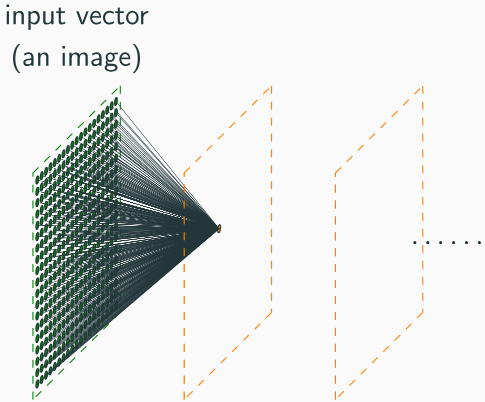

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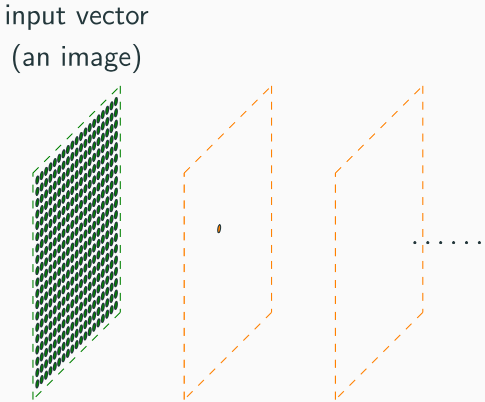

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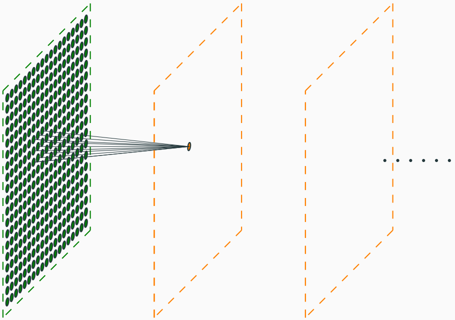

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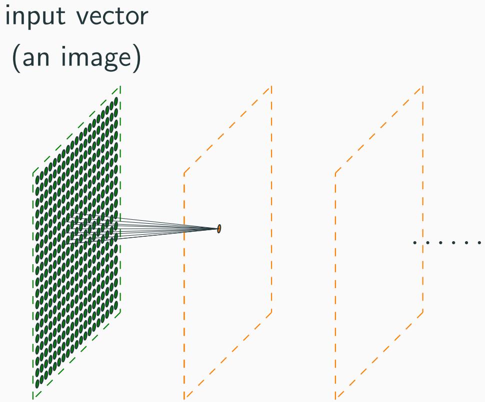

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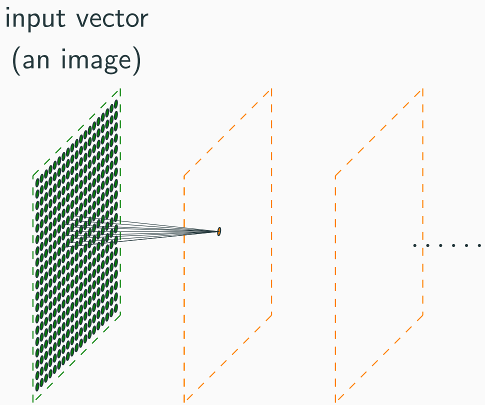

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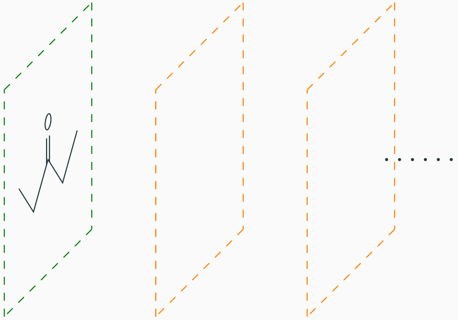
$\rightarrow$ fewer weights to learn (e.g, $500 * 9 = 4,500$ for the first layer)

$\rightarrow$ other advantage: recognize patterns that are local

Graph Neural Networks (GNNs)

input vector
(a molecule)

output:
is it poisonous? (e.g., [Duvenaud et al., 2015])



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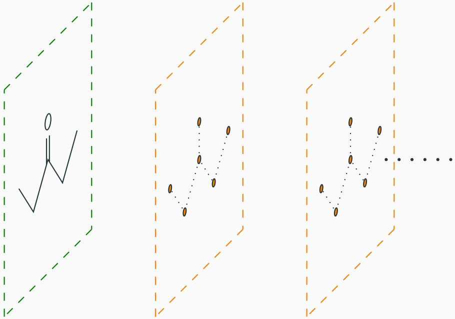

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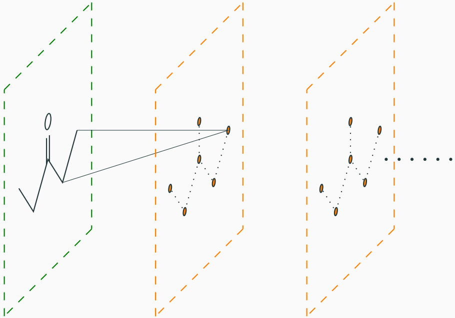

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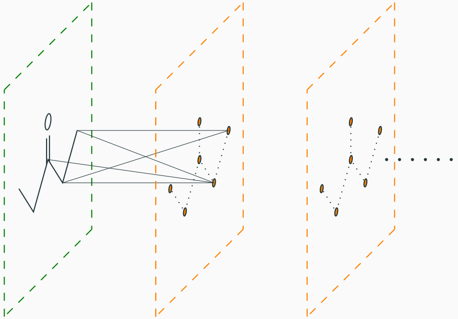

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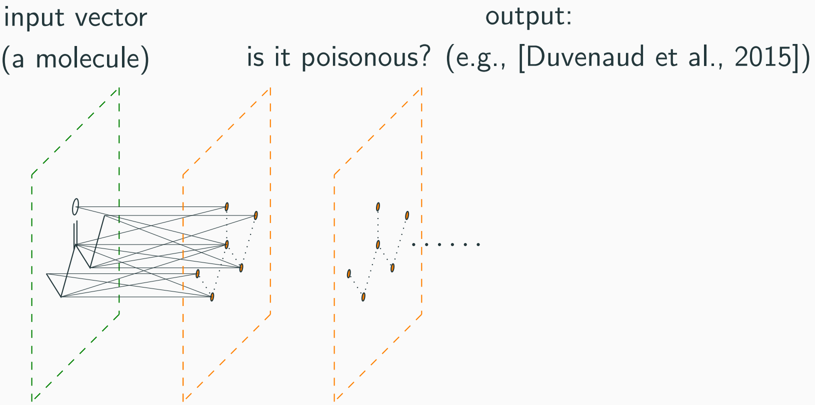

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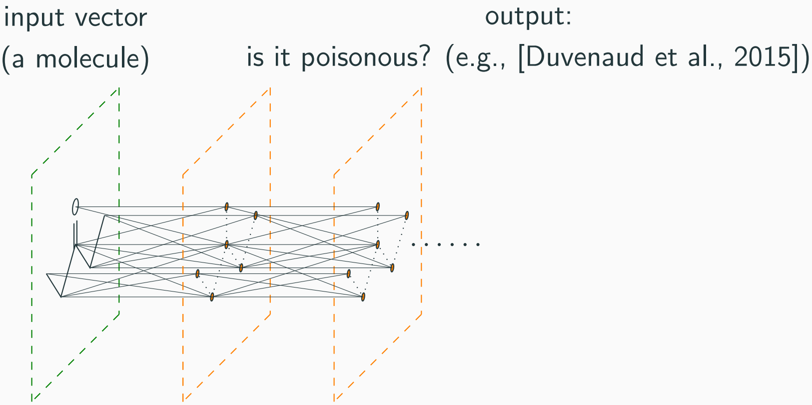

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Question: what can we do with graph neural networks? (from a *theoretical* perspective)

GNNs: formalisation

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- Where the $\mathrm{AGG}^{(i)}$ are called *aggregation functions* and the $\mathrm{COMB}^{(i)}$ *combination functions*
- Let us call such a GNN an aggregate-combine GNN (AC-GNN)

Link with Weisfeiler-Lehman

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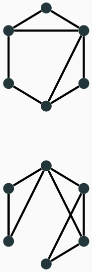
4. If the two graphs have the same multiset of colors, **accept**, else **reject**

Weisfeiler-Lehman: example 1



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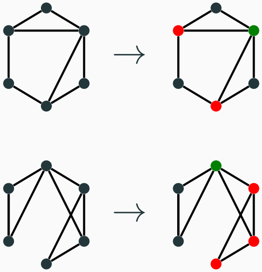

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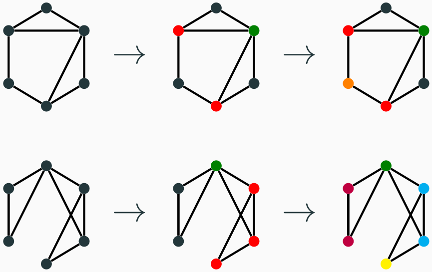

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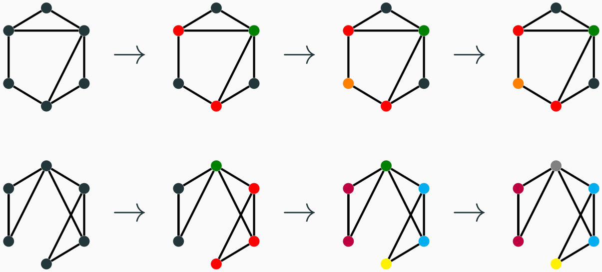

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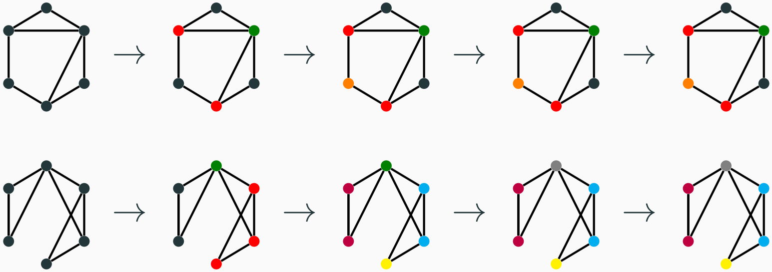

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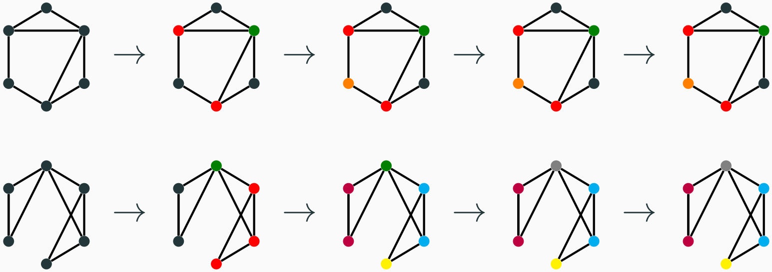
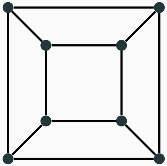


$$\{\{\textcolor{red}{\bullet}, \textcolor{red}{\bullet}, \textcolor{orange}{\bullet}, \bullet, \bullet, \textcolor{green}{\bullet}\}\} \neq \{\{\textcolor{purple}{\bullet}, \textcolor{purple}{\bullet}, \textcolor{gray}{\bullet}, \textcolor{cyan}{\bullet}, \textcolor{cyan}{\bullet}, \textcolor{yellow}{\bullet}\}\}$$

$\rightarrow$ **reject** (and this is correct)

Weisfeiler-Lehman: example 2



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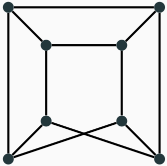

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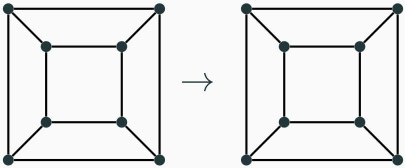

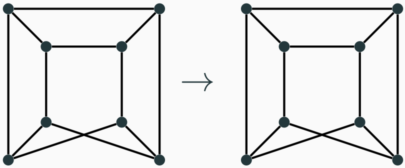

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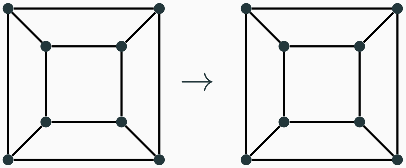

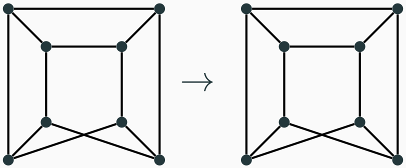

$$\{\{\bullet, \bullet, \bullet, \bullet, \bullet, \bullet, \bullet, \bullet, \}\} = \{\{\bullet, \bullet, \bullet, \bullet, \bullet, \bullet, \bullet, \bullet, \}\}$$

$\rightarrow$ **accept** (but this is incorrect!)

Link between AC-GNNs and Weisfeiler-Lehman

Weisfeiler-Lehman works like this:

- $\mathrm{WL}_{\mathrm{u}}^{(0)} \coloneqq \lambda(\mathrm{u})$
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Corollary ([Morris et al., 2019, Xu et al., 2019])

If WL assigns the same value to two nodes at round i, then any AC-GNN will also assign the same value to these two nodes at round i

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- For instance, **logical classifiers**?

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- Given these connections, we ask: let $\varphi(x)$ be a unary FOC_2 formula. Can we "capture" it with an AC-GNN?
  - (capture: after some number L of layers, we have $\boldsymbol{x}_u^{(L)} = 1$ if $(G,u) \models \varphi(x)$ and $\boldsymbol{x}_u^{(L)} = 0$ if $(G,u) \not\models \varphi(x)$)

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Theorem ([Cai et al., 1992])

We have $\mathsf{WL}_u^{(i)} = \mathsf{WL}_v^{(i)}$ if and only if u and v agree on all FOC_2 unary formulas of quantifier depth $\leq i$ in G

- Given these connections, we ask: let $\varphi(x)$ be a unary FOC_2 formula. Can we "capture" it with an AC-GNN?
  - (capture: after some number L of layers, we have $\boldsymbol{x}_u^{(L)} = 1$ if $(G, u) \models \varphi(x)$ and $\boldsymbol{x}_u^{(L)} = 0$ if $(G, u) \not\models \varphi(x)$)

$\rightarrow$ We answer this!

AC-GNNs for FOC_2: graded modal logic

- **Observation**: there are FOC_2 unary formulas that we cannot capture with any AC-GNN
  - $\rightarrow$ $\varphi(x) = \mathrm{Blue}(x) \wedge \exists y\, \mathrm{Red}(y)$

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$\rightarrow$ Graded modal logic [de Rijke, 2000]: syntactical fragment of FOC_2 in which quantifiers are only of the form $\exists^{\geq N} y\, (E(x,y) \wedge \varphi'(y))$

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Theorem

Let φ be a unary FOC formula. If φ is equivalent to a graded modal logic formula, then φ can be captured by an AC-GNN, otherwise it cannot.

Positive result: building simple GNNs

- We say that a GNN is simple if we update according to

$$\boldsymbol{x}_u^{(i+1)} := f\left(\boldsymbol{C}^{(i)}\boldsymbol{x}_u^{(i)} + \boldsymbol{A}^{(i)}\left(\sum_{v\in\mathcal{N}_G(u)} \boldsymbol{x}_v^{(i)}\right) + \boldsymbol{b}^{(i)}\right),$$

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$\rightarrow$ After L layers, we will have $\boldsymbol{x}_u^{(L)}(\varphi) = 1$ iff $u \models \varphi(x)$

Negative result: Van Benthem/Rosen characterization of GML

- We use the following [Otto, 2019]: let φ be an FOC unary formula that is not equivalent to any GML formula. Then there exist a graph G and two nodes $u, v \in G$ such that $u \models \varphi$ and $v \not\models \varphi$ and such that for all $i \in \mathbb{N}$ we have $\mathsf{WL}_u^{(i)} = \mathsf{WL}_v^{(i)}$

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$\rightarrow$ By [Morris et al., 2019, Xu et al., 2019], any AC-GNN must have $\boldsymbol{x}_u^{(i)} = \boldsymbol{x}_v^{(i)}$ for all $i \in \mathbb{N}$, so it cannot capture φ

ACR-GNNs for FOC_2

- Can we extend AC-GNNs so that they are able to capture any FOC_2 unary formula?

→ Yes: add global computations in between every layer.

→ $\boldsymbol{x}_u^{(i+1)} := \mathrm{COMB}^{(i+1)}(\boldsymbol{x}_u^{(i)}, \mathrm{AGG}^{(i+1)}(\{\{\boldsymbol{x}_v^{(i)} \mid v \in \mathcal{N}_G(u)\}\}), \mathrm{READ}^{(i+1)}(\{\{\boldsymbol{x}_v^{(i)} \mid v \in G\}\}))$

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→ Having readouts strictly increases the discriminative power of GNNs

Proofsketch

We use the following result of [Lutz et al., 2001]:

- Every FOC_2 formula φ can be rewritten as a FOC_2 formula φ' in which every unary subformula $\varphi''(x)$ starting with a quantifier is of one of the following form:
  - $\exists^{\geq N} y\, x = y \wedge \psi(y)$
  - $\exists^{\geq N} y\, E(x, y) \wedge \psi(y)$
  - $\exists^{\geq N} y\, \neg E(x, y) \wedge \psi(y)$
  - $\exists^{\geq N} y\, \neg E(x, y) \wedge x \neq y \wedge \psi(y)$
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We then build a simple ACR-GNN just like for AC-GNNs and GML, but, for instance:

- $\boldsymbol{x}_u^{(i+1)}(\exists^{\geq N} y\, \neg E(x, y) \wedge \psi(y)) = f(\sum_{v \in G} \boldsymbol{x}_v^{(i)}(\psi) - \sum_{v \in \mathcal{N}_G(u)} \boldsymbol{x}_v^{(i)}(\psi) - (N-1))$

Number of readouts

Theorem

Each FOC_2 *unary formula is captured by a simple ACR-GNN*

- How many readouts do we need? A fixed number? The quantifier depth of the formula?

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→ We show that one final readout is enough (but the ACR-GNN is no longer simple)

Theorem

Each FOC_2 unary formula is captured by an ACR-GNN with one final readout

Conclusion

- We have seen the relationship between GNNs and WL
- We started to study the relationships between GNNs and logic
  - $\rightarrow$ "$\mathrm{GML} = \mathrm{FOC} \cap$ AC-GNNs $\subseteq$ simple AC-GNNs"
  - $\rightarrow$ "$\mathrm{FOC}_2 \subseteq$ simple ACR-GNNs"
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- Open: $\mathrm{FOC} \cap$ ACR-GNNs $= \mathrm{FOC}_2$?

- Since then, GNNs have been compared to other known frameworks for local computations (message-passing, distributive local algorithms, etc). See, e.g., [Loukas, 2019, Sato et al., 2019]

Thanks for your attention!

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