Logical Expressiveness of Graph Neural Networks

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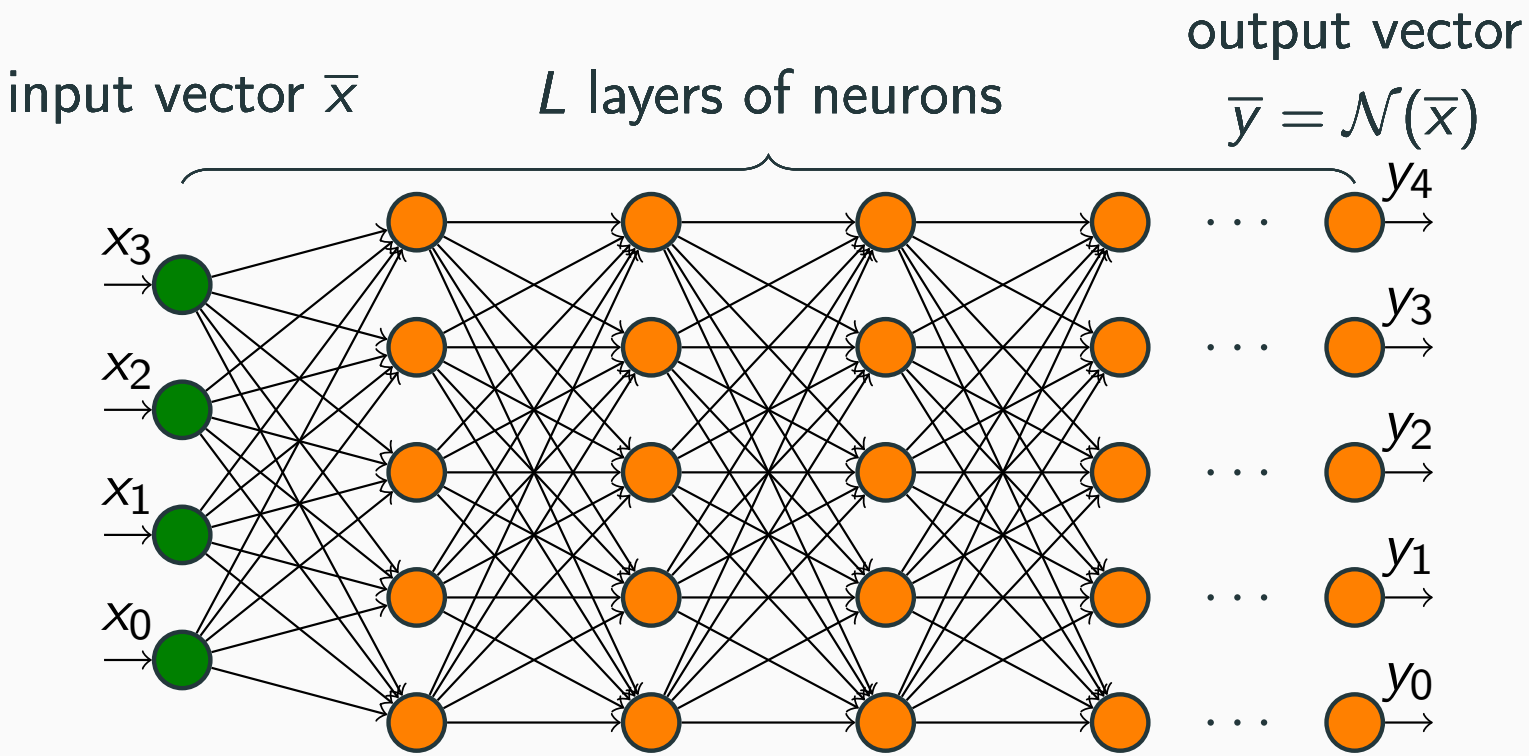
Millennium Institute for Foundational Research on Data, Chile

Graph Neural Networks (GNNs)

- **With:** Pablo Barceló, Egor Kostylev, Jorge Pérez, Juan Reutter, Juan Pablo Silva (ongoing work)
- 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 their theoretical properties

Neural Networks (NNs)



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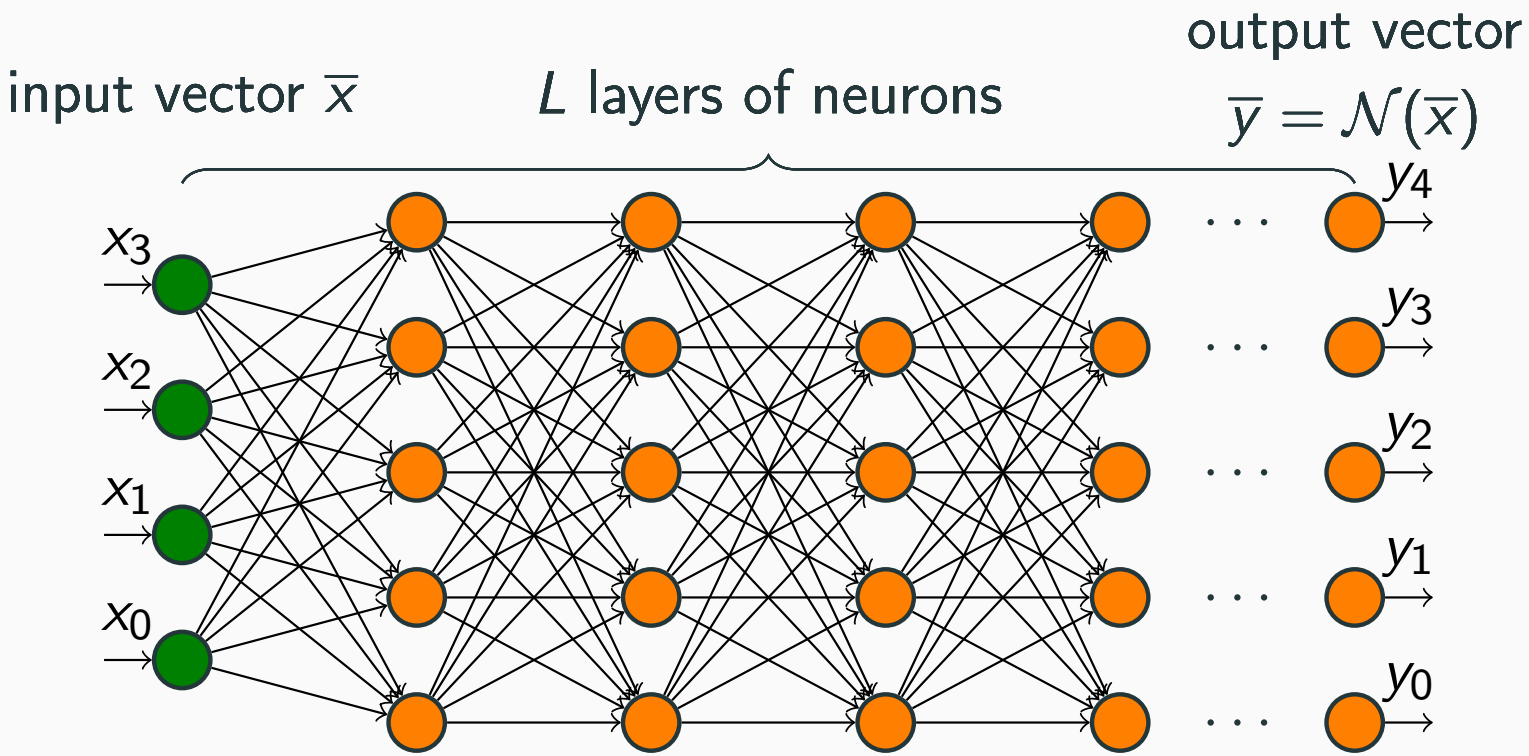

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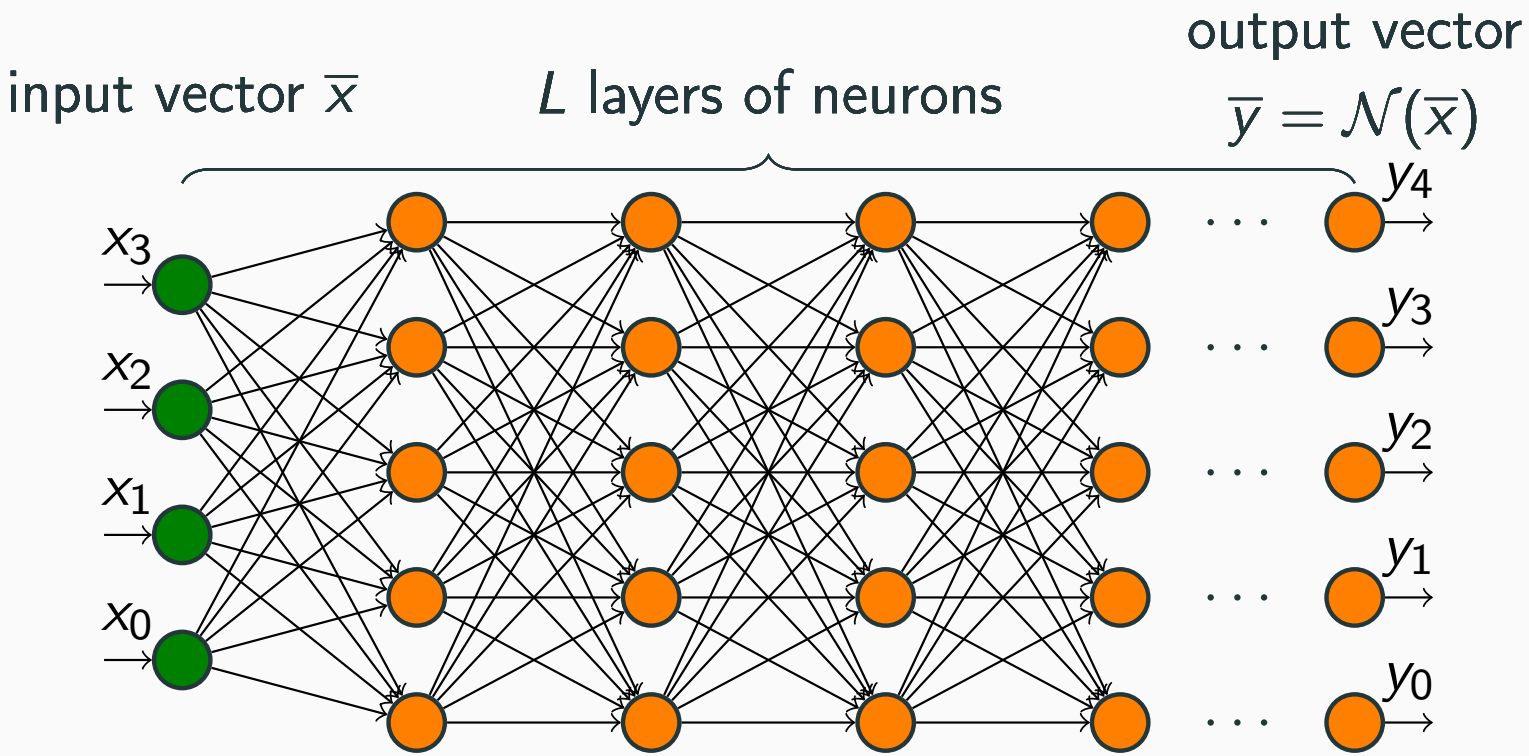

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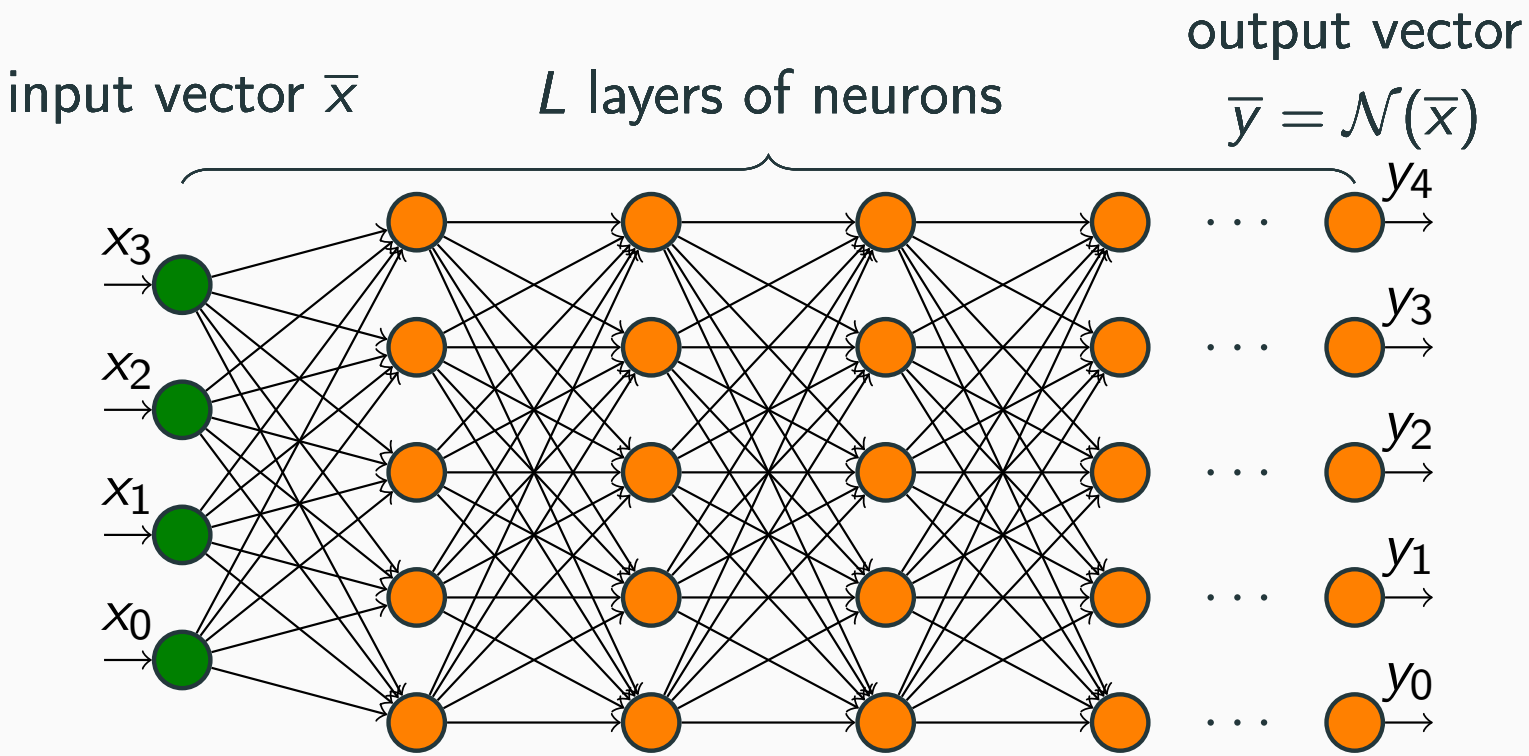

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- Goal: find the weights that "solve" your problem (classification, clustering, regression, etc.)

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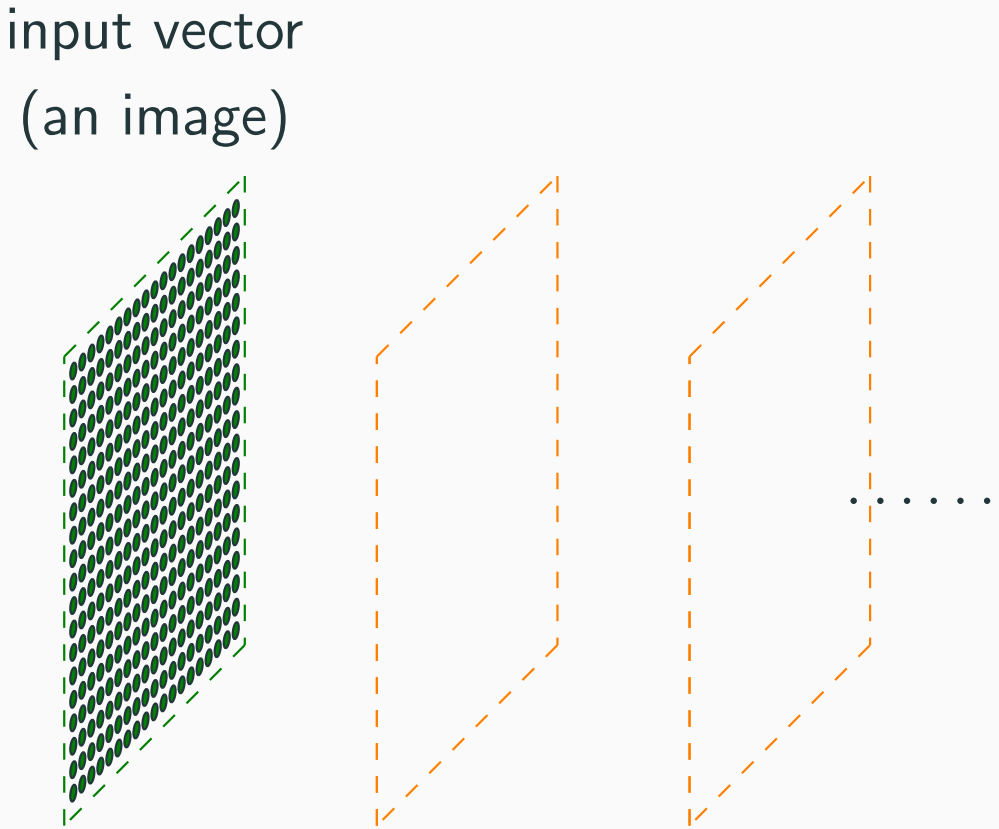
$\rightarrow$ example: input is a 250×250 pixels image, and we want to build a fully connected NN with 500 neurons per layer

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

Convolutional Neural Networks



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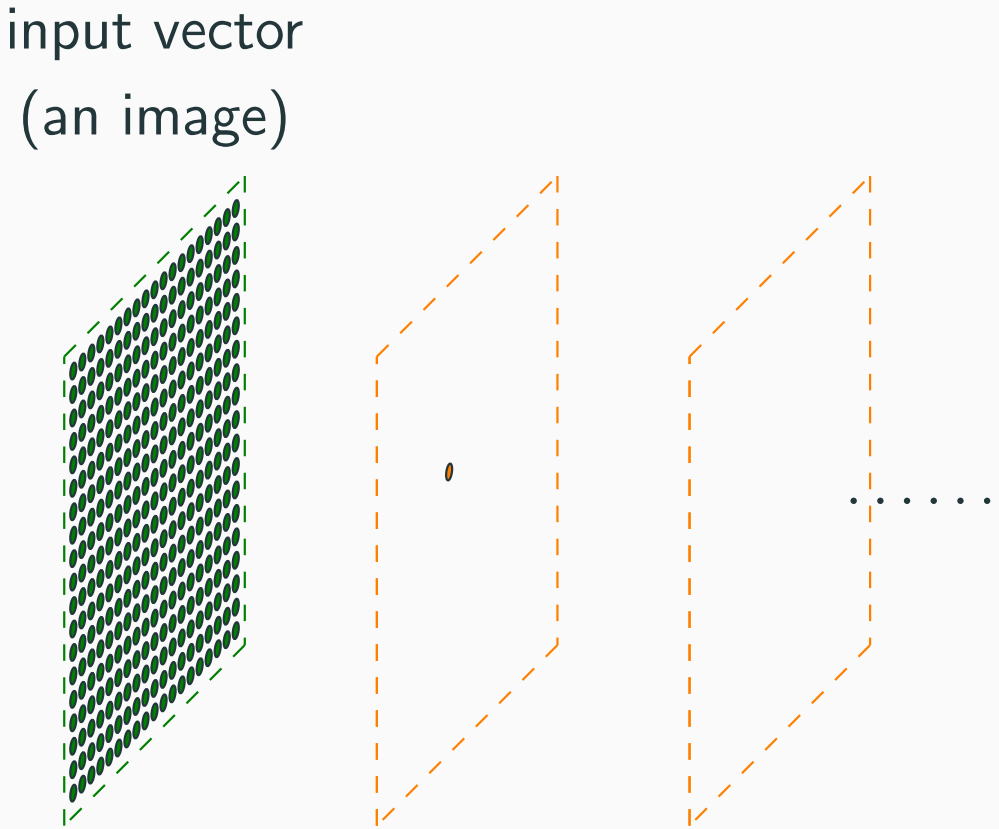

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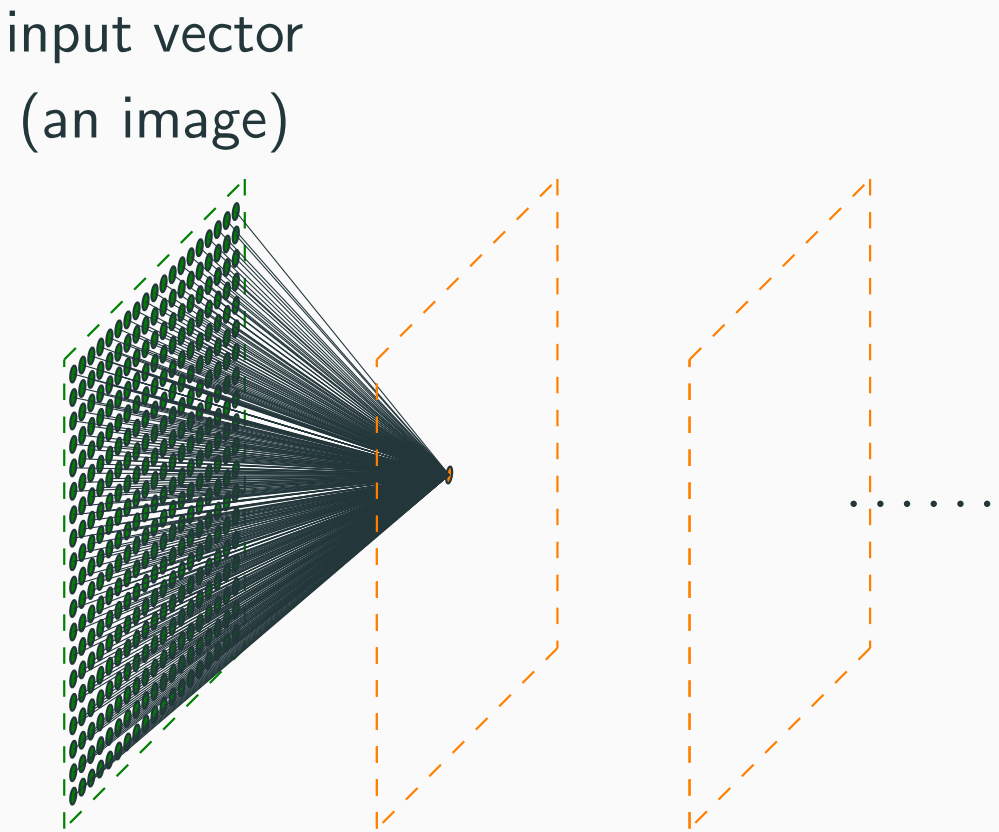

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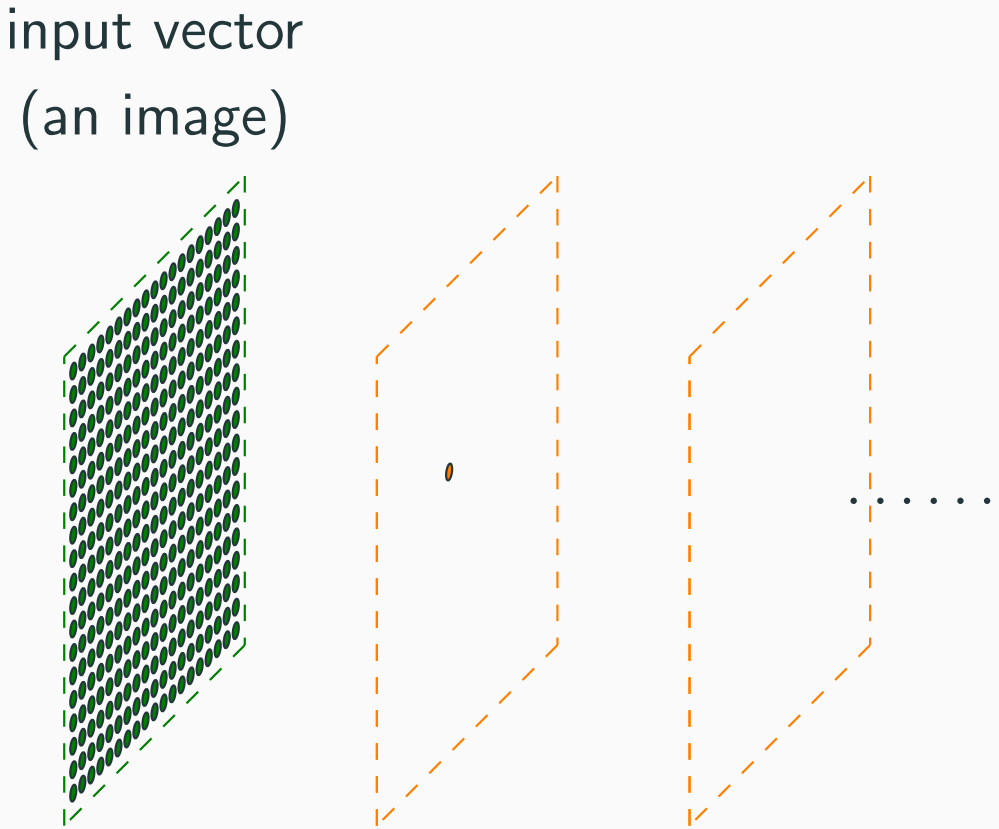

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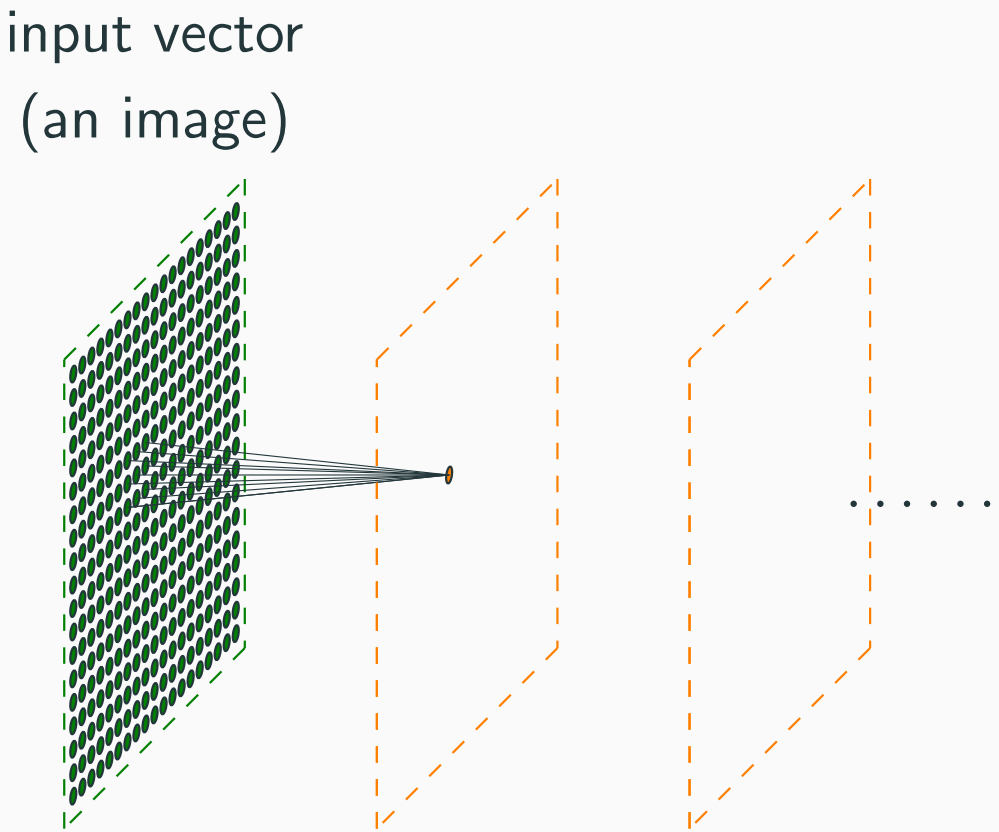

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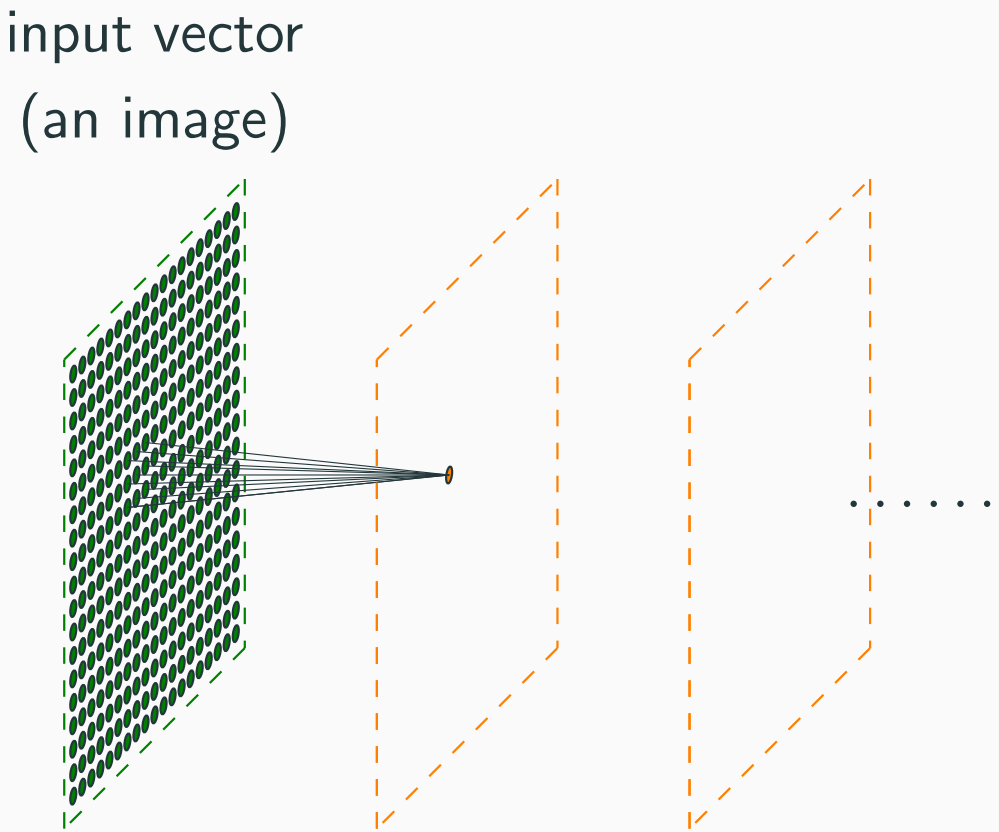

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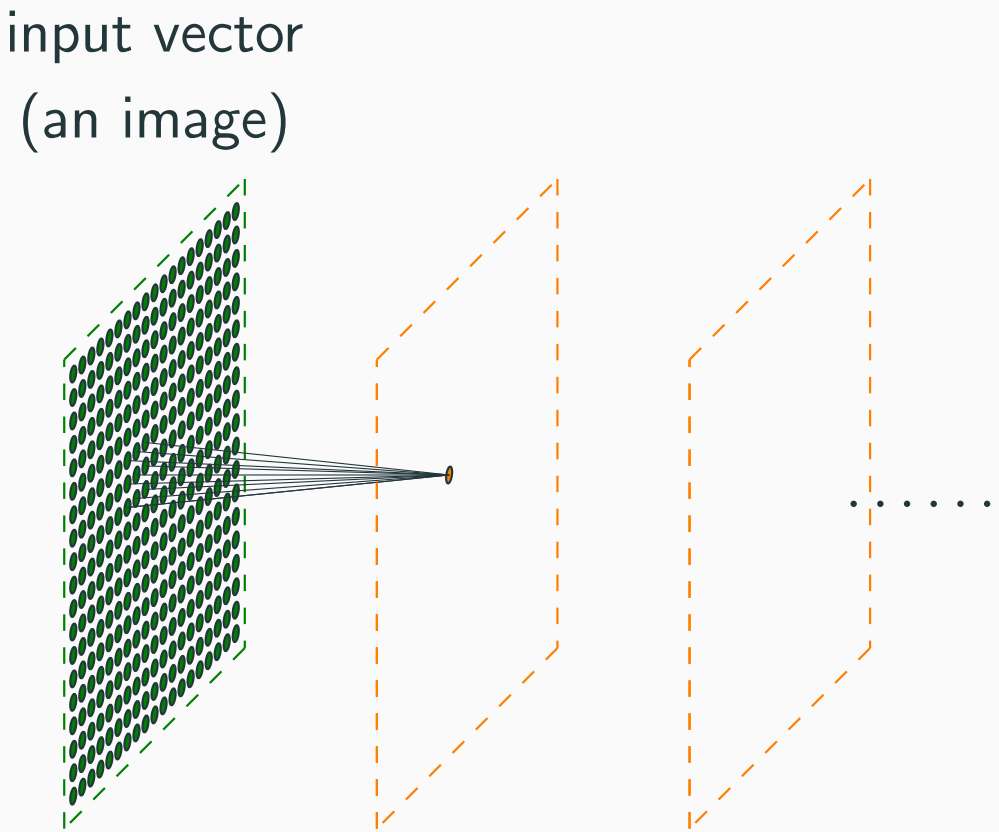

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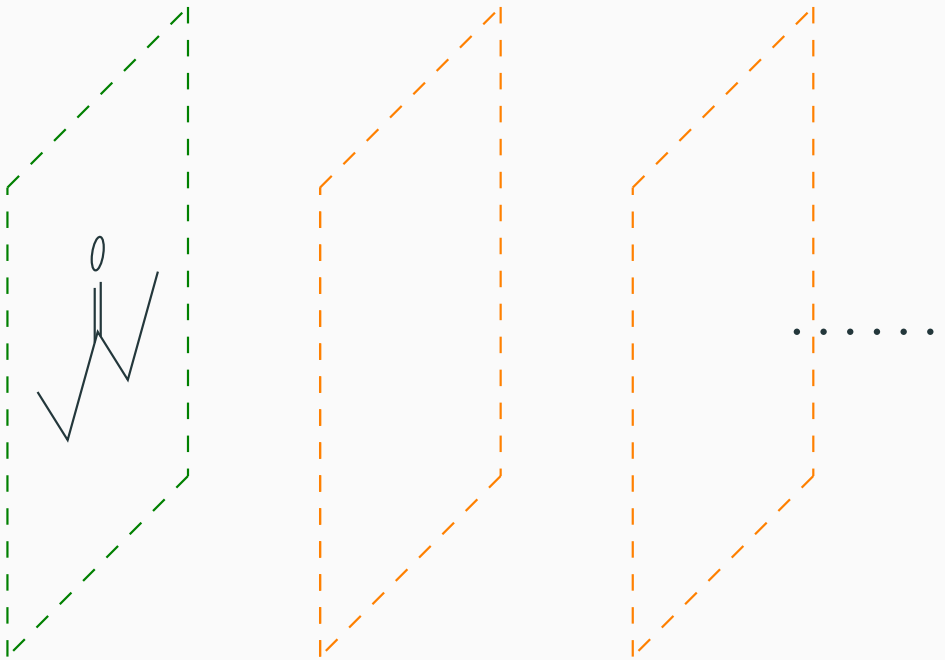
$\rightarrow$ other advantage: recognize patterns that are local

Graph Neural Networks (GNNs)

input vector (a molecule)

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



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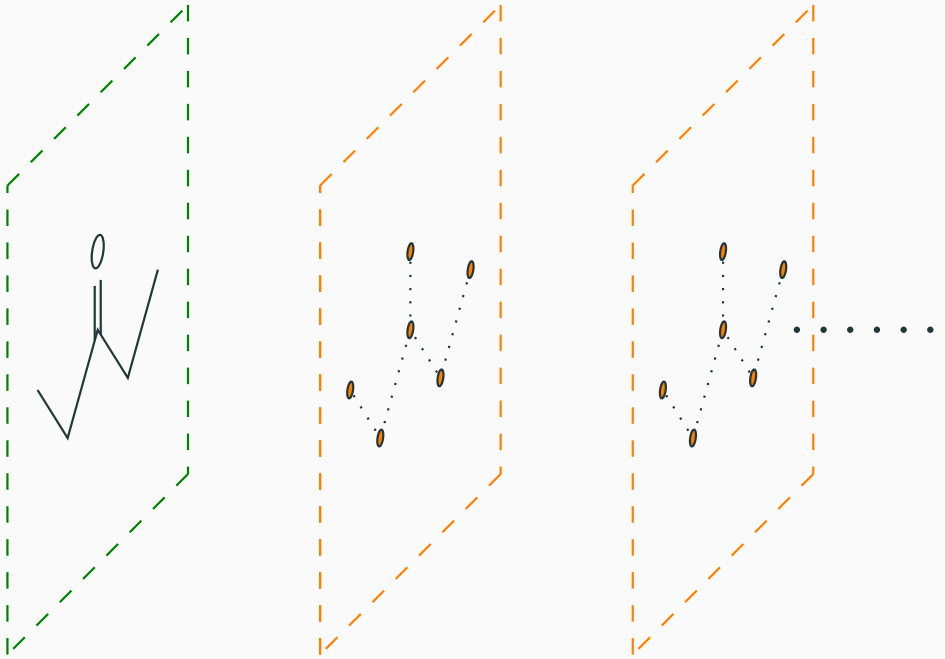

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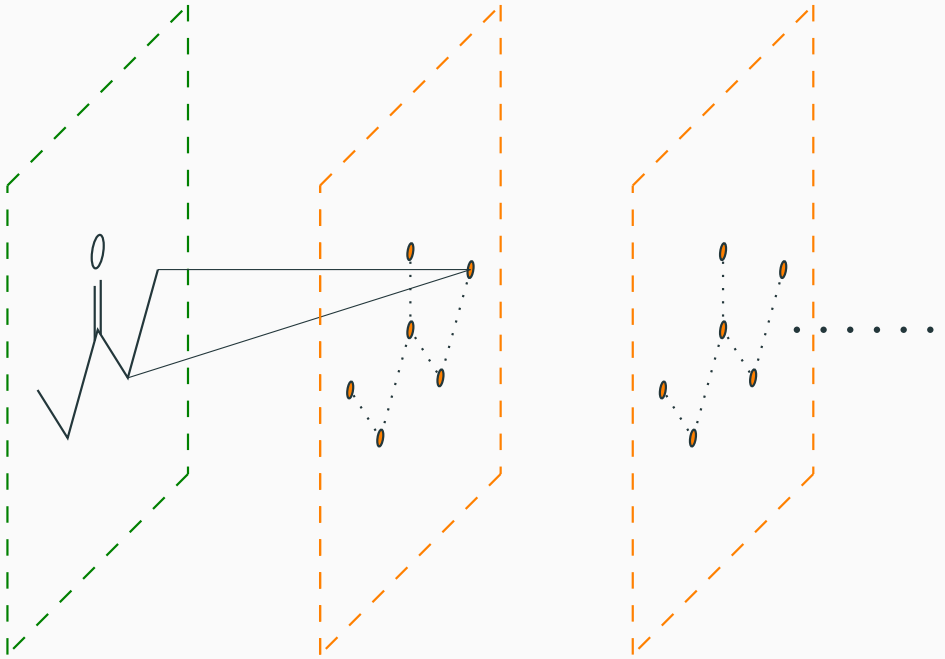

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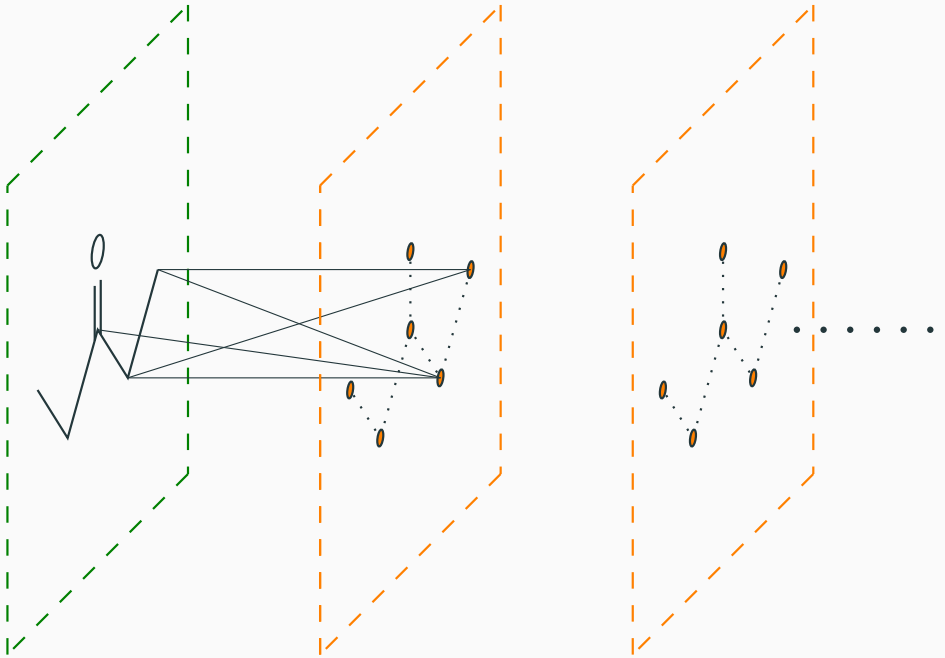

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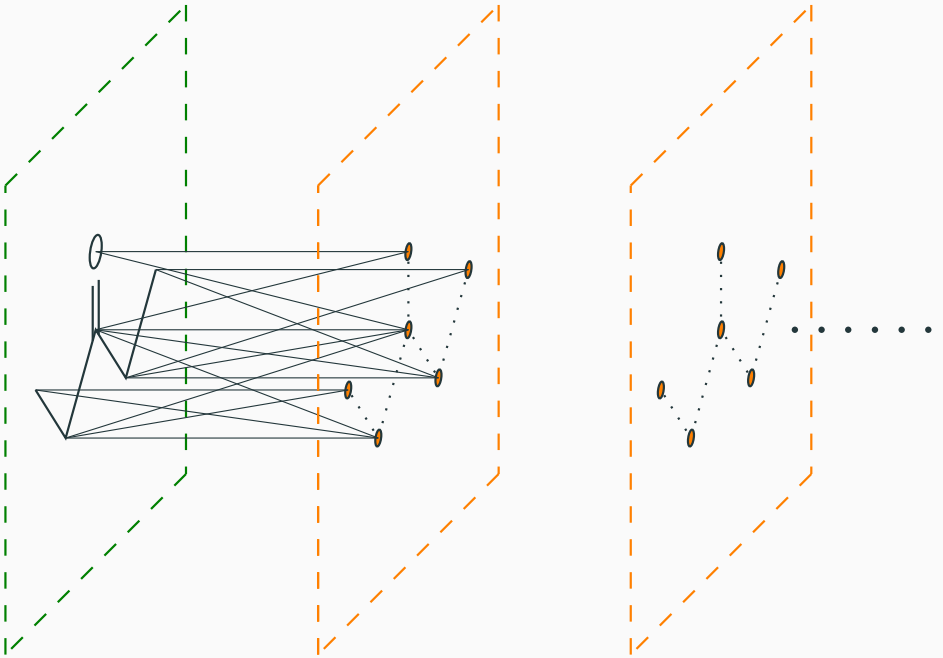

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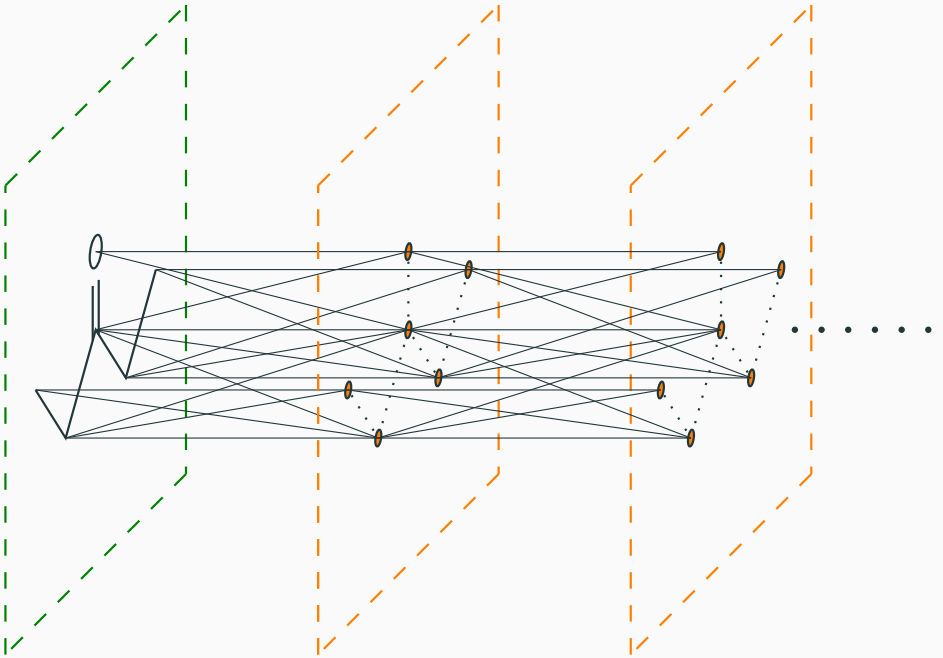

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Question: what can we do with graph neural networks? (from a *theoretical* perspective)

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)

AC-GNNs: what can they do? Related work (1/2)

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Corollary ([Morris et al., 2019, Xu et al., 2019])

If WL assigns the same value to two nodes in a graph, then any AC-GNN will also assign the same value to these two nodes

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- [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 φ be an FOC_2 formula. Can we "capture" it with an AC-GNN?

$\rightarrow$ 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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Theorem

Let φ be a unary FOC_2 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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  - $\boldsymbol{x}_u^{(i+1)}(\neg\varphi') = f(-\boldsymbol{x}_u^{(i)}(\varphi') + 1)$
  - $\boldsymbol{x}_u^{(i+1)}(\exists^{\geq N} y\, E(x,y) \wedge \varphi') = f(\sum_{v\in\mathcal{N}_G(u)} \boldsymbol{x}_v^{(i)}(\varphi') - (N-1))$

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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_2 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 $\boldsymbol{x}_u^{(i)} = \boldsymbol{x}_v^{(i)}$, 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?

$\rightarrow$ Yes: add global computations in between every layer.

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

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Theorem

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

$\rightarrow$ Having readouts strictly increases the discriminative power of GNNs

Conclusion and Future Work

- We started to study the relationships between GNNs and logic
  - $\rightarrow$ "$\mathrm{GML} = \mathrm{FOC}_2 \cap$ AC-GNNs $\subseteq$ simple AC-GNNs"
  - $\rightarrow$ "$\mathrm{FOC}_2 \subseteq$ simple ACR-GNNs"

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  - $\rightarrow$ "$\mathrm{FOC}_2 \subseteq$ simple ACR-GNNs"

Ideas of future work:

- $\mathrm{FOC} \cap$ ACR-GNNs $= \mathrm{FOC}_2$?
- A logic that fully captures all simple AC-GNNs?
- Given a GNN, find a formula that describes it?
- Which functions can be *approximated* by GNNs?
- Other architectures of NN?

Conclusion and Future Work

- We started to study the relationships between GNNs and logic
  - $\rightarrow$ "$\mathrm{GML} = \mathrm{FOC}_2 \cap$ AC-GNNs $\subseteq$ simple AC-GNNs"
  - $\rightarrow$ "$\mathrm{FOC}_2 \subseteq$ simple ACR-GNNs"

Ideas of future work:

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Thanks for your attention!

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