Logical Approach to Graph Neural Networks

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6. Expressiveness of Graph Neural Networks.

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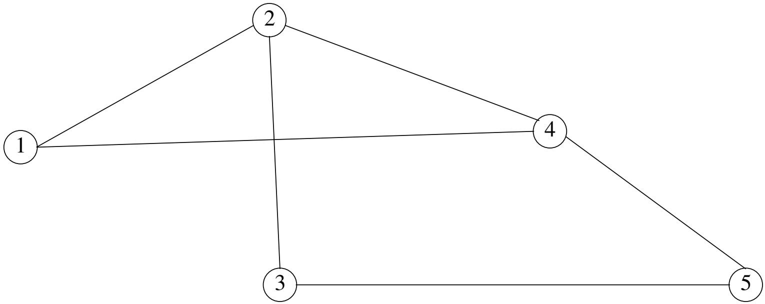
- Wide range of applications, e.g., computer vision, natural language processing, social network analysis, knowledge graphs, chemistry, and recommendation systems.
- We consider the core GNN architecture, known as Message Passing GNN or aggregate-combine GNN.
- There are many other variants, but they are mostly based in this core architecture.

GNN



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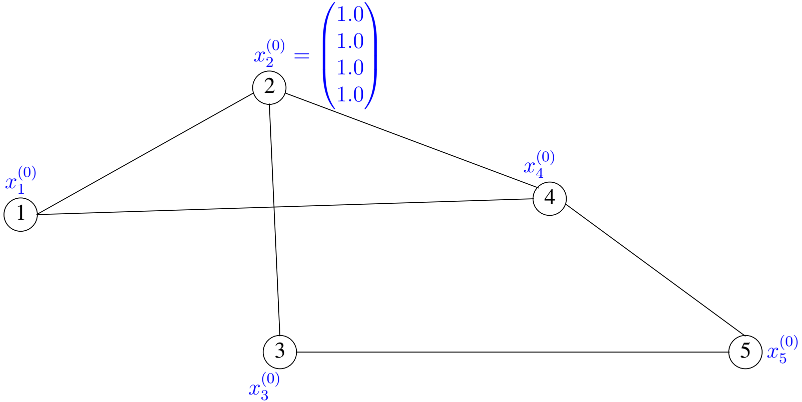
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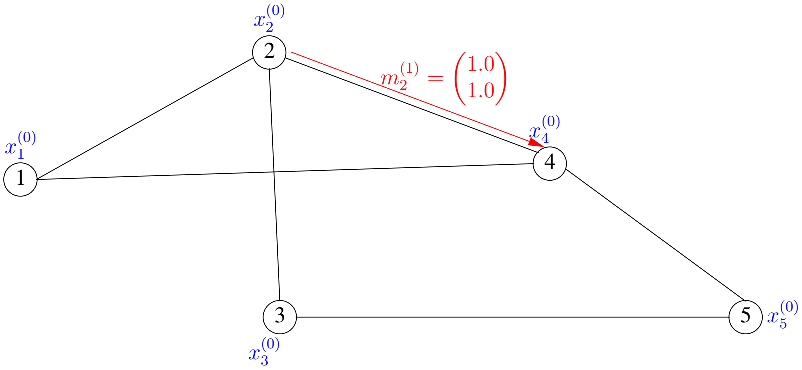

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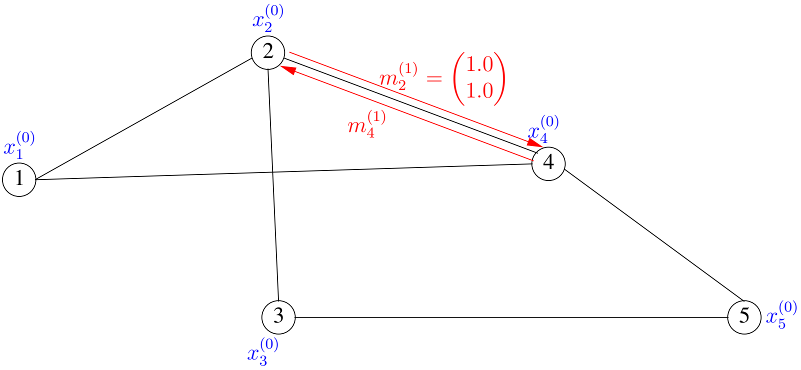

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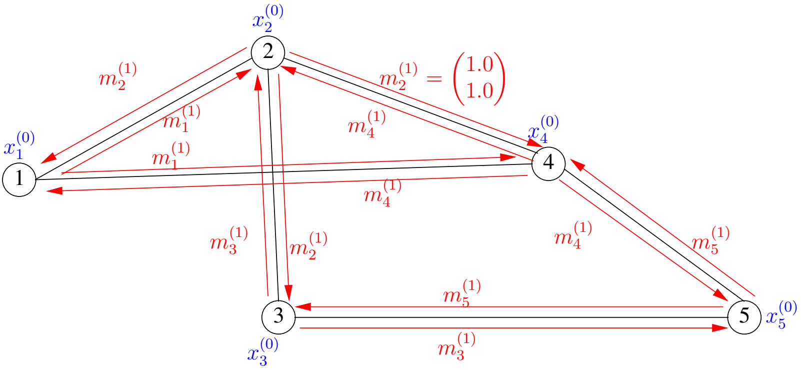

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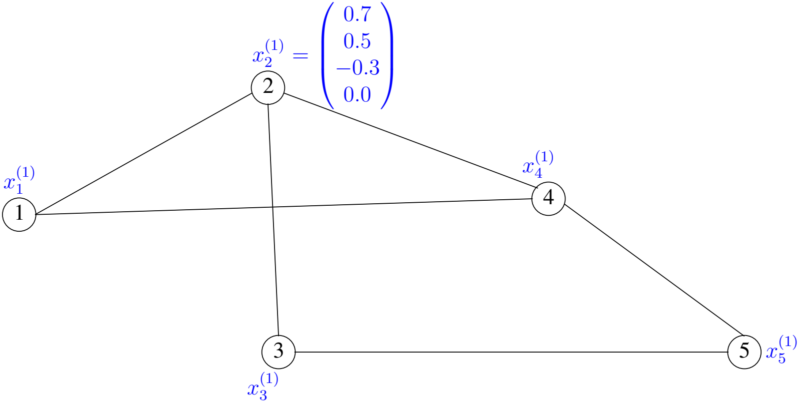
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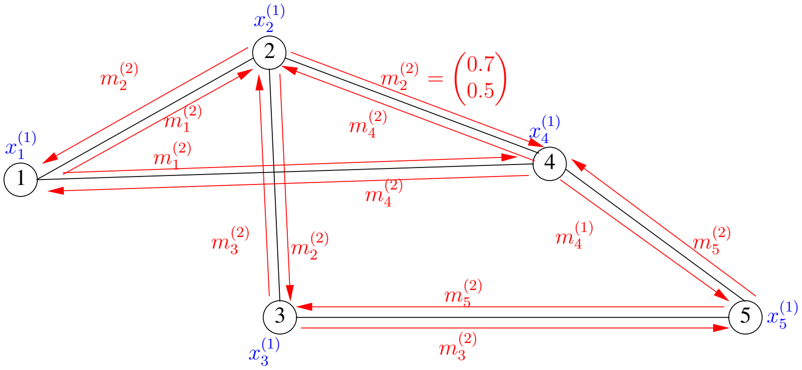

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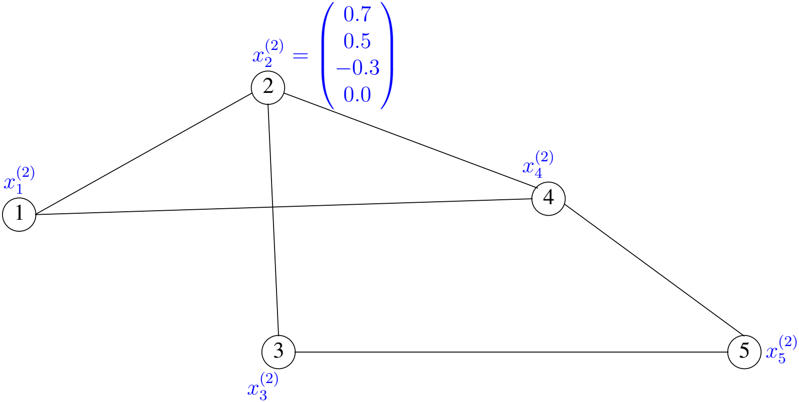

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Computation of GNN

A GNN $\mathcal{N}$ with d layers maps a vertex-labelled graph G with finite node set V to a sequence of functions

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  - Symmetric function, e.g., sum, mean, max.
  - Either applied directly to "states" $\zeta^{(t-1)}(w)$ or to some (learned) linear function of these states.

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To compute a graph level function f that maps graphs to $\mathbb{R}^q$, we apply an aggregate readout function aggro s.t.

$$f(G) = \mathrm{aggro}\big(\{\!\{\zeta^{(d)}(v) \mid v \in V\}\!\}\big)$$

(aggro is normally summation followed a FNN)

Properties of Functions Computed by GNNs

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Equivariance of Node Level Functions If f is a node level function computed by a GNN and h is an isomorphism from a graph G to a graph H, then for all node v of G we get

$$F(G)(v) = F(H)(h(v))$$

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The number of iterations might depend for instance on the size of the input graph or the evolution of the sequence $(\zeta^{(t)})_{t\geq 0}$.

No convergence is required, we can arbitrary decide when to stop.

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- If some colour appears different number of times in the histograms of two graphs G and H, then the graphs are non-isomorphic.
- Provides an efficient but incomplete isomorphism check.
  - $O((n+m)\log n)$ for n nodes and m edges.

Finite Variable Counting Logic

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Same expressiveness than FO,

$$\exists^{\geq p} x \varphi(x) \equiv \exists x_1 \ldots \exists x_p \Big(\bigwedge_{1 \leq i \leq j \leq p} x_i \neq x_j \wedge \bigwedge_{i=1,\ldots,p} \varphi(x_i) \Big)$$

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Translation from C to FO incurs an increase in the number of variables as well as the quantifier rank, e.g.,

$$\forall x \exists^{\geq d} y E(x,y) \quad \text{(uses 2 variables and quantifier rank 2)}$$

An equivalent FO formula needs at least $d+1$ variables and at least quantifier rank $d+1$.

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We are mainly interested in the 2-variable fragment GC^2, also known as graded modal logic.

Distinguishing Power of GNN

Theorem ([Immerman and Lander, 1990])

For all graph G, H, the following are equivalent:

- *Colour refinement does not distinguish G and H.*
- *G and H satisfy the same sentences of the logic C^2.*

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

For all graph G, H, the following are equivalent:

- *Colour refinement distinguishes G and H.*
- *G and H are distinguishable by a GNN, i.e., there is a graph level function f computed by a GNN N such that $f(G) \neq f(H)$.*

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- $(a_1, \ldots, a_k) \in Q(\mathrm{A})$ iff $(f(a_1), \ldots, f(a_k)) \in Q(\mathrm{B})$ for every isomorphism f from A to B and every $(a_1, \ldots, a_k) \in A^k$.

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Since there are only two 0-ary relations on a structure (true and false), a Boolean query Q is often identified with the class $\{\mathrm{A} \in \mathcal{C} \mid Q(\mathrm{A}) = \text{true}\}$.

Expressing Queries on Graphs

We say that a formula φ of a logic $\mathcal{L}$ *expresses* a k-ary query Q if for all graph G (in the considered class) and k-tuples $\bar{a}$ of nodes,

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More precisely, *$\mathcal{N}$ expresses the unary query Q* if there is an $\epsilon < 1/2$ such that for all graphs G and all nodes a,

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Similarly, if a GNN computes a graph level function, then it *expresses a Boolean query*

Expressiveness of GNNs

Theorem ([Barceló et al., 2020])

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  - E.g. a GNN can decide decide whether a node a has twice as many neighbours with a given label L_1 as it has with label L_2.

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- It is not obvious how to adapt the result to other activation functions (beyond ReLU).
- The converse inclusion does not (fully) hold.
  - E.g. a GNN can decide decide whether a node *a* has twice as many neighbours with a given label L_1 as it has with label L_2.

But there is a partial converse...

Theorem ([Barceló et al., 2020])

If Q is a unary query expressible by a GNN and also expressible in first-order logic, then Q is expressible in GC^2.

Final Consideration

- The described results provide clear evidence in favour of:
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  - Pursuing a precise understanding of the expressive power of NNs through well established methods from logic.
- Possible line of work (among others):
  - To explore the design space of GNNs by considering the impact in their expressive power of different features such as recurrence, activation functions (beyond ReLu) and alternative ways of assuring isomorphism invariance.

Thank you!!!

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