RWTH AACHEN UNIVERSITY

Logic and the Power of Recurrent Graph Neural Networks

Martin Grohe

Graph Neural Networks

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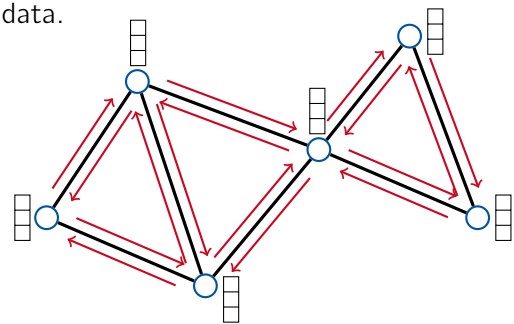

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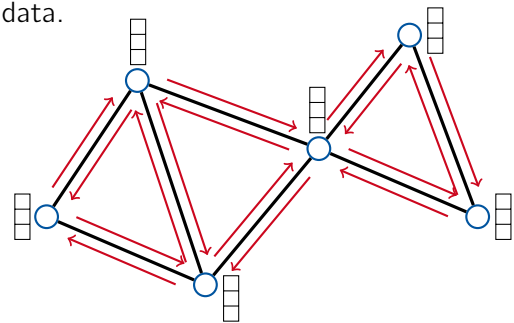


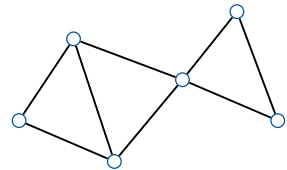
- In this talk, we study the expressiveness of GNNs:

  Which functions on graphs can be computed by a GNN?

Computation of GNNs

GNN N with d layers maps graph G to sequence of signals

$$\mathcal{I}^{(t)} : V(G) \to \mathbb{R}^{p_t} \quad \text{for } t = 0, \ldots, d$$



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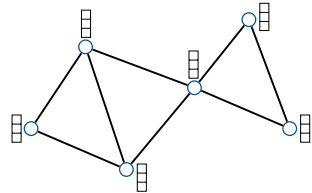

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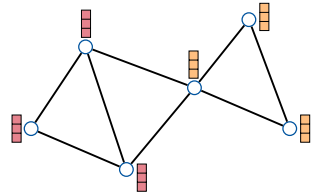

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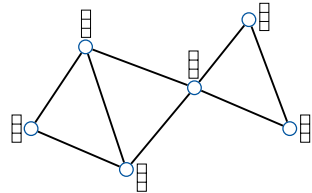

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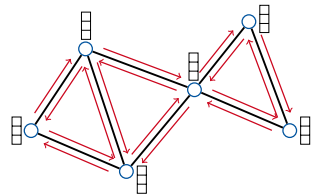

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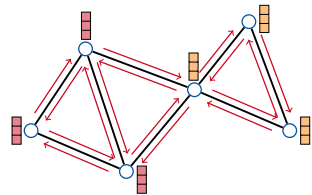

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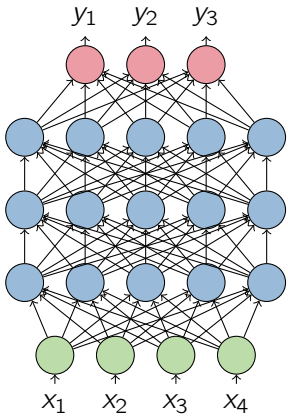
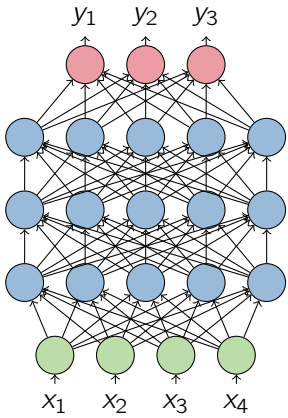
Feedforward Neural Networks





Feedforward Neural Networks

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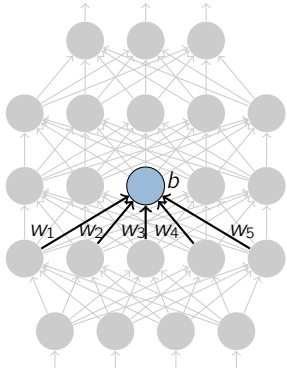

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- Nodes and edges are weighted.
- Node with weight $b \in \mathbb{R}$ and incoming edges with weights $w_1, \ldots, w_k \in \mathbb{R}$ computes function

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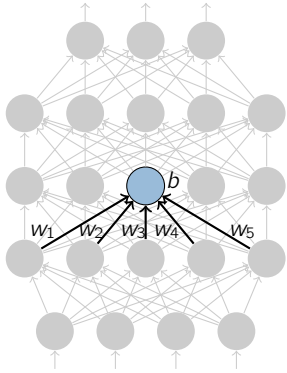

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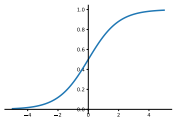
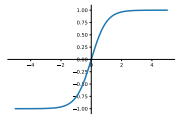
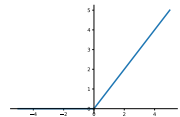


sigmoid



hyperbolic tangent



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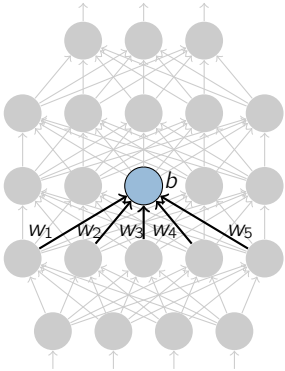

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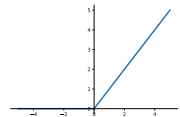
In this talk, we always use

$$\mathrm{ReLu}(x) \coloneqq \max\{0, x\}$$

as activation function.



rectified linear unit (ReLU)

Universal Approximation Theorem

Theorem (Cybenko 1989, Hornik 1991)

Let $f : K \to \mathbb{R}^n$ be a continuous function defined on a compact set $K \subseteq \mathbb{R}^m$. Then for every $\epsilon > 0$ there is a feedforward neural network N computing a function f_N such that

$$\sup_{\mathbf{x} \in K} \|f(\mathbf{x}) - f_N(\mathbf{x})\| < \epsilon.$$

Computation of GNNs (revisited)

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Then combination becomes

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Random Initialisation

$\mathscr{j}^{(0)}(v) = (s_1, \ldots, s_{p_0}, s_{p_0+1}) \in \mathbb{R}^{p_0+1}$ where $(s_1, \ldots, s_{p_0})$ endodes node labels or initial signal and s_{p_0+1} is chosen uniformly at random from $[0, 1]$.

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In this talk, we always consider GNNs with global aggregation. We sometimes consider random initialisation, but mention it explicitly when we do.

Node-Level Functions

GNNs compute a function $\mathscr{f}$ that maps each graph G (possibly with node labels or an initial signal) to a signal $\mathscr{f}(G, \cdot) : V(G) \to \mathbb{R}^q$ defined by

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To compute a function $\mathscr{F} : \mathscr{G} \to \mathbb{R}^q$ mapping graphs to vectors of real numbers, we aggregate the values and then apply a readout function:

$$\mathscr{F}(G) = \mathrm{ro}\Big(\mathrm{agg}\Big(\Big\{\!\!\Big\{ \mathscr{z}^{(d)}(v) \;\Big|\; v \in V(G) \Big\}\!\!\Big\}\Big)\Big).$$

- agg aggregation function: sum, mean or max
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To compute a function, we can run the GNN several times with independent random initialisations and then take the average value, or for Boolean functions, the majority.

The Logic of GNNs

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- An $FO^2{+}C$-formula expressing that vertex x has even degree:

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4. *G and H are fractionally isomorphic, that is, there is a doubly stochastic matrix X such that $A_G X = X A_H$.*
5. *For all trees T, the number of homomorphisms from T to G equals the number of homomorphisms from T to H.*

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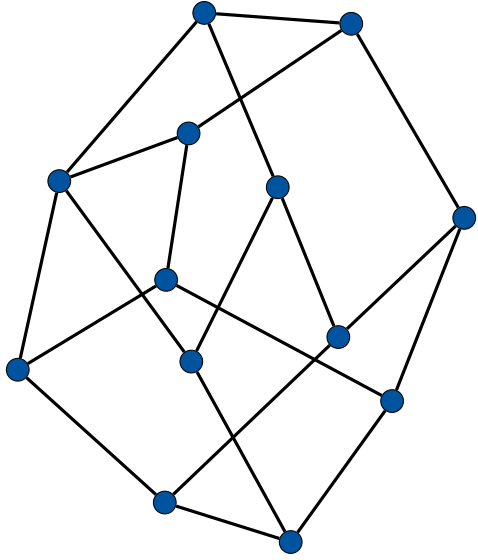
Remark

The algorithm is also refered to as naive vertex classification and as 1-dimensional Weisfeiler-Leman algorithm. One needs to be careful though, because there are two slightly different versions of the algorithm, and this difference does play a role in our work (though not in this talk).

Example



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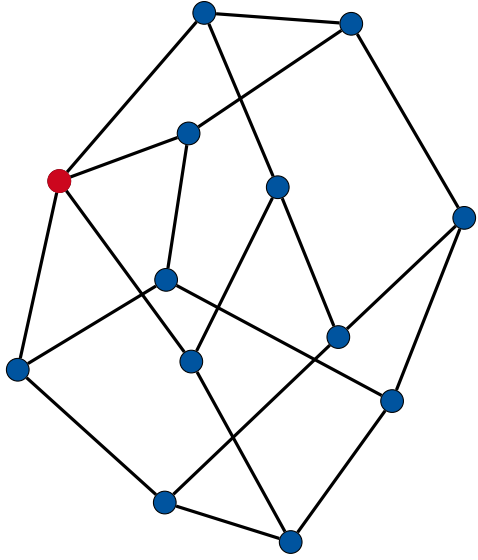

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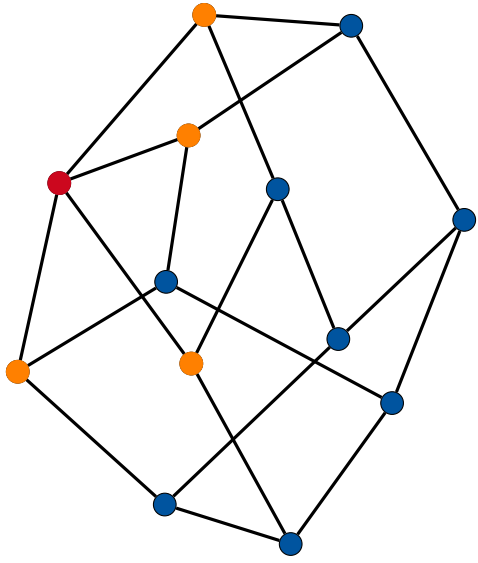

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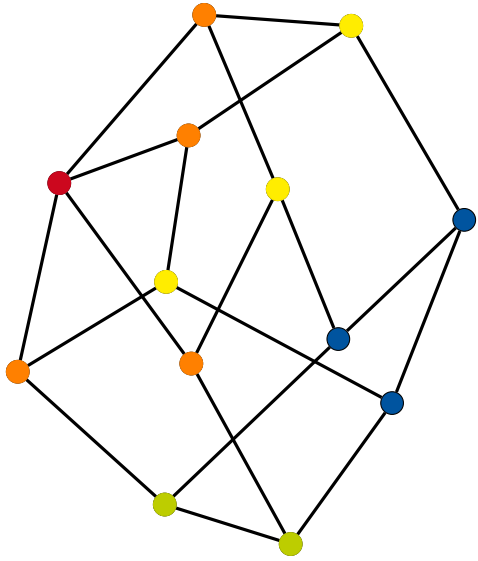

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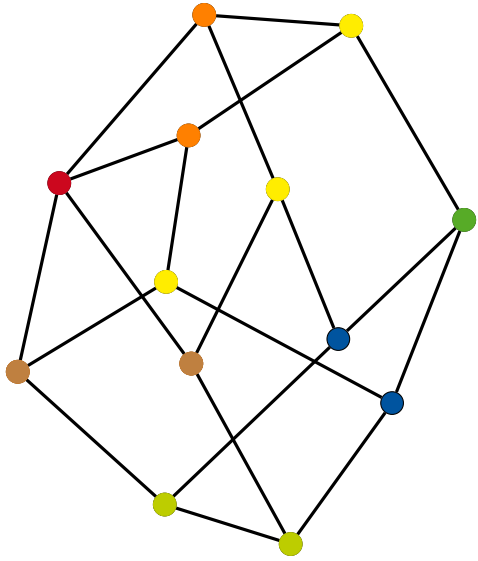

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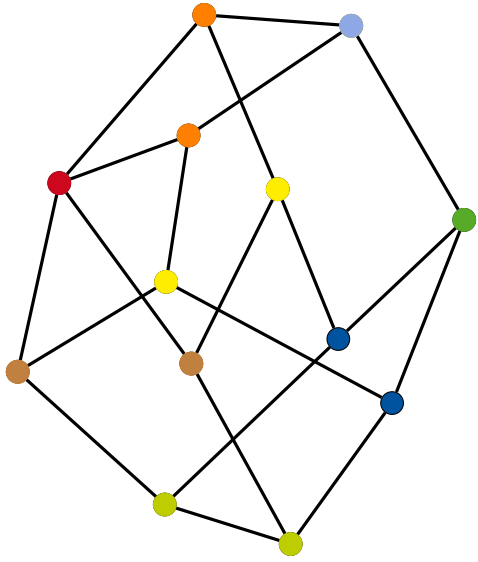

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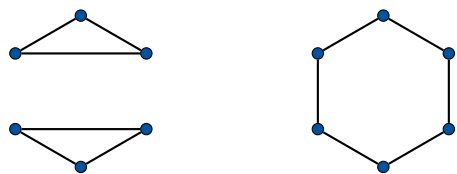

The Distinguishing Power of GNNs

Theorem (Morris, Ritzert, Fey, Hamilton, Lenssen, Rattan, G. 2019, Xu, Hu, Leskovec, Jegelka 2019)

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

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Remark

(Morris et al. 2019) ensure that graphs G, H that are not C^2-equivalent can be distinguished by a GNN N of size polynomial in $|G|, |H|$.

Expressing Graph Properties

Theorem (Barceló, Kostylev, Monet, Pérez, Reutter, Silva 2019)

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It can be shown that both inclusions are strict.

Theorem (G. 2023)

For all graph properties $\mathscr{P}$, the following are equivalent.

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4. *$\mathscr{P}$ is in the complexity class TC^0.*

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Recurrent GNN Computation

A recurrent GNN has a single layer and applies it repeatedly. That is, we have aggregation functions $\mathrm{agg}, \mathrm{agg}'$ and a combination function comb and for $t \geq 1$ let:

$$\jmath^{(t)}(v) = \mathrm{comb}\Big(\jmath^{(t-1)}(v), \mathrm{agg}\big(\{\!\{\jmath^{(t-1)}(w) \mid w \in N_G(v)\}\!\}\big), \mathrm{agg}'\big(\{\!\{\jmath^{(t-1)}(w) \mid w \in V(G)\}\!\}\big)\Big)$$

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We do not require convergence of the signals.

Universality of Recurrent GNNs

Theorem (Rosenbluth and G. 2025+)

Let $\mathscr{F} : \mathscr{G} \to \mathbb{Q}^n$ be computable. Then the following are equivalent.

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Furthermore,

- *we may choose the GNN in (ii) to have rational weights and to only use SUM aggregation;*
- *if $\mathscr{F}$ is computable in polynomial time then the GNN stops after polynomially many iterations and only uses internal states of polynomial bitlength.*

Corollary

Every computable function $\mathscr{F} : \mathscr{G} \to \mathbb{Q}^n$ is computable by a recurrent GNN with random initialisation only using rational weight and SUM aggregation.

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- There are also a versions of the results for node-level functions (actually, we prove these first and derive the graph-level results as a consequence).

Proof of the Theorem (Outline)

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Thus after Phase 3, every node holds the correct function value, and readout becomes trivial.

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Thus we can use the following result

Theorem (Siegelmann and Sontag 1992)

Every computable function $f : \mathbb{Q}^m \to \mathbb{Q}^n$ is computable by a recurrent feedforward neural network.

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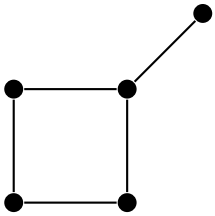

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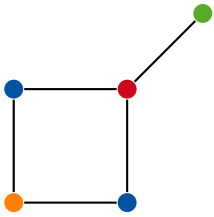

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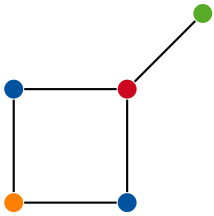

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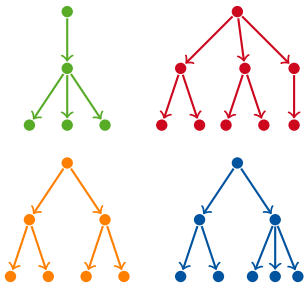

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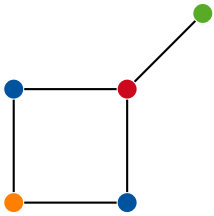

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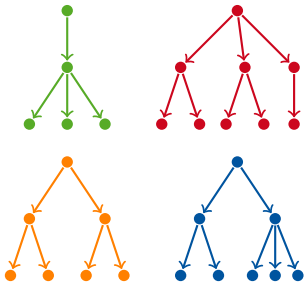

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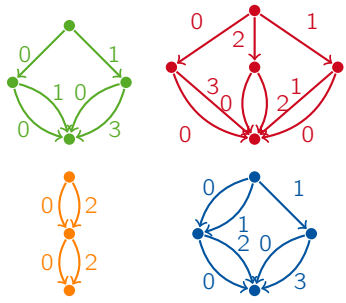

Compact dag representation

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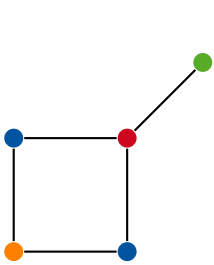

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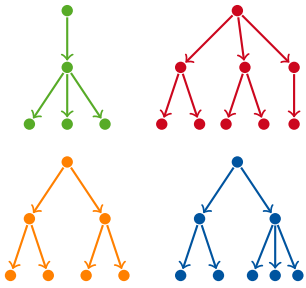

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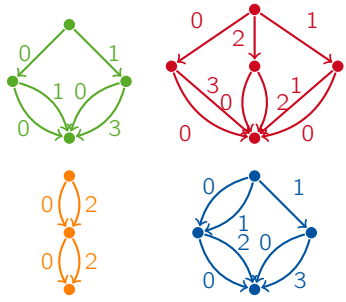

Compact dag representation

To simulate colour refinement by a recurrent GNN, we encode the compact dag representation of colours by rational numbers and in several rounds by decreasing c for each node v count the number of neighbours of v of colour c.

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Lemma (Otto 1997)

There is a polynomial time algorithm that, given the dag representation D_v of the colour of a node v in a graph G, computes a graph G_v that is C^2-equivalent to G.

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If you are looking for a postdoc position, please contact me.

A Few References

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