RWTH AACHEN UNIVERSITY

The Descriptive Complexity of Graph Neural Networks

Martin Grohe

Graph Neural Networks

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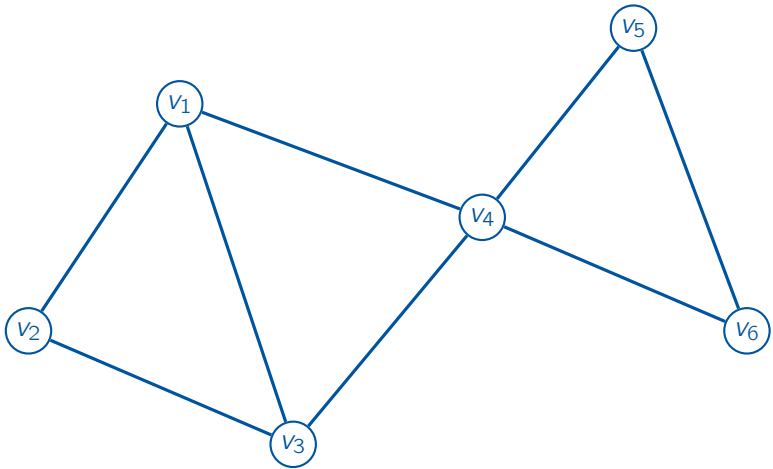
- GNNs have a wide range of applications, for example, in computational biology, chemical engineering, physics, etc.
- By now, there is a large variety of GNN architectures.
  In this talk, we focus on the core GNN architecture known as message passing graph neural network or aggregate-combine graph neural network.

Graph Neural Networks



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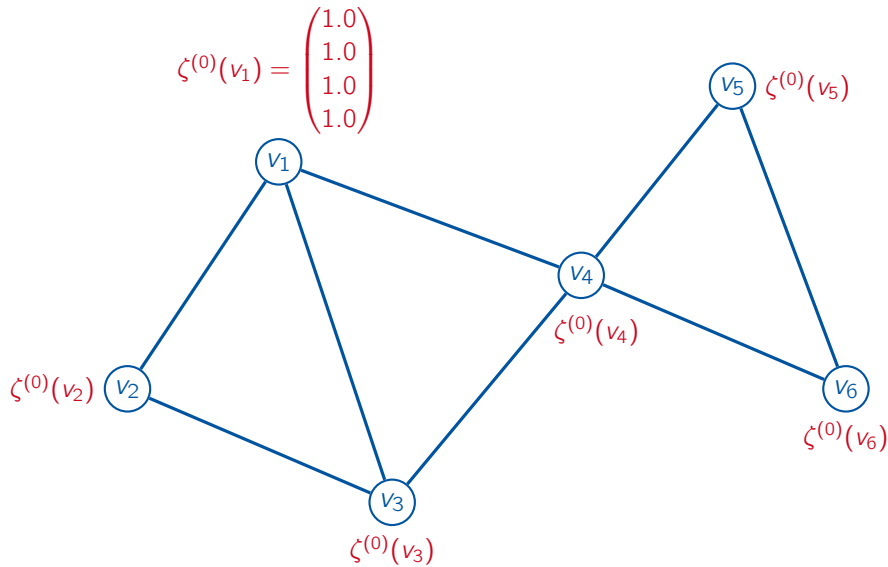

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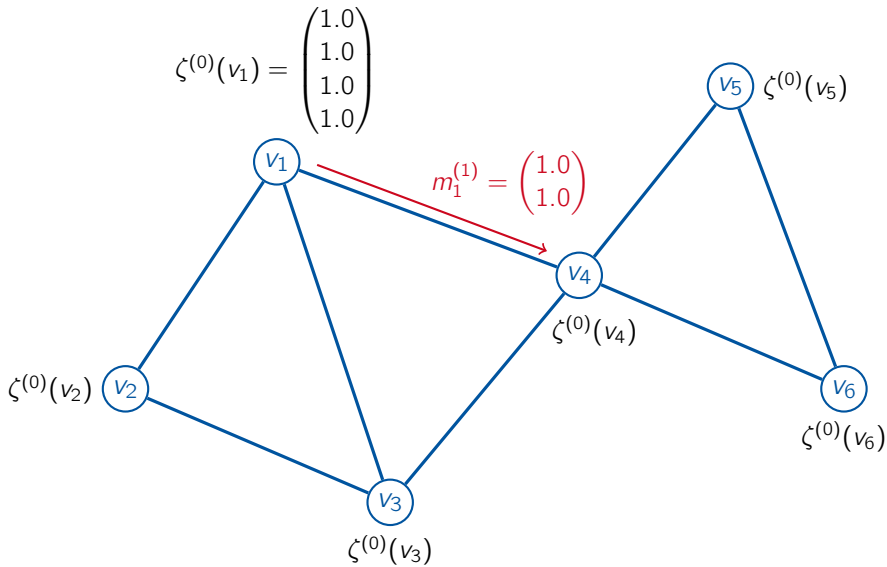

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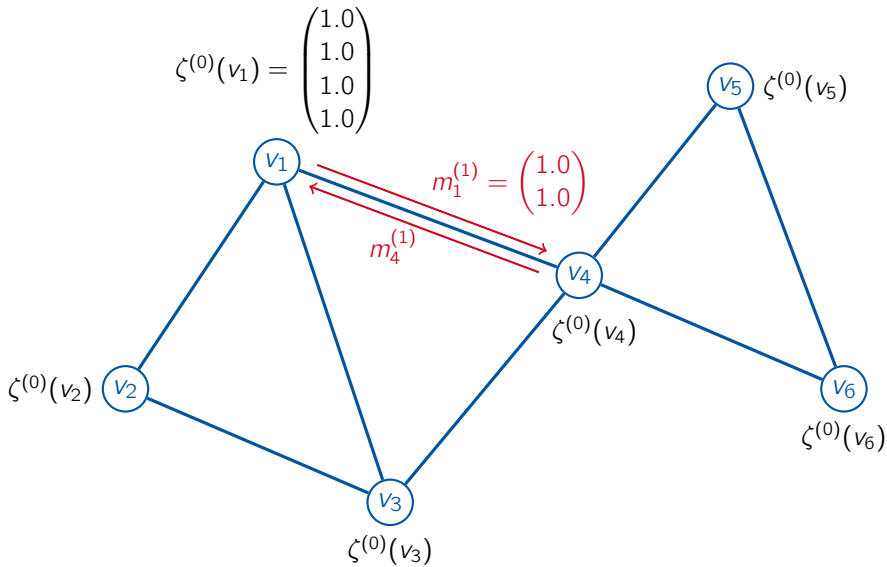

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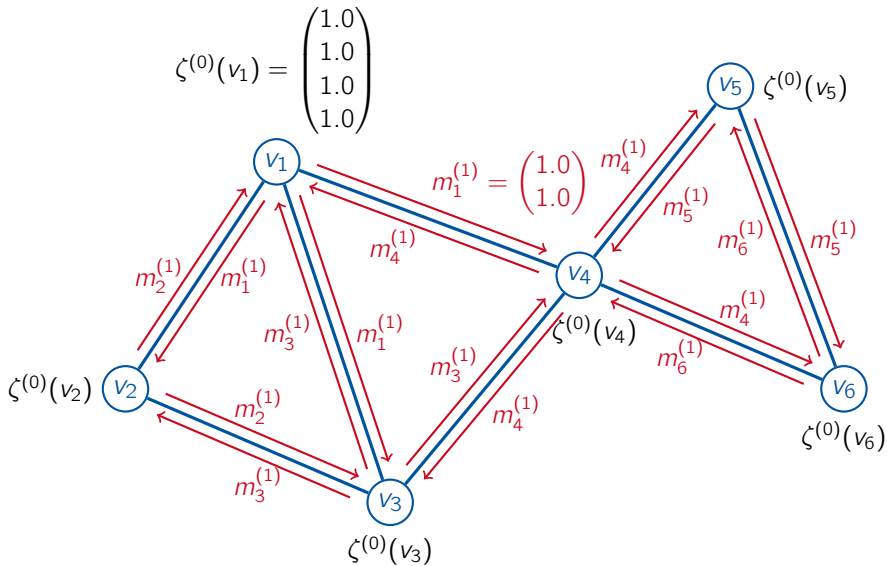

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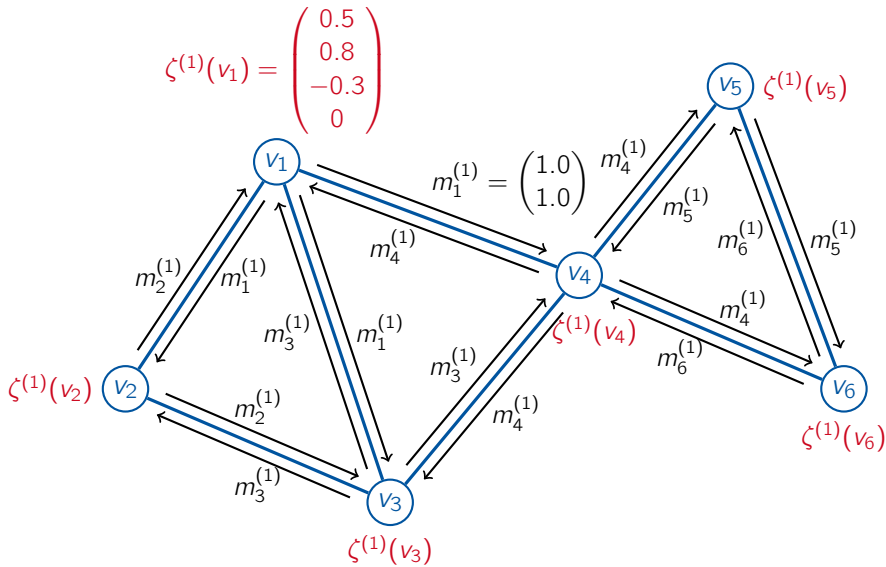

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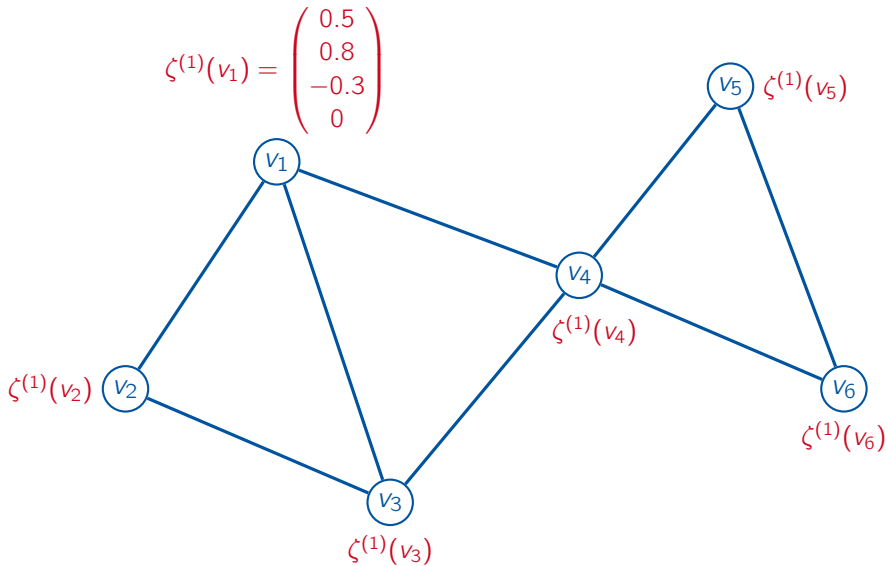

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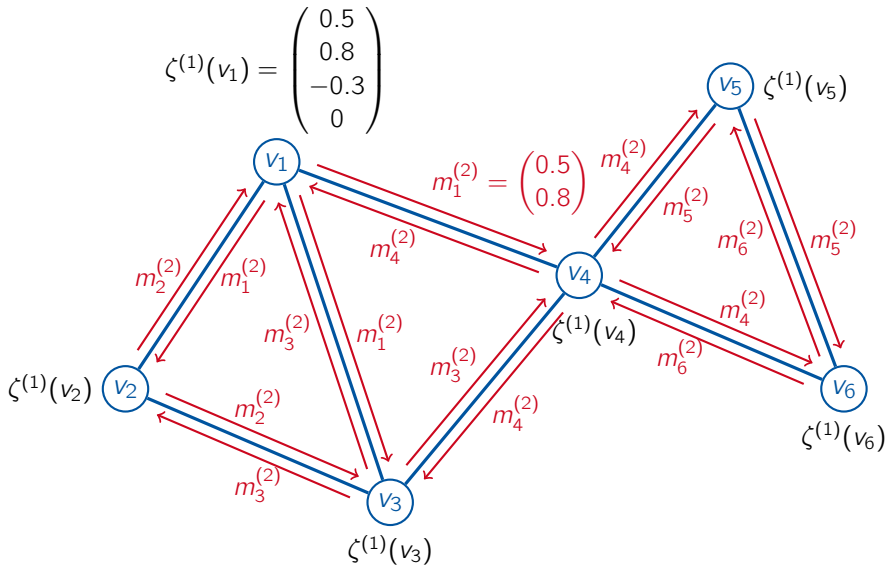

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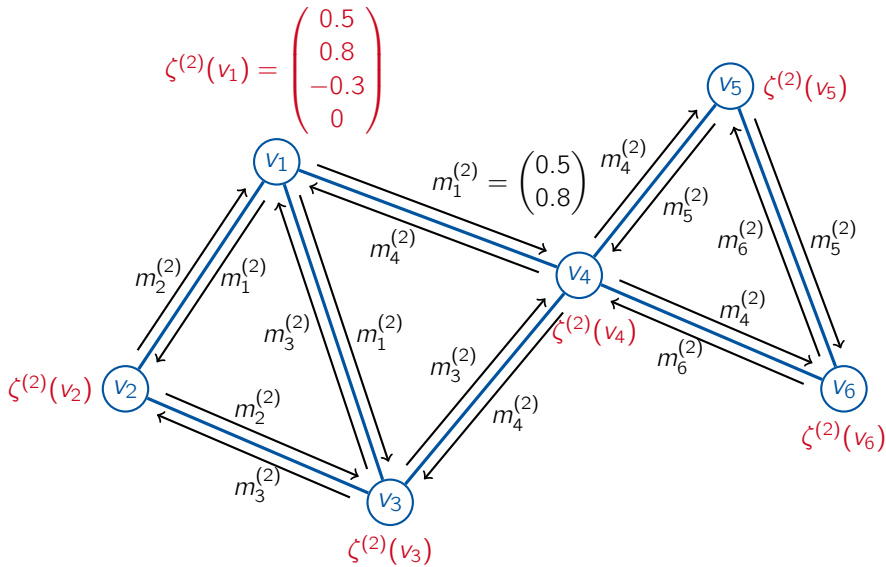

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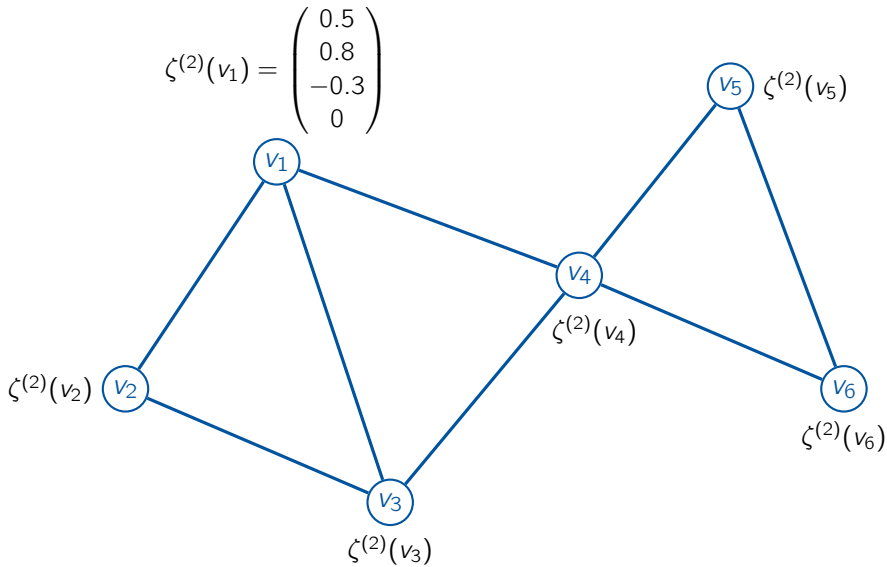
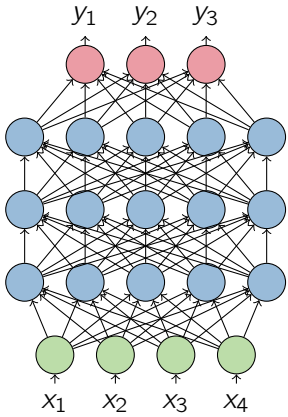
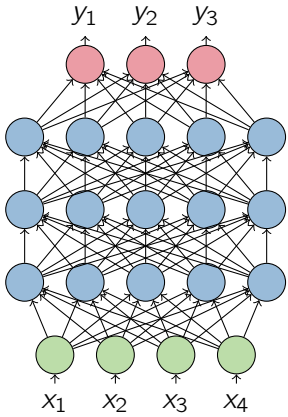


Feedforward Neural Networks





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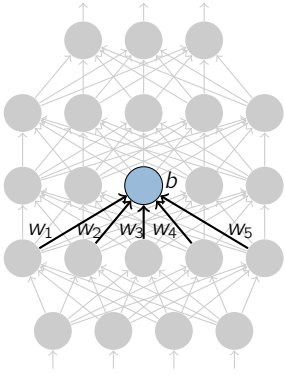

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- Node with weight $b \in \mathbb{R}$ and incoming edges with weights $w_1, \ldots, w_k \in \mathbb{R}$ computes function

$$x_1, \ldots, x_k \mapsto \sigma\left(b + \sum_{i=1}^{k} w_i x_i\right),$$

where $\sigma : \mathbb{R} \to \mathbb{R}$ is the activation function.

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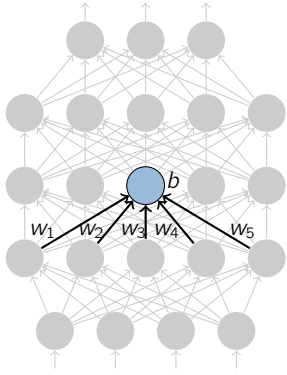

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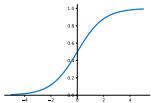
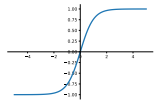
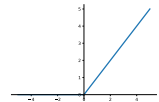
Typical activation functions are:



sigmoid



hyperbolic tangent



rectified linear unit (ReLU)

Universal Approximation Theorem

Theorem (Cybenko 1989, Hornik 1991)

Let

- $\sigma : \mathbb{R} \to \mathbb{R}$ *be be continuous and not polynomial,*
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Then there is a depth-2 feedforward neural network N *with activation functions*

- σ *on layer* 1*,*
- *the identity on layer 2*

computing a function f_N *such that*

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

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

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Combination: $\zeta^{(t)}(v) \coloneqq \mathrm{comb}_t\big(\zeta^{(t-1)}(v), \alpha^{(t)}(v), \gamma^{(t)}\big)$

- $\mathrm{comb}_t : \mathbb{R}^{2p+p'} \to \mathbb{R}^p$ function computed by a feedforward neural network

Node-Level Functions

To compute a function Φ that maps each graph G to a signal $\Phi(G, \cdot) : V(G) \to \mathbb{R}^q$, we apply a readout function ro such that

$$\Phi(G, v) = \mathrm{ro}\big(\zeta^{(d)}(v)\big).$$

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Functions Computed by GNNs

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Graph-Level Functions

To compute a function φ that maps graphs to $\mathbb{R}^q$, we apply an aggregate readout function aggro such that

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

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We are mainly interested in Boolean queries and unary queries, that is, invariant graph level functions $G \mapsto \{0, 1\}$ and equivariant node-level functions $G \mapsto \{0, 1\}^{V(G)}$.

Recurrent GNNs

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As before, we apply the readout function to the dth layer.

Digression: The Weisfeiler-Leman Algorithm

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Remark

Colour Refinement is essentially the same as the 1-dimensional Weisfeiler-Leman algorithm. There is a subtle difference that is actually relevant here (but we ignore it in the talk).

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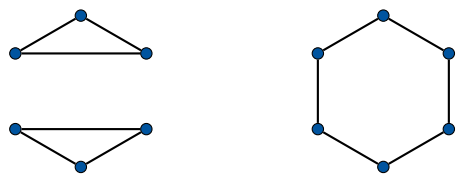
- works on almost all graphs (Babai, Erdös, Selkow 1980)
- fails on some very simple graphs:



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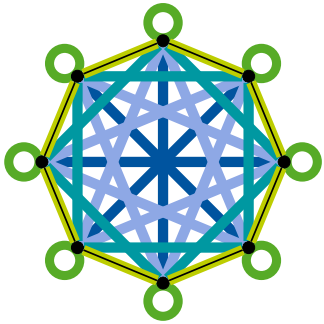
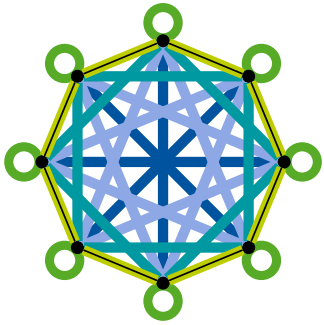
3. *G and H are fractionally isomorphic, that is, there is a doubly stochastic matrix X such that $A_G X = X A_H$.*
4. *For all trees T, the number of homomorphisms from T to G equals the number of homomorphisms from T to H.*



Higher-Dimensional Weisfeiler-Leman

The k-dimensional Weisfeiler-Leman algorithm (k-WL) iteratively colours k-tuples of nodes (Weisfeiler and Leman 1968, Babai $\sim$1980)



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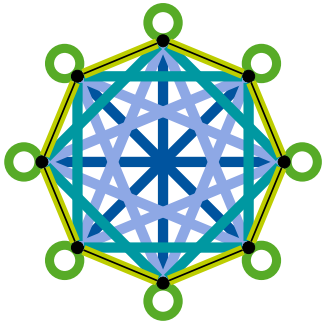

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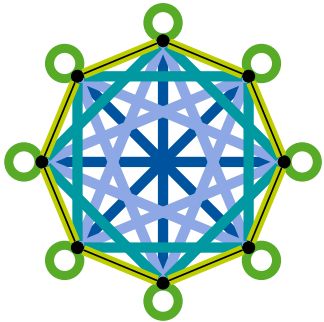

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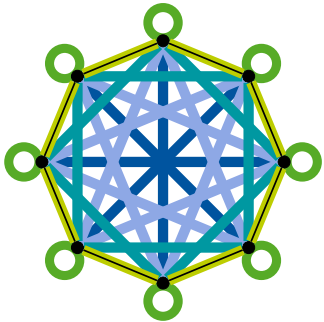

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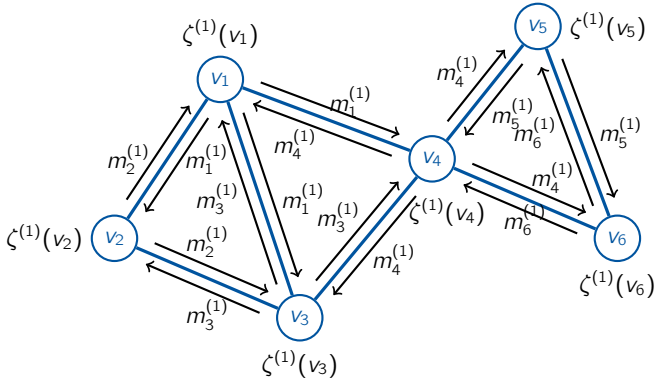
- The characterisations of Colour Refinement in terms of logic, linear (in)equalities, and homomorphism counts can be generalised to k-WL.

Weisfeiler and Leman go Neural

GNNs Revisited



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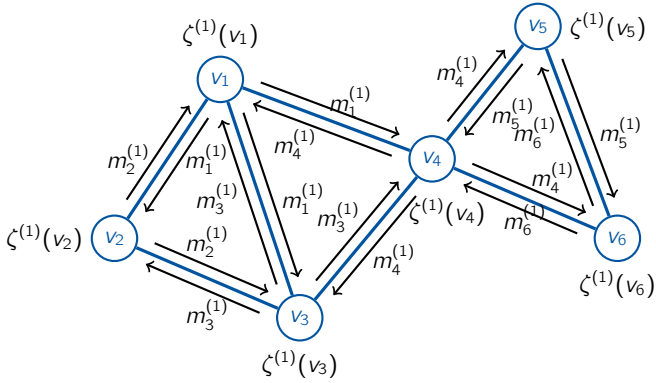

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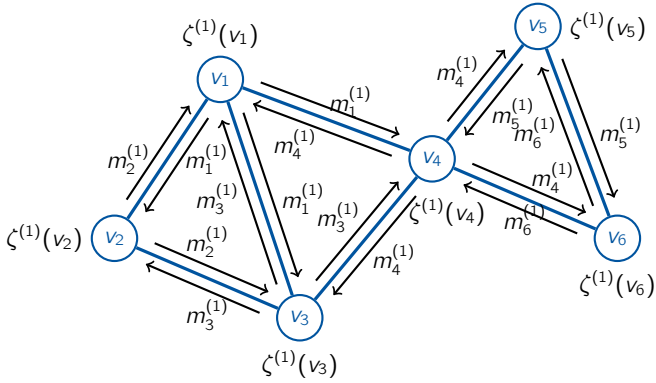

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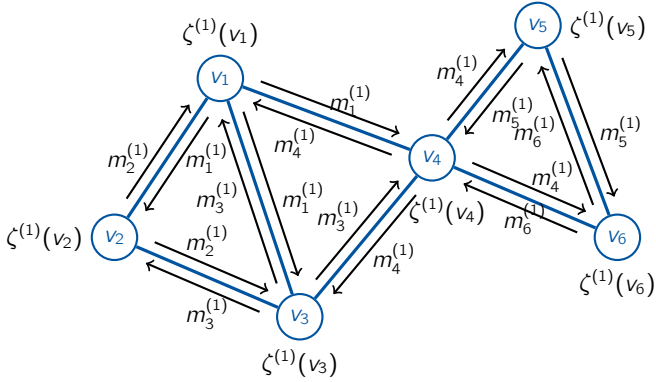

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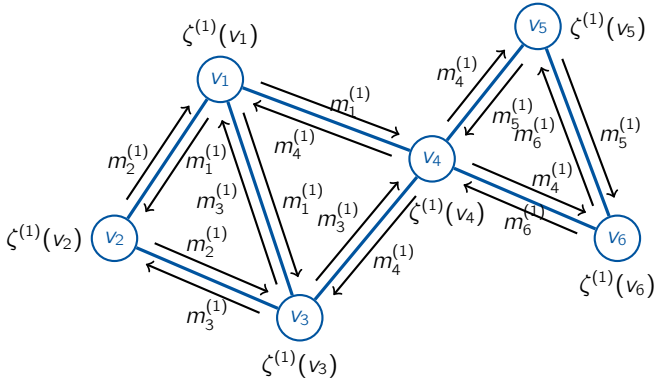

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Notation: Index N refers to GNN N

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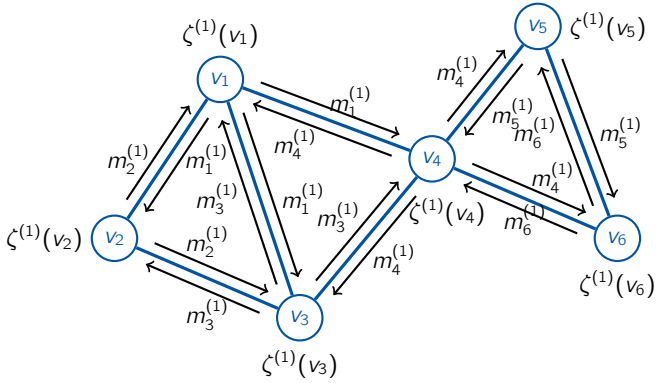

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$\varphi_N(G) \coloneqq \mathrm{ro}(\mathrm{agg}(\{\!\{\zeta^{(d)}(v)) \mid v \in V(G)\}\!\}))$ (graph level)

Distinguishing Graphs

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

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

1. *G and H are distinguishable by a GNN, that is, there is a GNN N such that $\varphi_N(G) \neq \varphi_N(H)$;*
2. *1-WL distinguishes G and H.*

Expressing Graph Properties

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

Let $\mathcal{Q}$ be a query expressible in the logic C^2. Then there is a GNN computing $\mathcal{Q}$.

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- Barceló et al. also prove a converse of the theorem for queries expressible in first-order logic.
- This is a uniform expressibility result: the property can be expressed by a single GNN across input graphs of all sizes.
- The proof assumes activation functions like ReLU or linearised sigmoid. It is open whether the theorem also holds for GNNs with logistic (sigmoid) or tanh activations.

Higher-Order Graph Neural Networks

We also proposed a model of higher-order GNNs passing messages between tuples of vertices.

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Theorem (Morris, Ritzert, Fey, Hamilton, Lenssen, Rattan, G. 2019)

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

1. *G and H are distinguishable by a GNN, that is, there is a order $(k+1)$-GNN N such that $\varphi_N(G) \neq \varphi_N(H)$;*
2. *k-WL distinguishes G and H.*

Random Node Initialisation

Suppose we initialise the states of the nodes of a GNN randomly:

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- (Sato et al. 2020) proved that many interesting combinatorial problems can be expressed by GNNs with RI.

Universality of GNNs with RI

Theorem (Abboud, Ceylan, G., Lukasiewicz 2021)

Let $\epsilon, \delta > 0$ *and* $n \in \mathbb{N}$ *and* $\psi : \mathscr{G}_n \to [0, 1]$.

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Graphs of order n

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- There is also a node-level version of this result.
- These approximation results are non-uniform, that is, for each size of the input graph we need a separate GNN.
- The size of the GNN N can be exponential in n.

The Descriptive Complexity of GNNs

Goal

Understand the power of GNNs to compute queries and compare it to classical models of complexity theory and logic.

Circuits with Threshold Gates

We consider Boolean circuits with threshold gates. For all $t \in \mathbb{N}$, a t-threshold gate evaluates to 1 if at least t of its inputs are 1.

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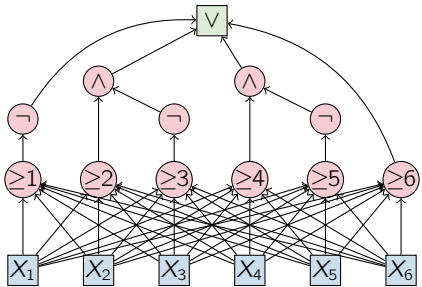
Example

The following threshold circuit evaluates to 1 if an even number of input bits is 1.



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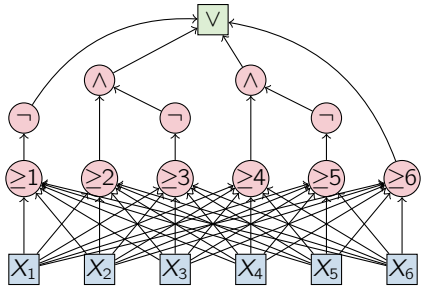

TC^0 is the class of all languages in $\{0,1\}^*$ decidable by a polynomial-size, bounded-depth family of threshold circuits.

Theorem (Maass 1997)

Let $\mathscr{f} = (f_n)_{n \geq 1}$ be a family of Boolean functions $f_n : \{0,1\}^n \to \{0,1\}$. Then the following are equivalent.

1. *$\mathscr{f}$ is in TC^0.*
2. *$\mathscr{f}$ is computable by a bounded-depth polynomial-size family of feedforward neural networks with piecewise polynomial activation functions.*

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Theorem (Barrington, Immerman, Straubing 1990)

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Nonuniform Version: *A language $L \subseteq \{0,1\}^*$ is in (nonuniform) TC^0 if and only if it is definable in* FO+C *with built-in relations.*

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Corollary

Combined with Barcelo et al. (2019), we get

$$\mathrm{C}^2 \quad \subseteq \quad \mathrm{GNN} \quad \subseteq \quad \mathrm{FO}^2\text{+C}.$$

Both inclusions are strict.

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Theorem (G. 2023)

For all queries $\mathcal{Q}$, the following are equivalent.

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2. *$\mathcal{Q}$ is computable by a polynomial-size bounded-depth family of GNNs with random initialisation and with rational weights and ReLU activations, using only sum aggregation.*
3. *$\mathcal{Q}$ is expressible in $\mathsf{FO}^2{+}\mathsf{C}$ with built-in relations.*
4. *$\mathcal{Q}$ is in TC^0.*

Lemma

Let $\mathcal{Q}$ be a query that is computable by a polynomial-size bounded-depth family of graph neural networks with random initialisation and with arbitrary real weights and rpl approximable activation functions.
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Proof Ideas

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- Trade randomness for non-uniformity.

Lemma

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Lemma

Let $\mathcal{Q}$ be a query that is expressible in FO^2+C *with built-in relations.*
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Proof Ideas

- Transform FO^2+C-formula into a guarded (local) form.
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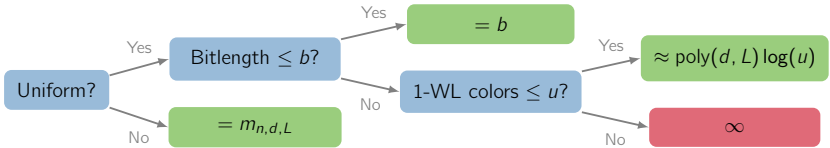
- Random initialisation is used to obtain linear order.

Learning and Generalisation

The VC Dimension of GNNs



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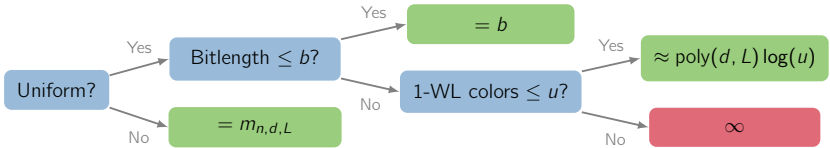

Theorem (Morris, Geerts, G. 2023)

1. *In the non-uniform regime, the VC-dimension of GNNs is essentially the number of of Colour-Refinement equivalence classes.*
2. *In the uniform regime, the VC-dimension of GNNs is linear in the bitlength of the GNN's weights.*

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- Expressiveness results only tell half the story, because they ignore learning. However, most of the results presented here have good experimental support.

A Few References

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