Lecture 5: Expressive Power of Message Passing Neural Networks

Relational Learning

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Advanced Topics in Machine Learning, University of Oxford

01.02.2021

Overview

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- A journey into model representation capacity

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- Graph isomorphism and colour refinement

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- Summary

A Journey into Model Representation Capacity

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From a learning perspective, universal approximation is only the first step — it does not imply that the functions can be learned efficiently (e.g., we might need exponentially many neurons etc)!

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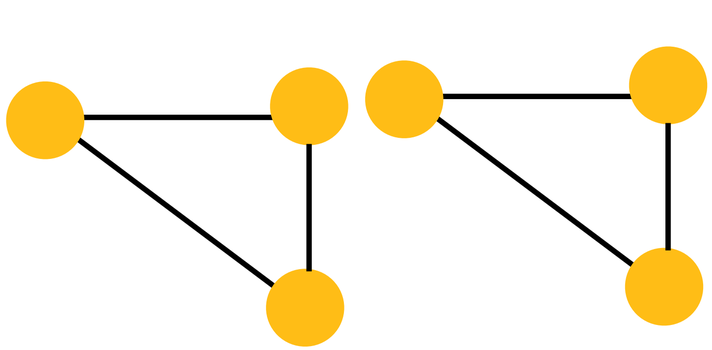
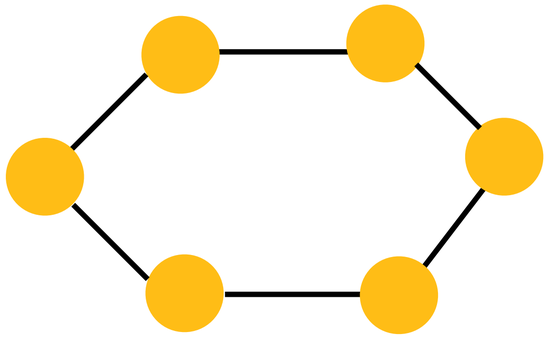
This would be desirable, as it implies we can distinguish all structures, and this paves the way for learning more general classes of functions over graphs.

A Tale of Two Graphs





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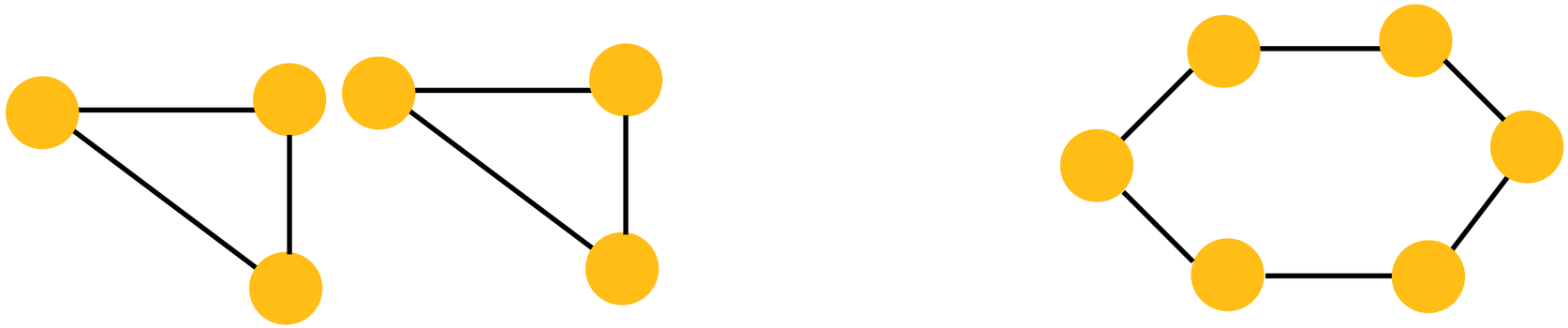

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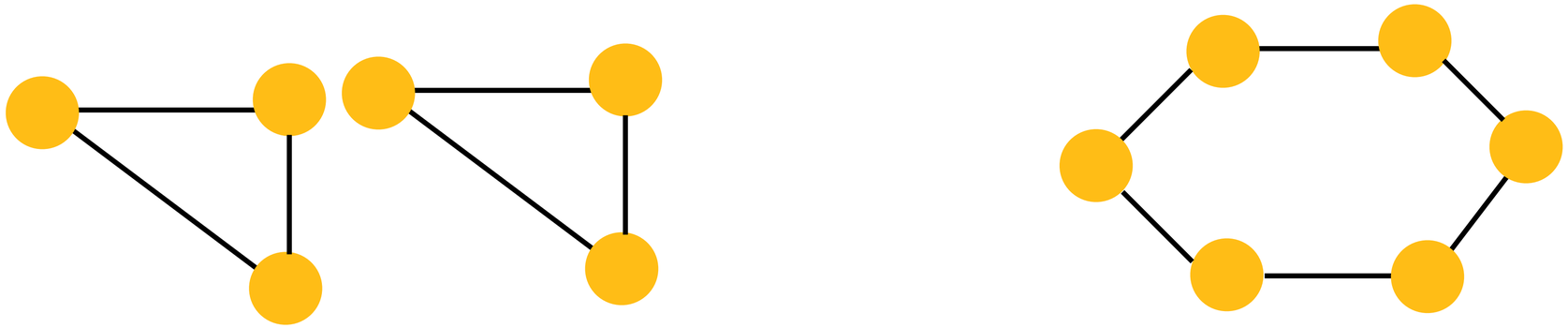

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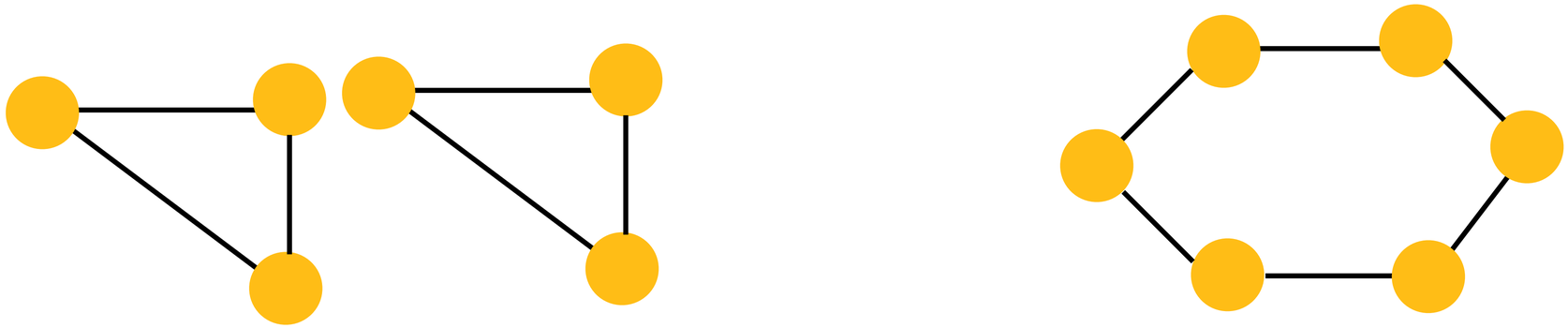

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Is this only a problem for graph classification?

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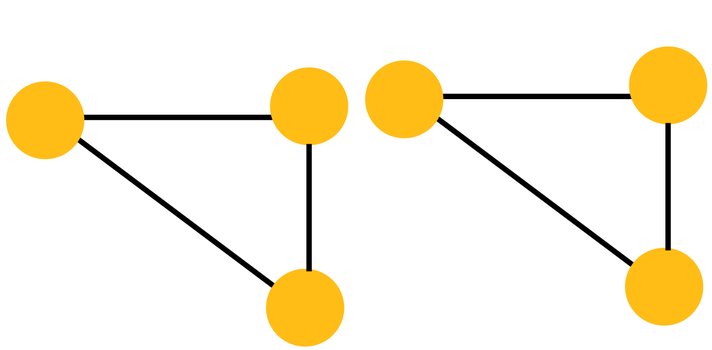

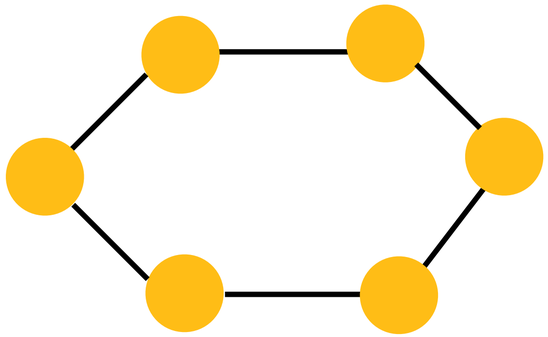

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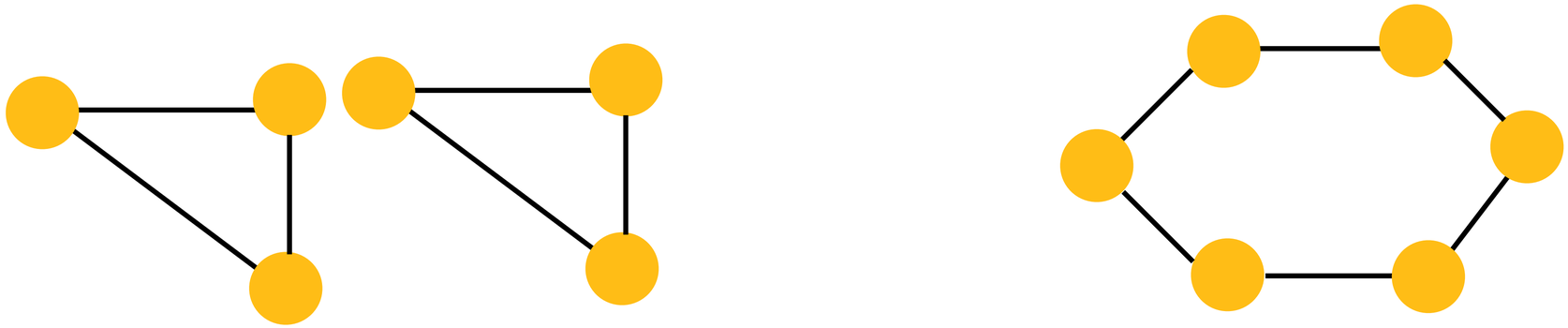

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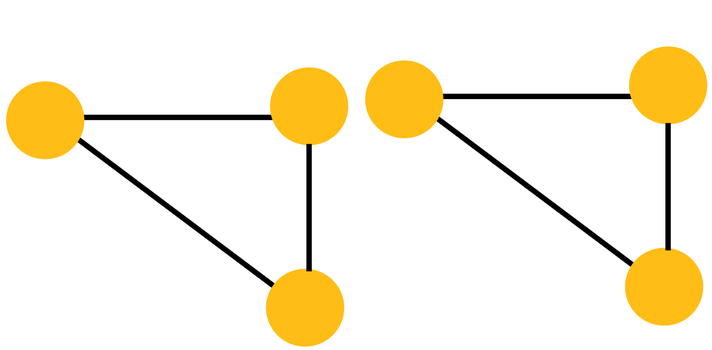

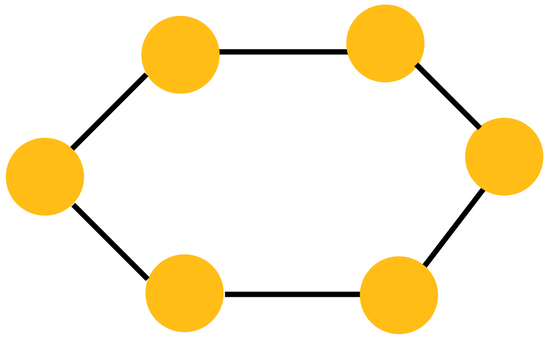

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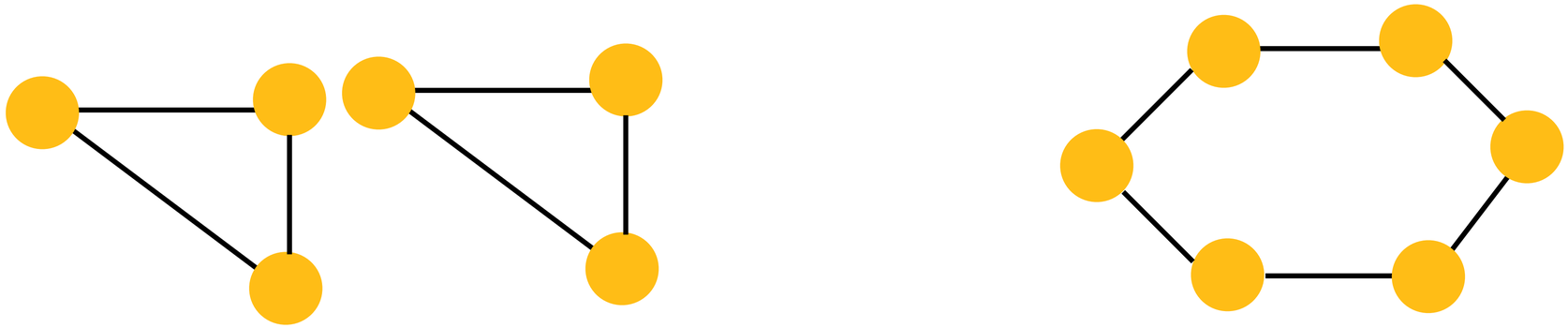

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An MPNN will either predict all nodes to be separator nodes, or all of them as non-separator nodes, regardless of training choices etc — either case, a random answer with exactly $50\,\%$ accuracy.

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Recall that we can define an embedding of a graph G as a multi-layer perceptron:

$$f(G) = \text{MLP}(\mathbf{A}^G_{[1]} \oplus \ldots \oplus \mathbf{A}^G_{[|V_G|]}),$$

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This is a trade-off: We want to constrain the learning space (e.g., incorporating inductive bias) as much as possible, but not so much that we induce strong limitations in the representation capacity.

Graph Isomorphism and Color Refinement

Graph Isomorphism

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Graph isomorphism testing is one of the most fundamental tasks in graph theory:

We say that two graphs G and H are isomorphic if there is a bijection between the vertex sets V_G and V_H:

$$f : V_G \mapsto V_H$$

such that any two vertices u and v of G are adjacent in G if and only if $f(u)$ *and* $f(v)$ are adjacent in H.

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We can restate this with features and using matrices:

If we have two graphs G and H, represented with adjacency matrices $\mathbf{A}^G$and $\mathbf{A}^H$, as well as associated with node features $\mathbf{X}^G$and $\mathbf{X}^H$, we say that two graphs are isomorphic if and only if there exists a permutation matrix $\mathbf{P}$ such that:

$$\mathbf{P}\mathbf{A}^G\mathbf{P}^\top = \mathbf{A}^H \text{ and } \mathbf{P}\mathbf{X}^G = \mathbf{X}^H.$$

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There are, however, many practical — approximate — algorithms for graph isomorphism testing that work on broad classes of graphs, including colour refinement.

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Observe that the stopping condition is well-defined, since $\pi(\lambda^{(i+1)}) \preceq \pi(\lambda^{(i)})$ for any $i \geq 0$, i.e., each iteration corresponds to a refinement, and there exists a minimal integer j such that $\pi(\lambda^{j}) \equiv \pi(\lambda^{(j+1)})$.

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Colour refinement is also known as naive vertex refinement, or 1-dimensional Weisfeiler Lehman (1-WL) algorithm.

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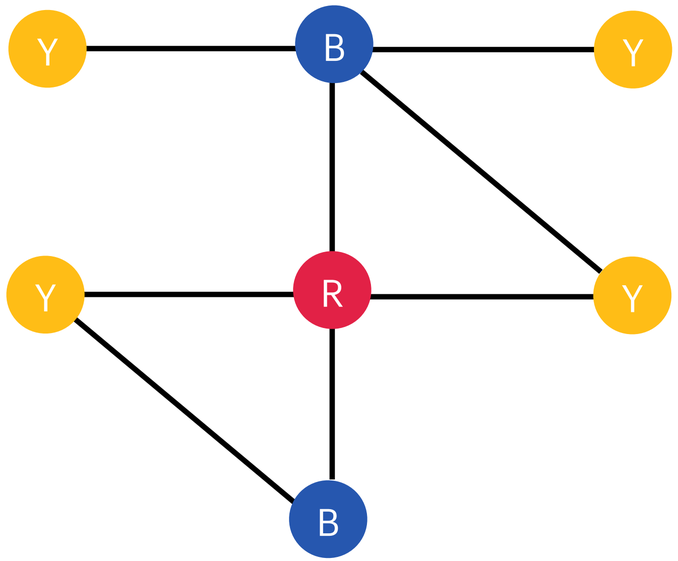

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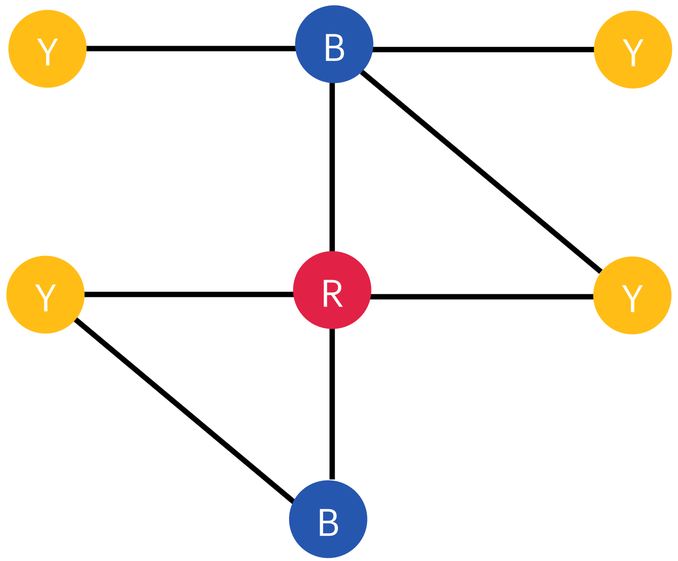

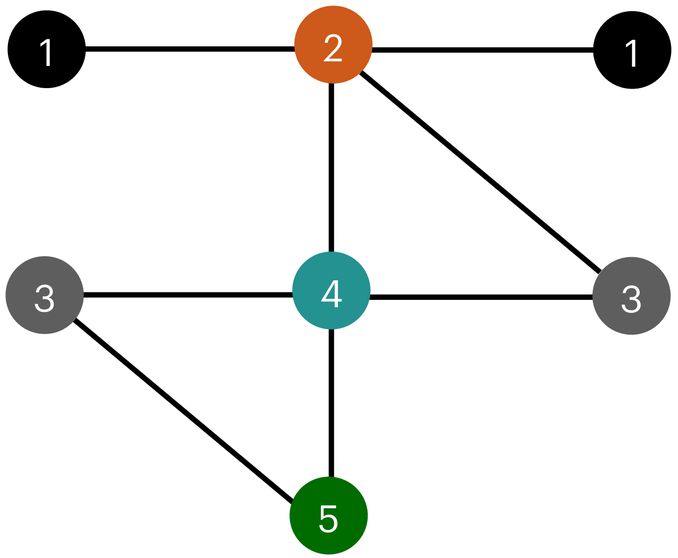

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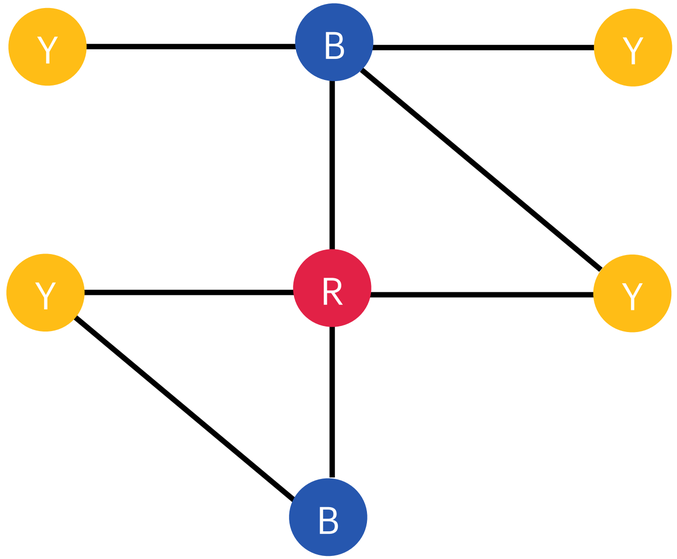

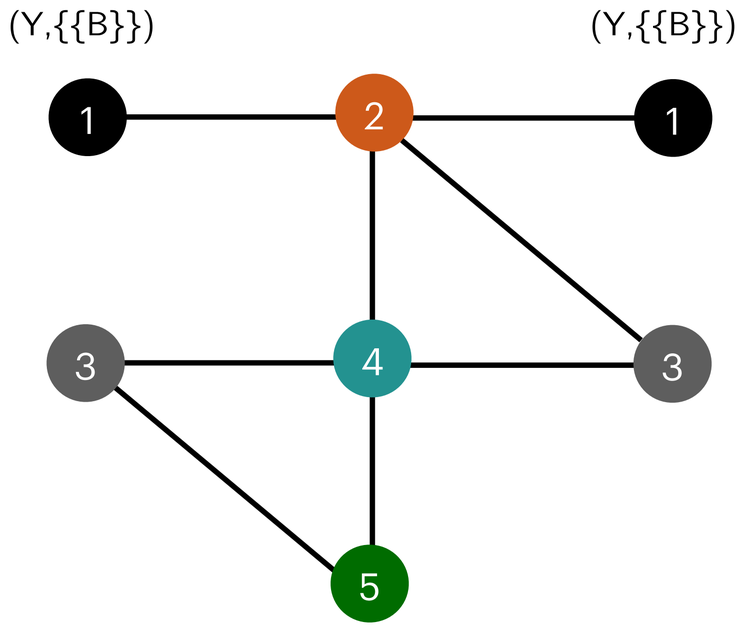

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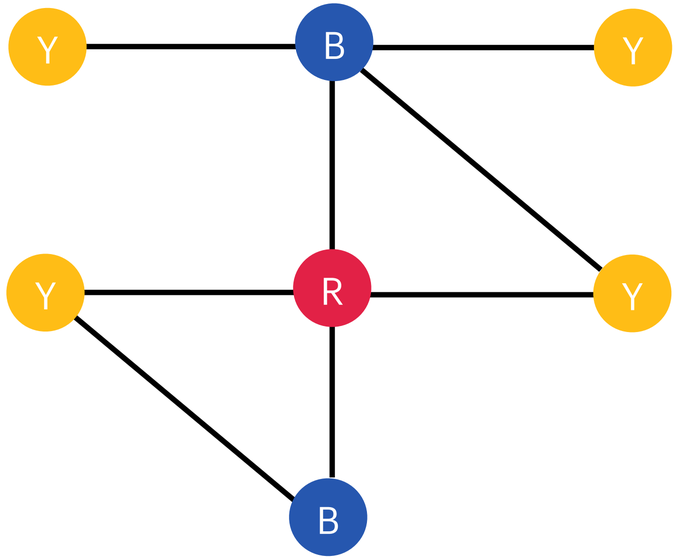

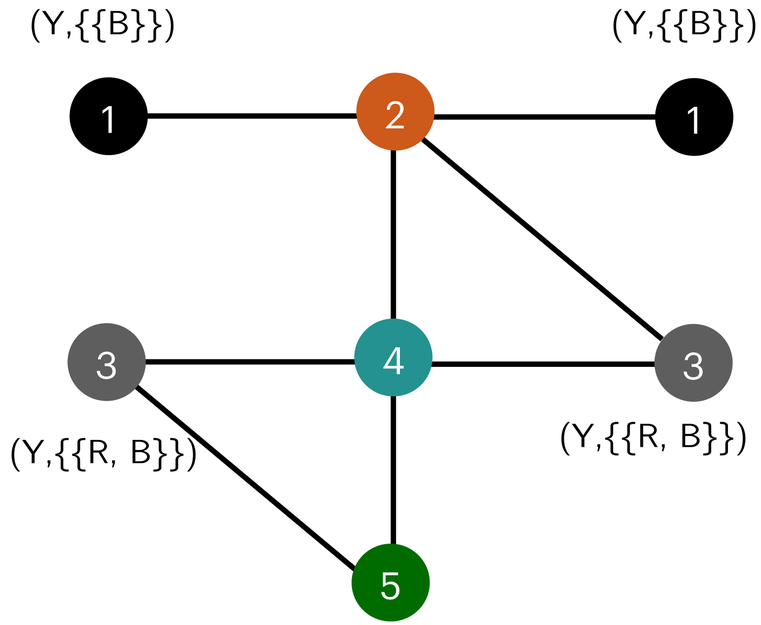

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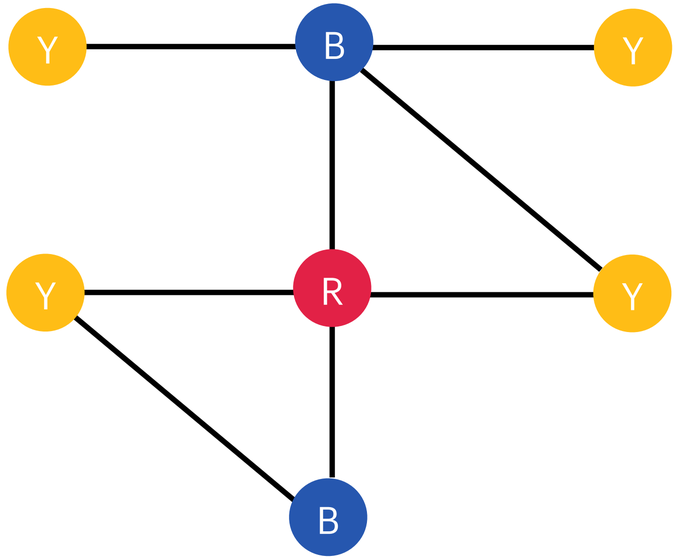

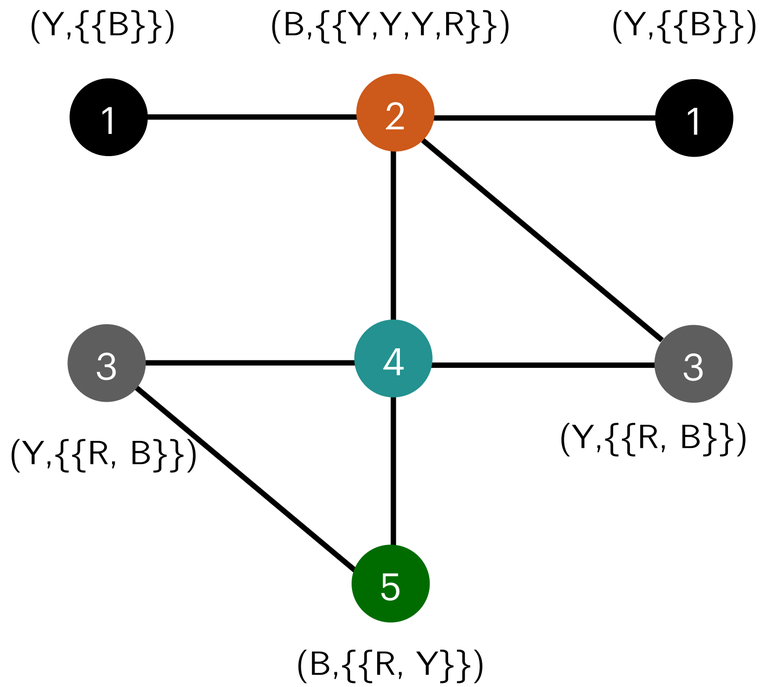

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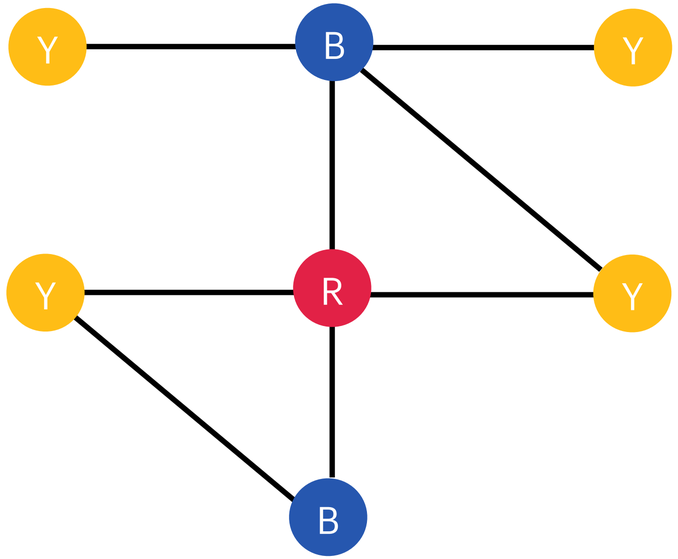

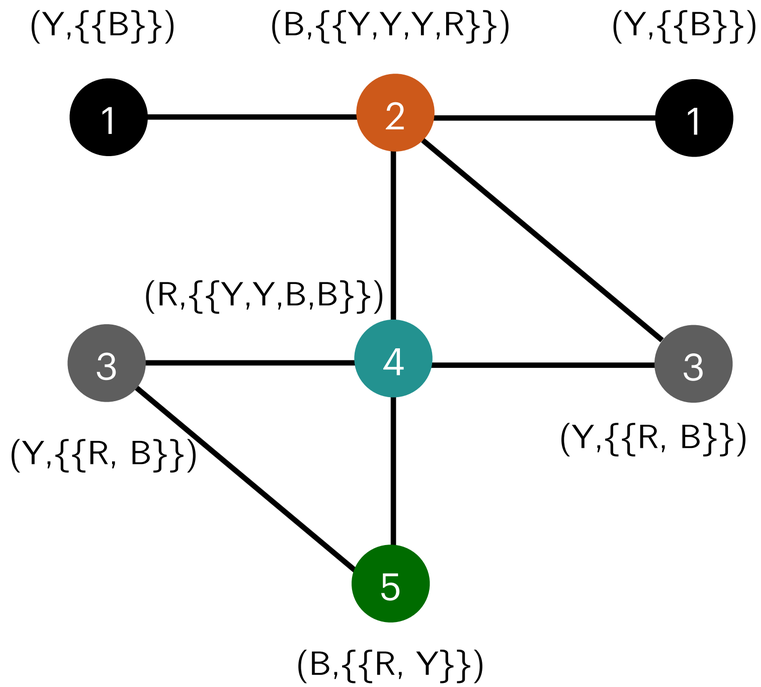

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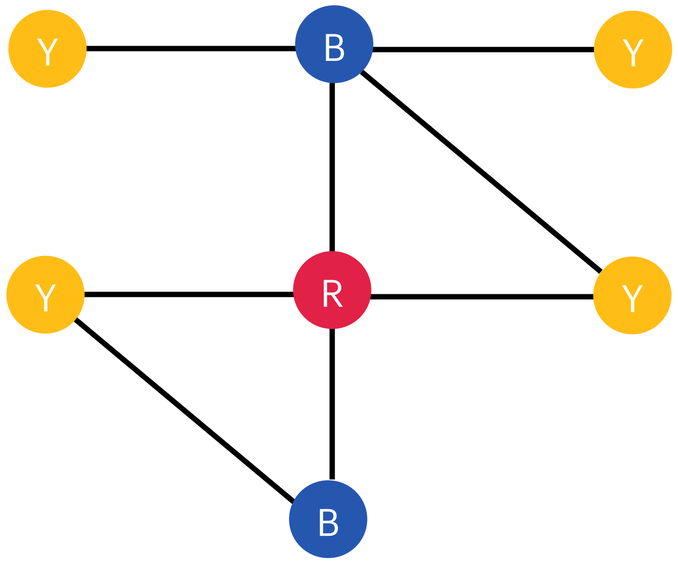

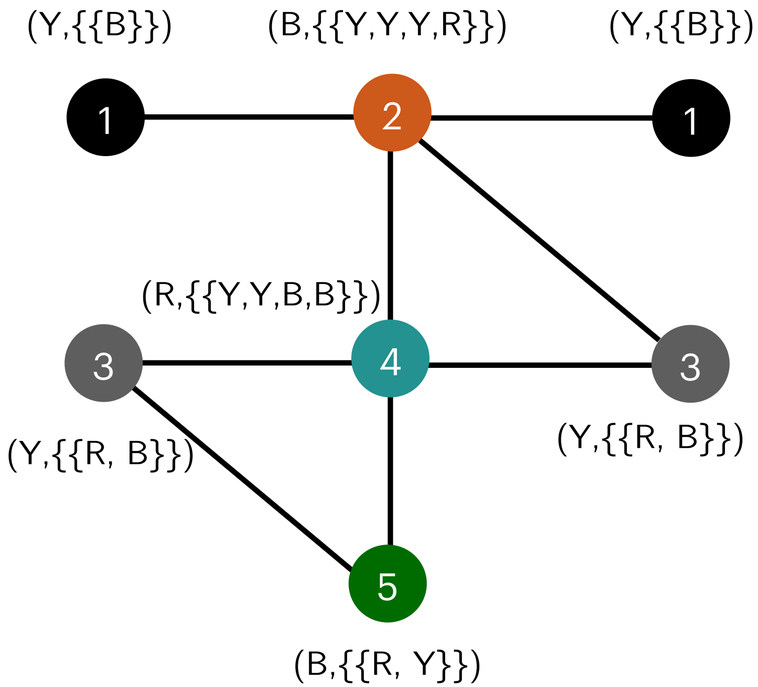

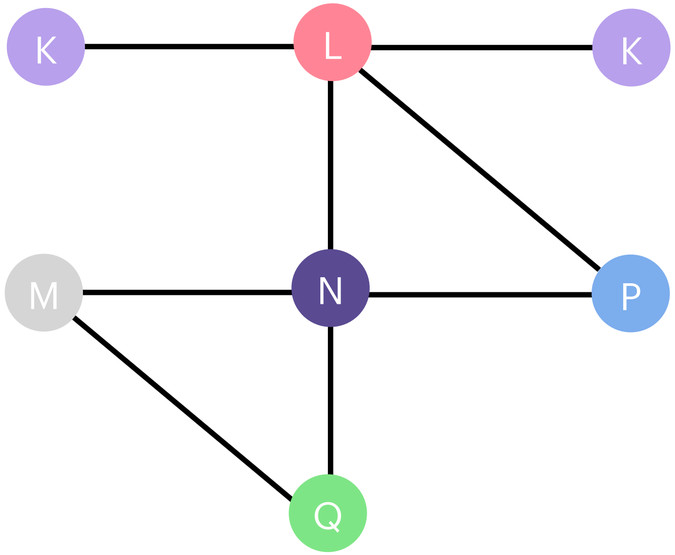

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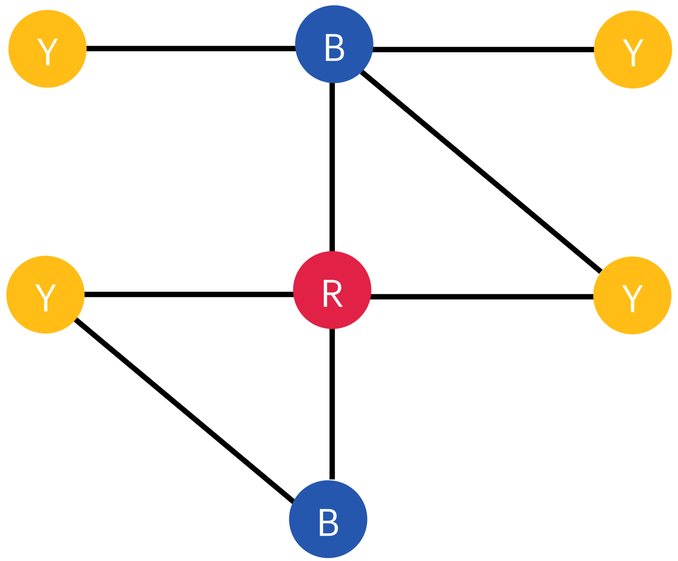

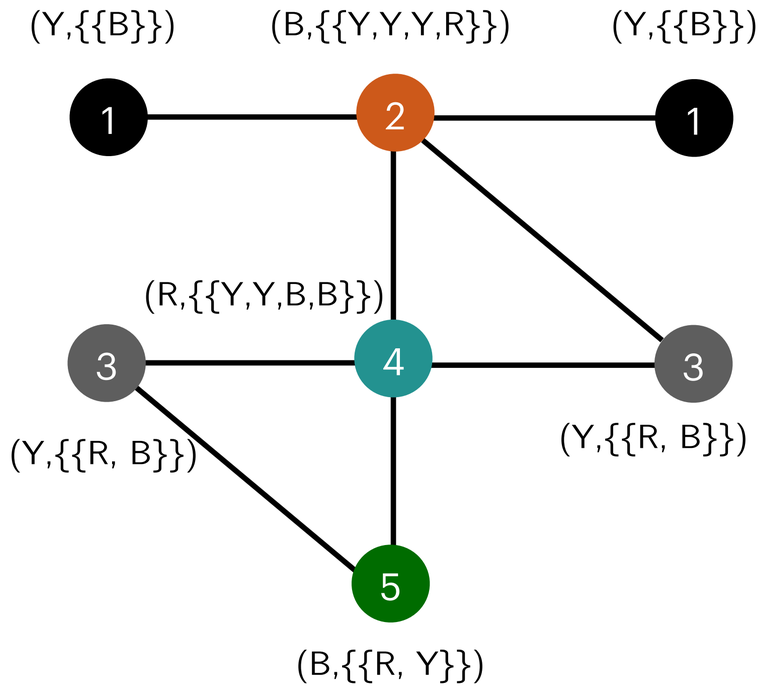

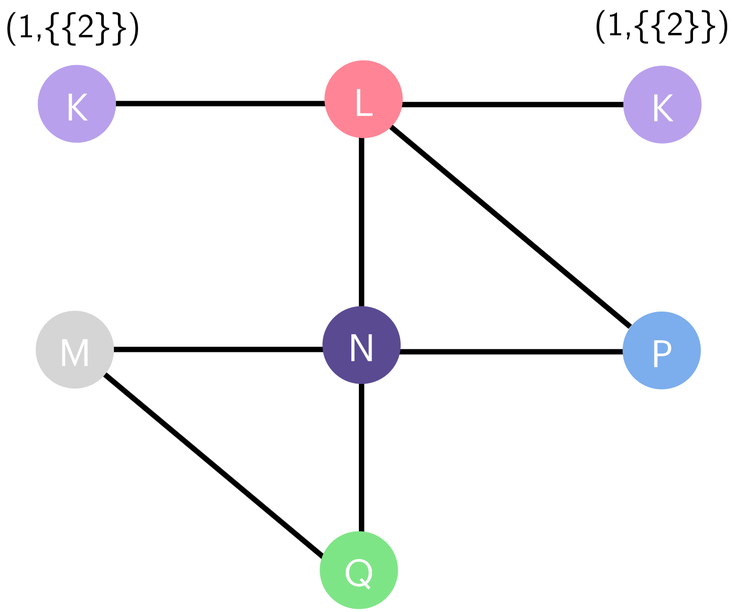

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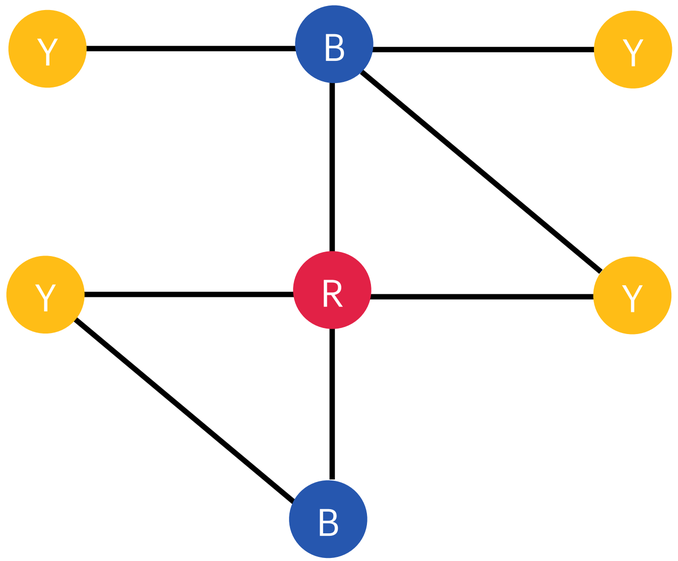

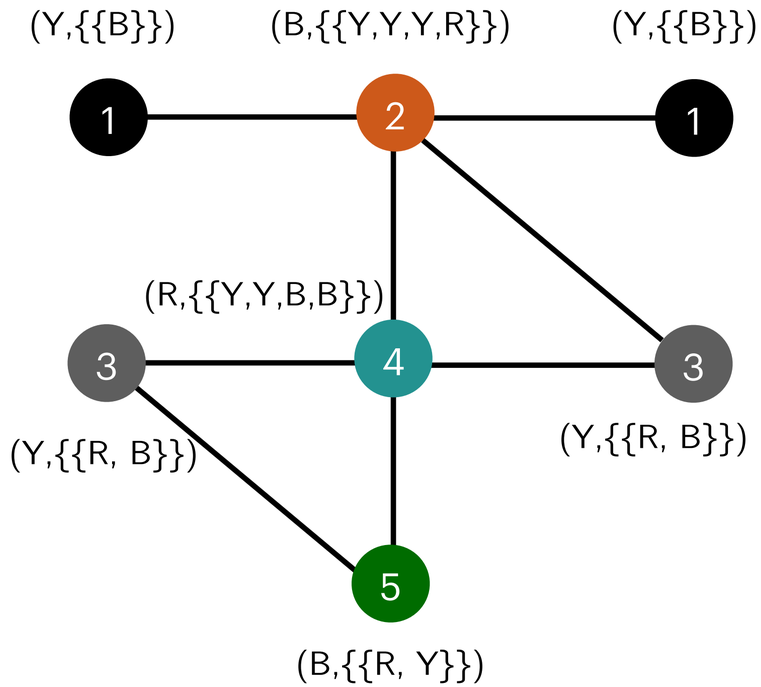

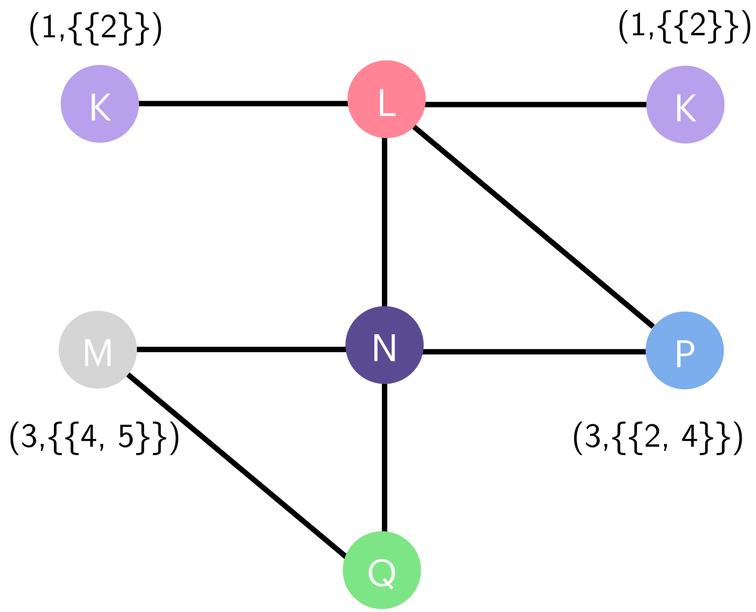

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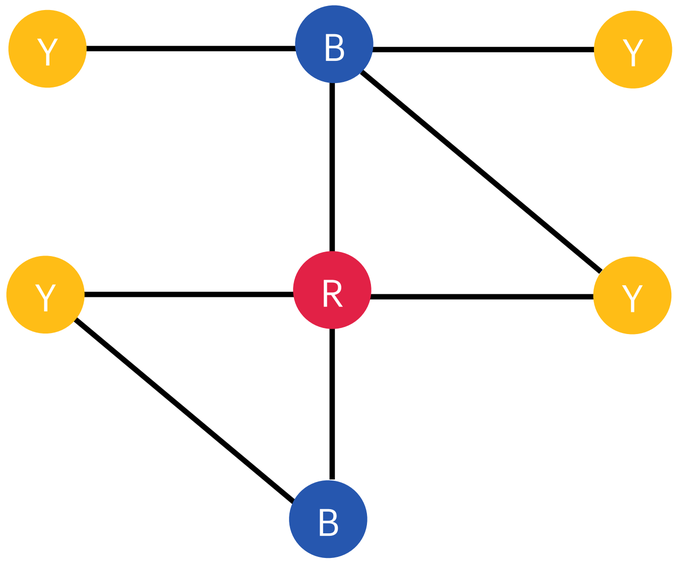

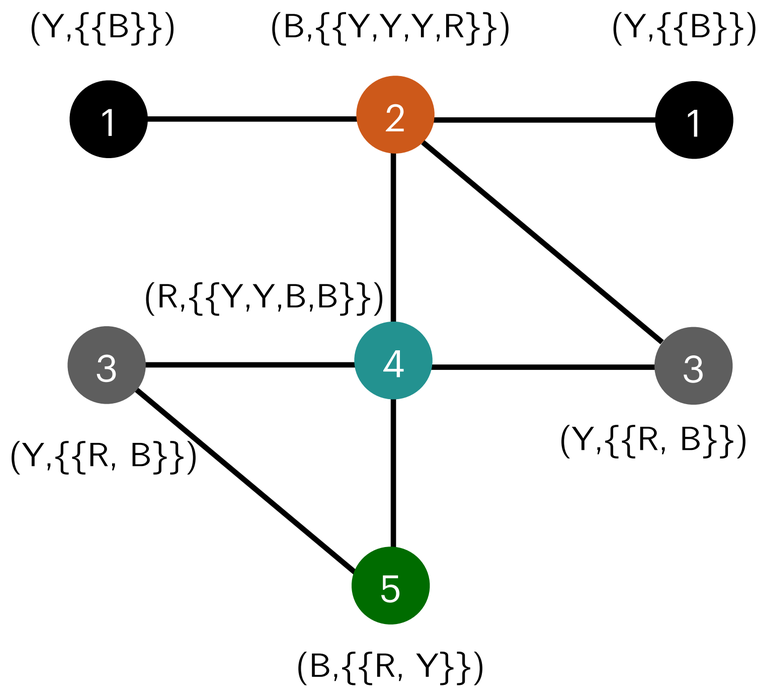

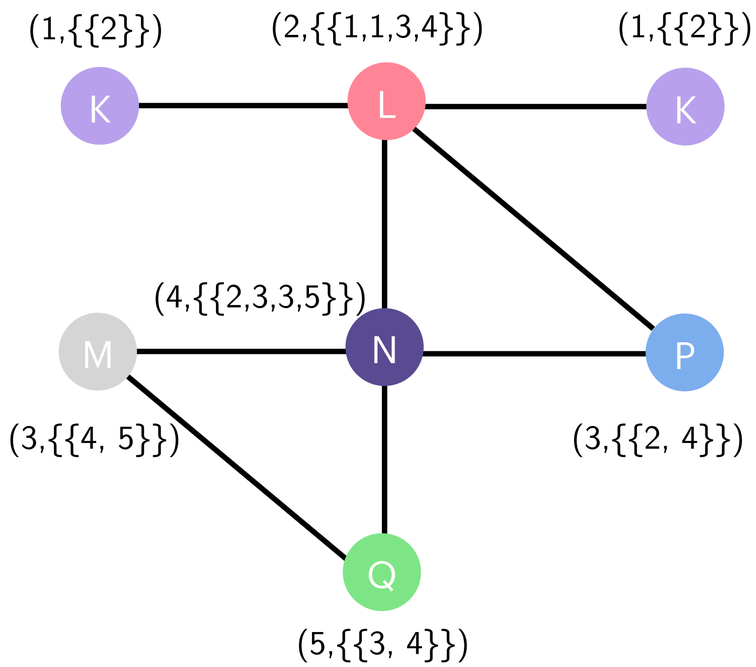

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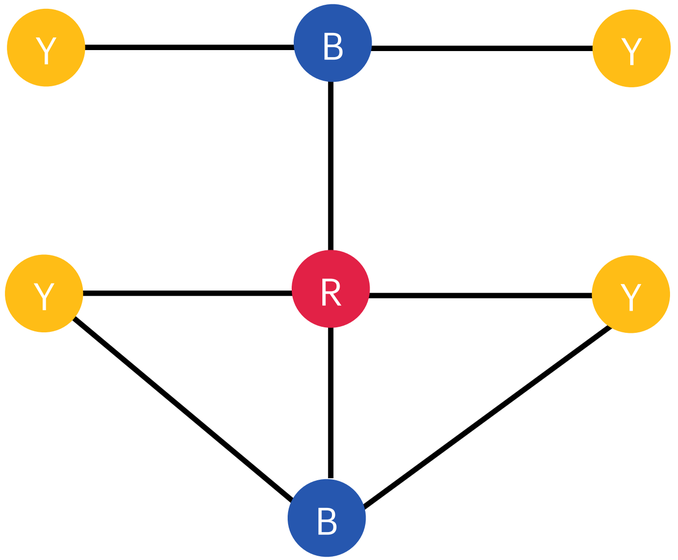

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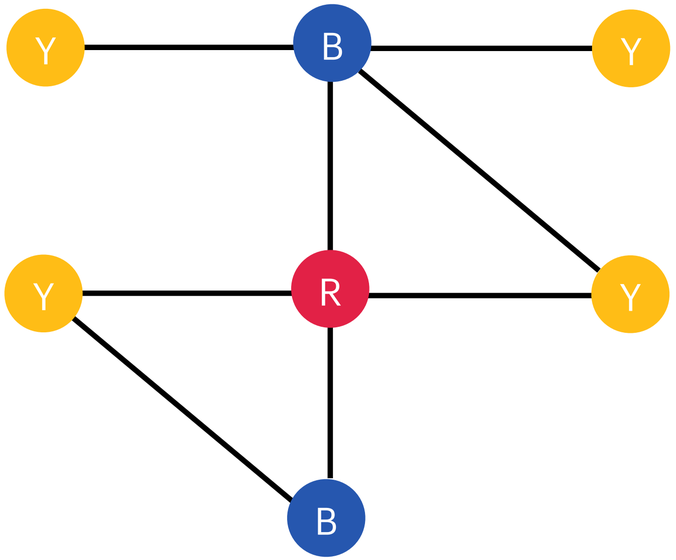

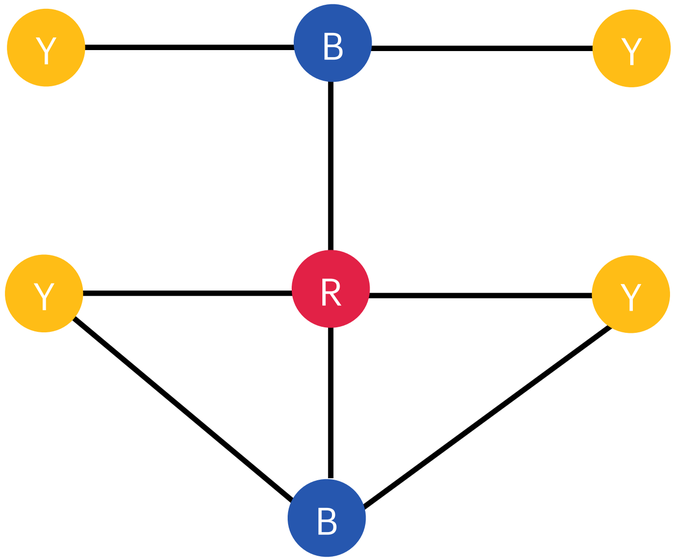

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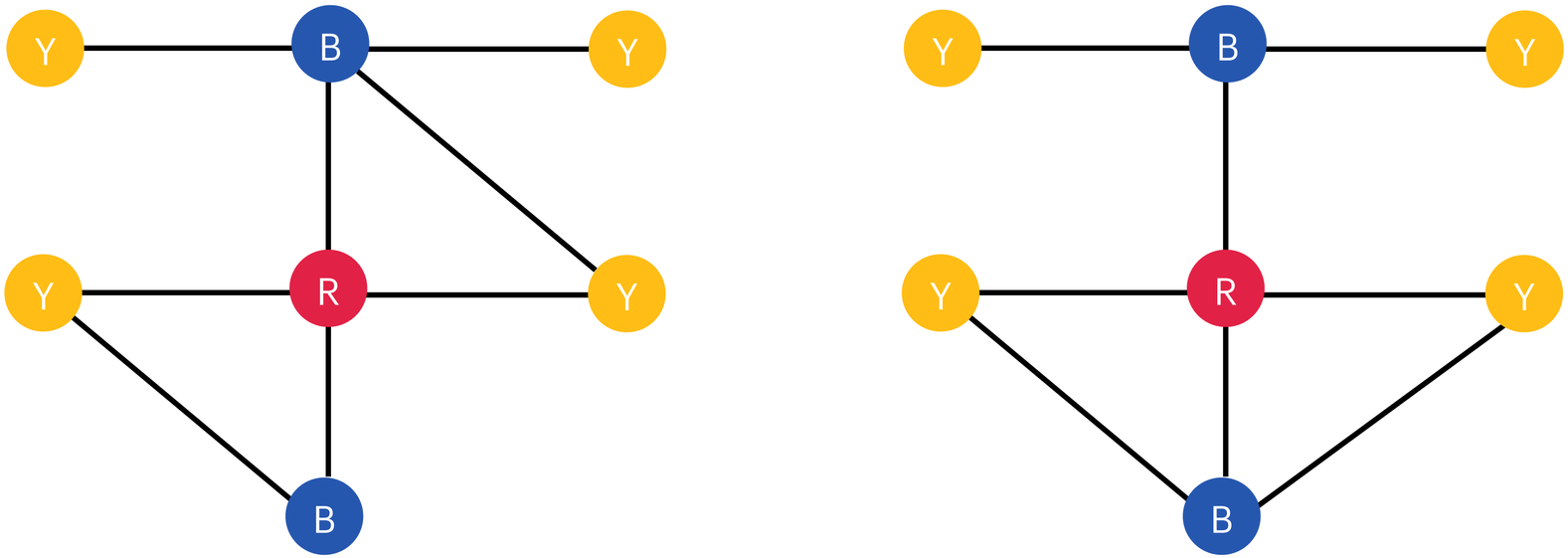

Vertex colour classes will be different for these two graphs, and so colour refinement can distinguish these non-isomorphic graphs.

Expressive Power of MPNNs

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Are MPNNs (at most) as powerful as 1-WL?

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Theorem ([Morris et al., 2019, Xu et al., 2019]). Consider any MPNN that consists of k message-passing layers of the following form:

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where $aggregate^{(t)}$ is a permutation-invariant differentiable function and $combine^{(t)}$ a differentiable function. Assuming only discrete input features $\mathbf{h}_u^{(0)} = \mathbf{x_u} \in \mathbb{Z}^d$, we have that $\mathbf{h}_u^{(k)} \neq \mathbf{h}_v^{(k)}$ only if the nodes u and v have different labels after k iterations of the 1-WL algorithm.

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MPNNs are as powerful as 1-WL test under mild assumptions.

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Proposition (Morris et al., 2019; Xu et al., 2019). Two graphs G and H are indistinguishable by all MPNNs if and only if they satisfy the same C^2 -sentences.

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Together with the results of (Morris et al., 2019; Xu et al., 2019), this implies the following:

Proposition (Morris et al., 2019; Xu et al., 2019). Two graphs G and H are indistinguishable by all MPNNs if and only if they satisfy the same C^2 -sentences.

This is the territory of descriptive complexity — a branch of complexity theory, where the goal is to characterise complexity classes in terms of the logics that can capture the complexity classes (Immerman, 1995).

Logic of Graphs

First-Order Logic: Syntax

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Basics: A (first-order) relational vocabulary denoted by σ, consists of sets $\mathbf{R}$ of relation, $\mathbf{C}$ of constant, and $\mathbf{V}$ of variable names. A term is either a constant or a variable. An atom is of the form $P(s_1, \ldots, s_n)$, where P is an n-ary relation, and $s_1, \ldots, s_n$ are terms. A ground atom is an atom without variables.

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Formulas: First-order logic (FO) formulas are inductively built from atomic formulas using the logical constructors and quantifiers based on the grammar rule:

$$\Phi = \; P(s_1, \ldots, s_n) \;\mid\; \neg\Phi \;\mid\; \Phi \wedge \Phi \;\mid\; \Phi \vee \Phi \;\mid\; \exists x \,.\, \Phi \;\mid\; \forall x \,.\, \Phi,$$

where P is an n-ary relation, $s_1, \ldots, s_n$ are terms, and x is a variable.

Note: We are using upper-case letters to denote relation names, and lower case letters to denote variables/ constants — In Lecture 1 & 2, we used lower case for everything to align with conventions in node embeddings.

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As usual, some constructors are only syntactic sugar, i.e., we use usual abbreviations:

$$\forall x \,.\, \Phi \equiv \neg\, \exists x \,.\, \neg \Phi,$$

$$\Phi \vee \Psi \equiv \neg(\neg \Phi \wedge \neg \Psi),$$

$$\Phi \rightarrow \Psi \equiv \neg \Phi \vee \Psi,$$

and so we define the semantics based on the constructors $\neg$, $\wedge$, $\exists$.

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We assume that constants are mapped to themselves by any interpretation (i.e., unique name assumption).

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Logic can be used to characterise graph properties and we can view graphs as interpretations, where the domain is simply the set of vertices!

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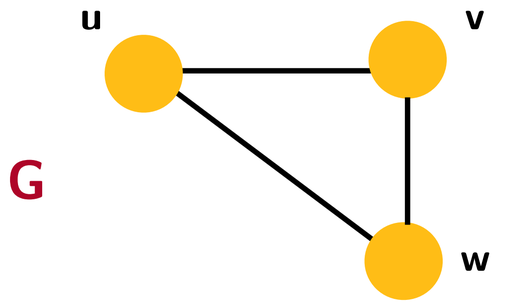

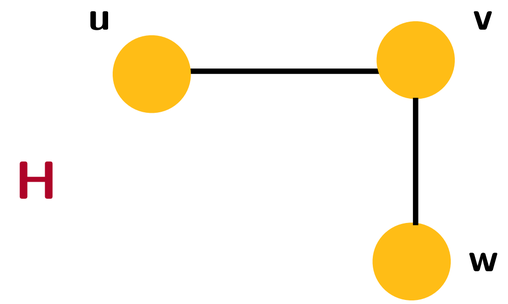

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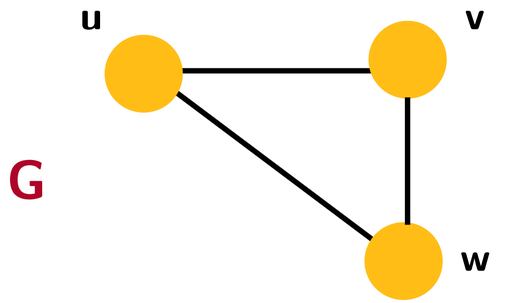

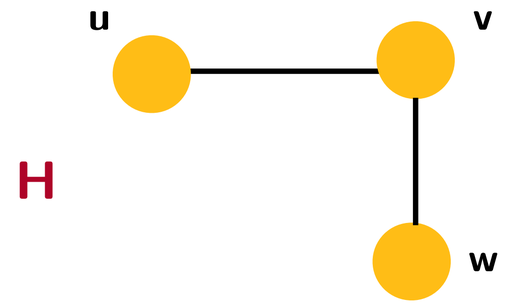

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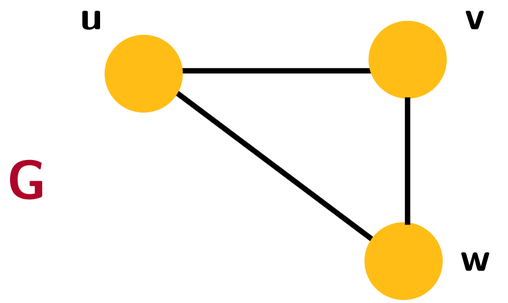

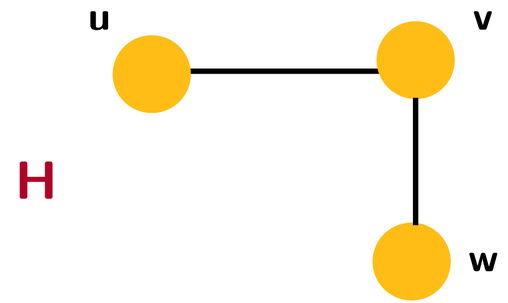

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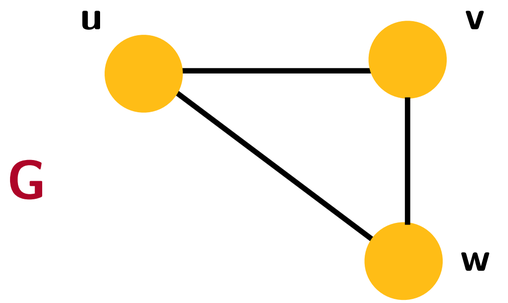

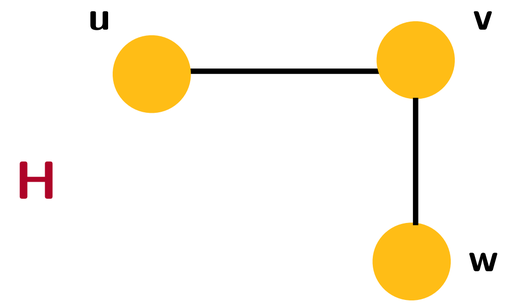

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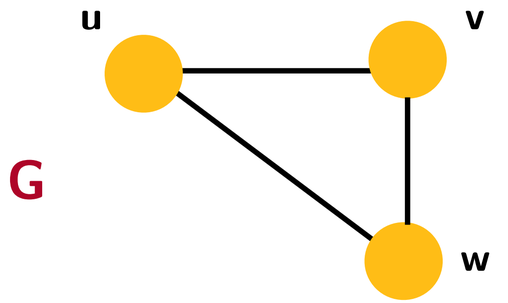

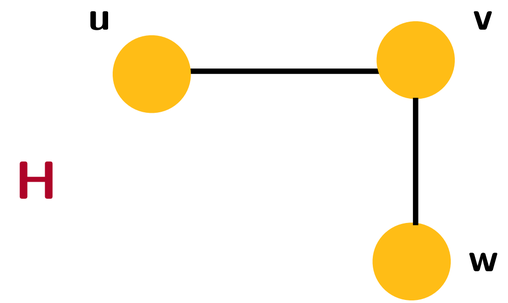

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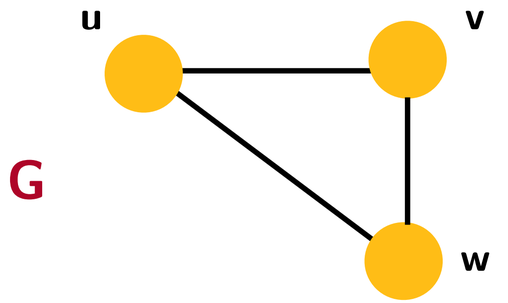

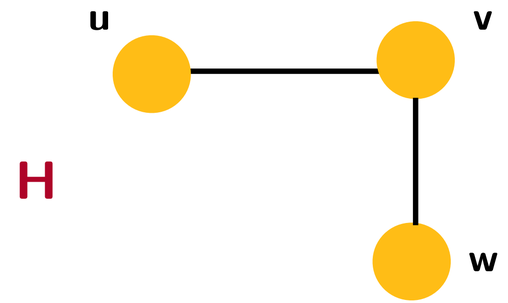

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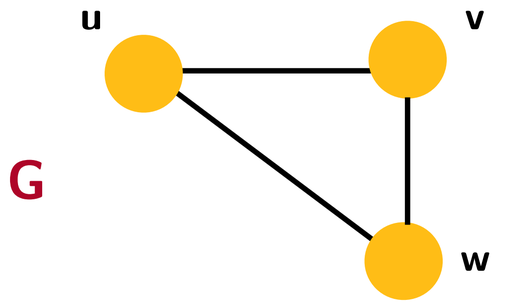
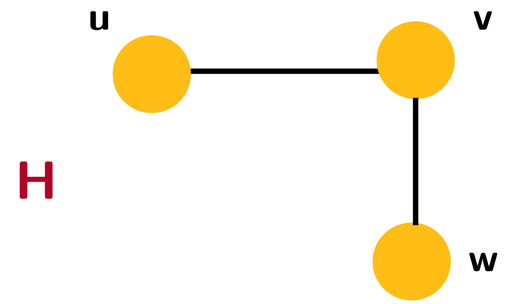
Intuitively, any graph relative to a node a which takes part in a triangle is a model of $\Phi(a)$.





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Consider, for example, the formula:

$$\Psi(x) = \mathit{Red}(x) \wedge \exists y \Big(E(x, y) \wedge \mathit{Blue}(y) \wedge \exists z \Big(E(x, z) \wedge \mathit{Green}(z) \Big) \Big).$$

This formula is satisfied by nodes nodes $u \in V_G$ such that $G \vDash \Psi(u)$, i.e., red nodes that are connected to a blue and a green node.

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This works, intuitively, because the variables refer to different things in the scope of different quantifiers. This trick is not always possible: Indeed FO^2 is strictly contained in FO, i.e, there are formulas in FO that cannot be expressed in FO^2.

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C extends first-order logic with counting quantifiers of the form $\exists^{\geq k} x$ for $k \geq 0$, where $\exists^{\geq k} x \Phi(x)$ means that there are at least k elements x satisfying Φ. As before, C^{k} denotes the k-variable fragment of C.

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It is well-known that C is only a syntactic extension of FO, as counting quantifiers of the form $\exists^{\geq k} x$ can be simulated with standard existential quantifiers, and using k variables. However, counting quantifiers add expressiveness if we restrict the number of variables.

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Our goal is to identify a logic that is captured by MPNNs — identifying the expressive power of MPNNs.

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"...there are AC-GNNs that can reproduce the WL labelling, and hence AC-GNNs can be as powerful as the WL test for distinguishing nodes. This does not imply, however, that AC-GNNs can capture every node classifier—that is, a function assigning true or false to every node — that is refined by the WL test. In fact, it is not difficult to see that there are many such classifiers that cannot be captured by AC-GNNs; one simple example is a classifier assigning true to every node if and only if the graph has an isolated node."

(Barcelo et al., 2020)

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For example, MPNNs without any readouts cannot capture the function described by the following formula (Barcelo et al., 2020):

$$\gamma(x) = Red(x) \wedge \exists y \Big(\neg E(x, y) \wedge \exists^{\geq 2} x \Big(E(y, x) \wedge Blue(x) \Big) \Big),$$

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An obvious candidate is MPNNs with global readout in the sense we defined earlier, i.e., there is a global feature computation happening at every layer.

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This result is also strengthened in another direction: It holds also for MPNNs with a single (final) global readout, but in this case we require MPNN to be non-homogeneous.

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This result is not complete: MPNNs with global readout can capture C^2, but is this all what MPNNs can capture? Is there a logic which MPNNs with global readout can capture, but cannot capture anything beyond?

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- Graph isomorphism, colour refinement, 1-WL
- MPNNs are at most as powerful as 1-WL test
- MPNNs with injective aggregation and combine functions are as powerful as 1-WL test.
- The logic of graphs: FO, C, FO^2, C^2 — an interesting connection to descriptive complexity!
- Logical characterisation of MPNNs
  - Each C^2 classifier can be captured by an MPNNs with global readout (even with a final readout)!
  - MPNNs without global readout cannot capture C^2, but can capture graded model logic.
- We have not discussed the practical implications of the limitations in expressive power, and neither the proposed tools to address such limitations — Lecture 6 & 7.

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