Lecture 7: Message Passing Neural Networks and Randomisation

Relational Learning

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Advanced Topics in Machine Learning, University of Oxford

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Overview

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- The quest for expressive and scalable models

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- MPNNs with random features

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- MPNNs with random features
- Universality of MPNNs with random node initialisation

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- Benchmarking expressiveness evaluation

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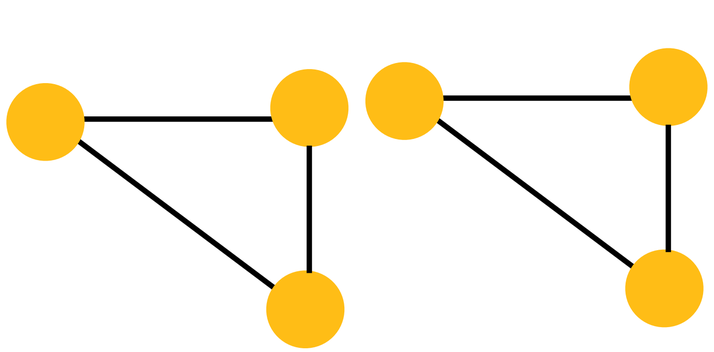
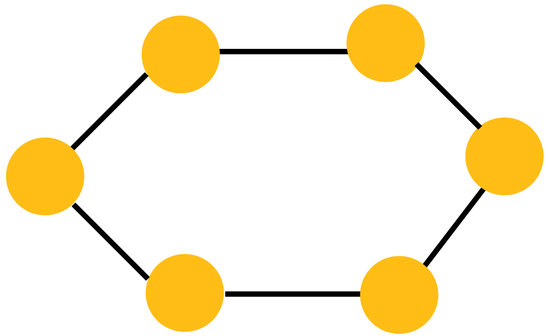
- Summary

The Quest for Expressive and Scalable Models

A Tale of Two Graphs





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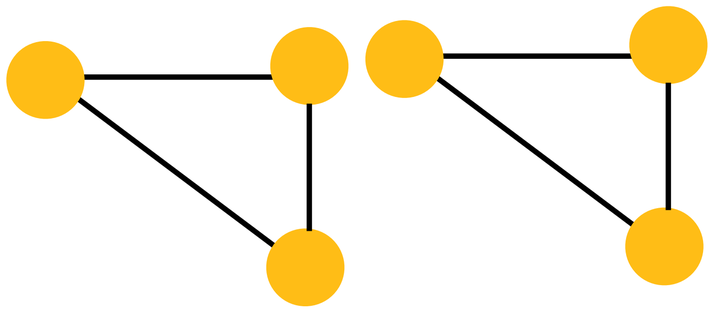

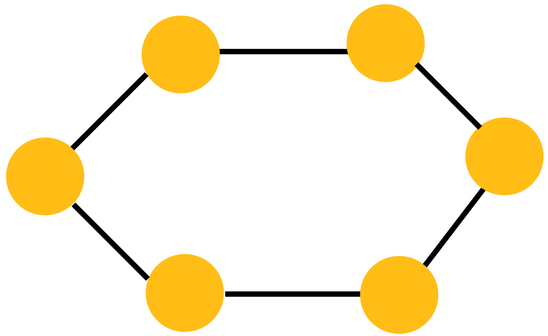

A brief recap

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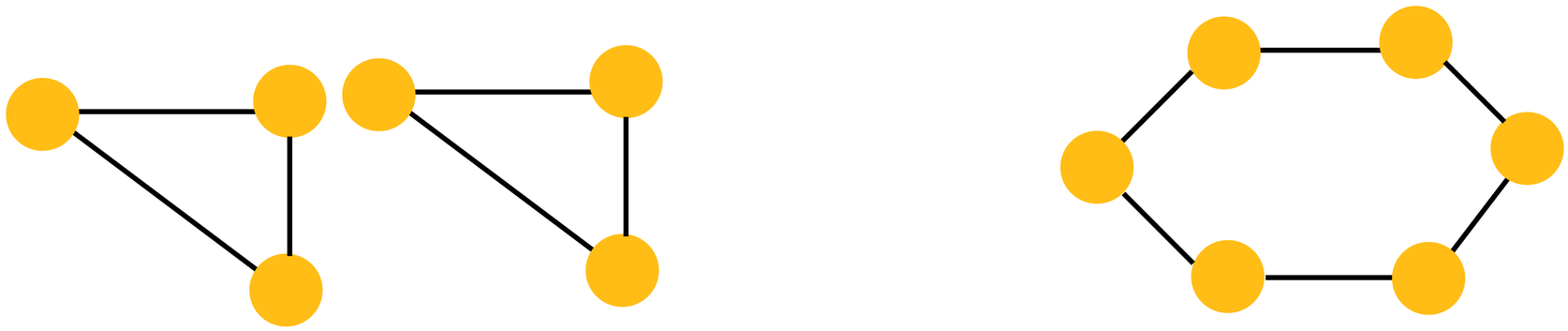

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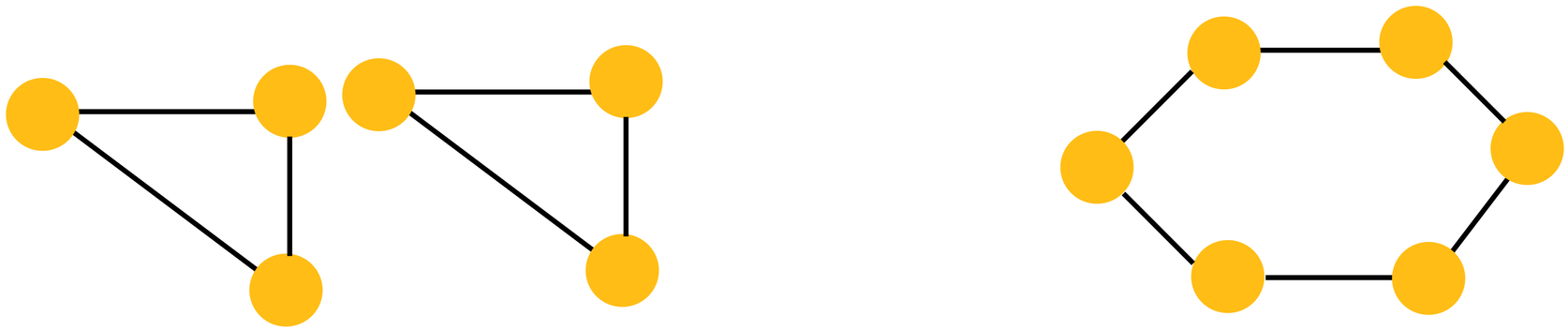

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2. The embedding learned for the graph on the left-hand side will be exactly the same as the embedding of the graph on the right-hand side for MPNNs!

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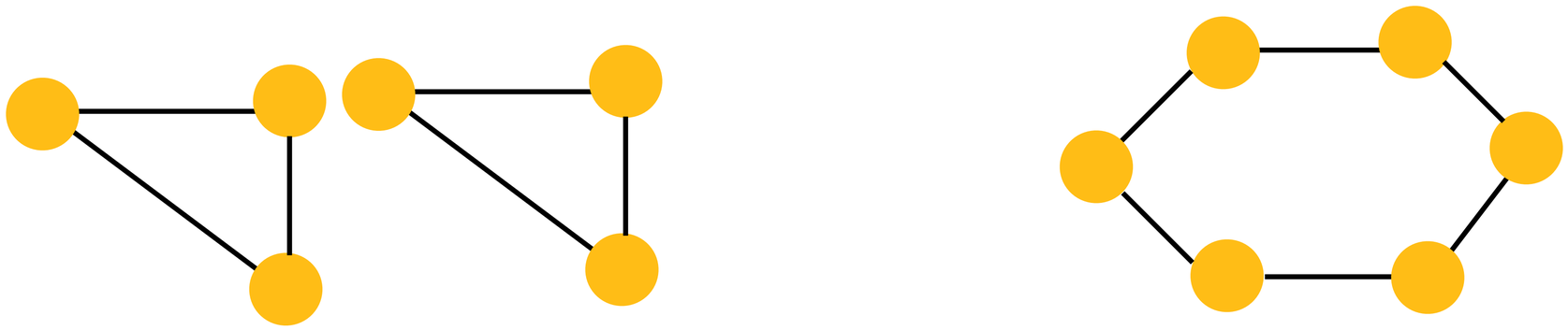

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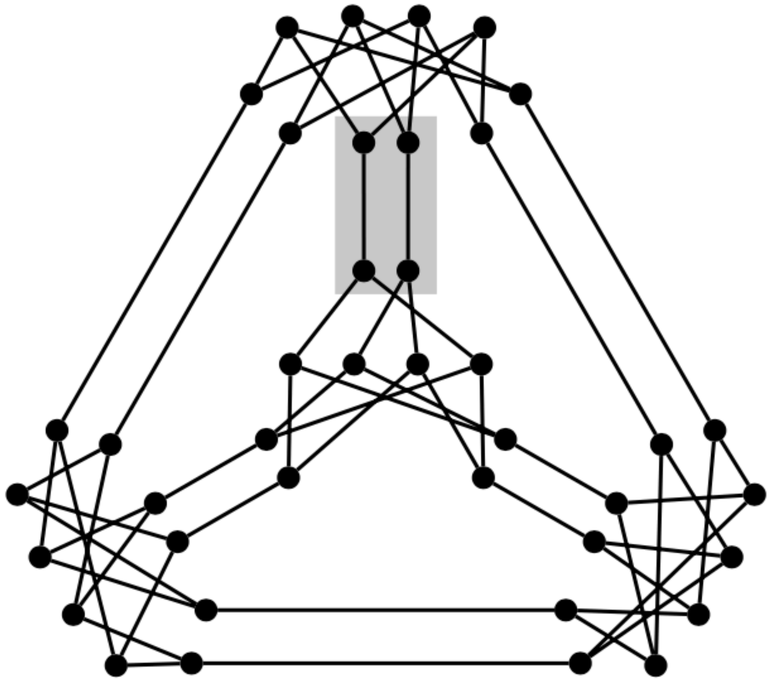
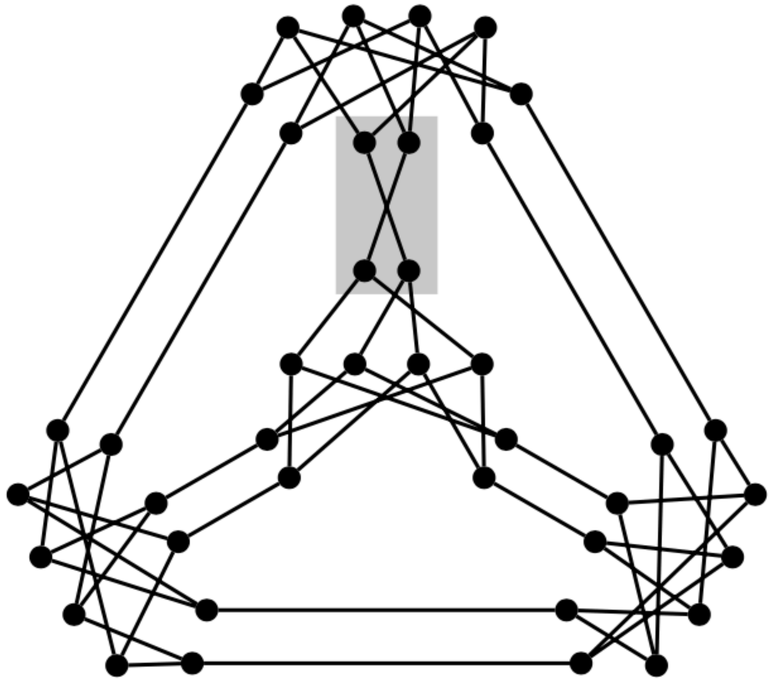
2. The embedding learned for the graph on the left-hand side will be exactly the same as the embedding of the graph on the right-hand side for MPNNs!
3. There is a pair of non-isomorphic graphs distinguishable by $(k+1)$-WL but not by k-WL for each $k \geq 1$.

Graph Distinguishability





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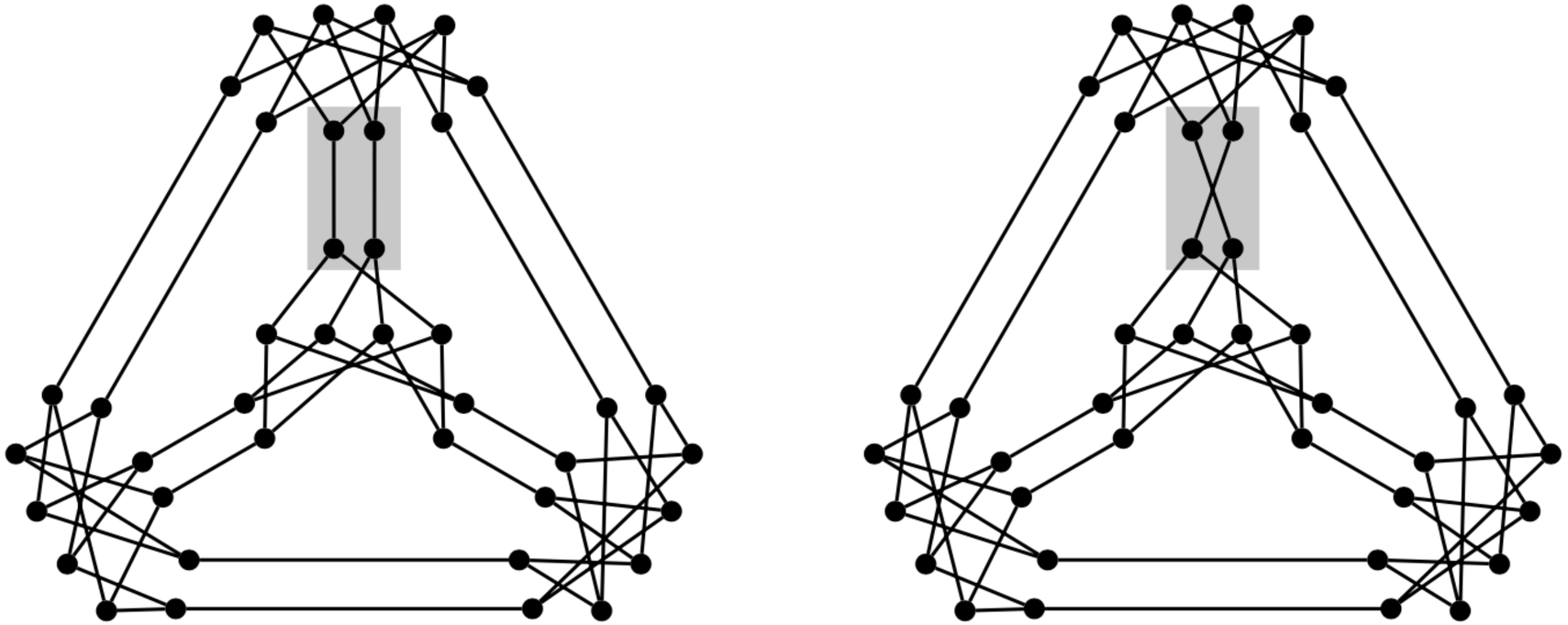

Example: 2WL cannot distinguish the shown graphs which differ only in the grey area (Grohe, 2017), i.e., even higher-order models such as 3-GNNs do not possess sufficient expressive power to distinguish these graphs.

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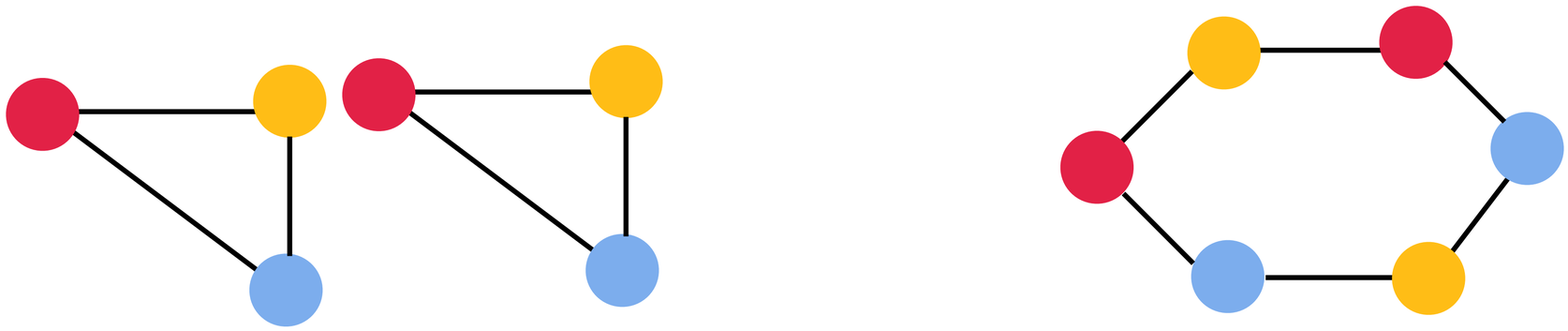

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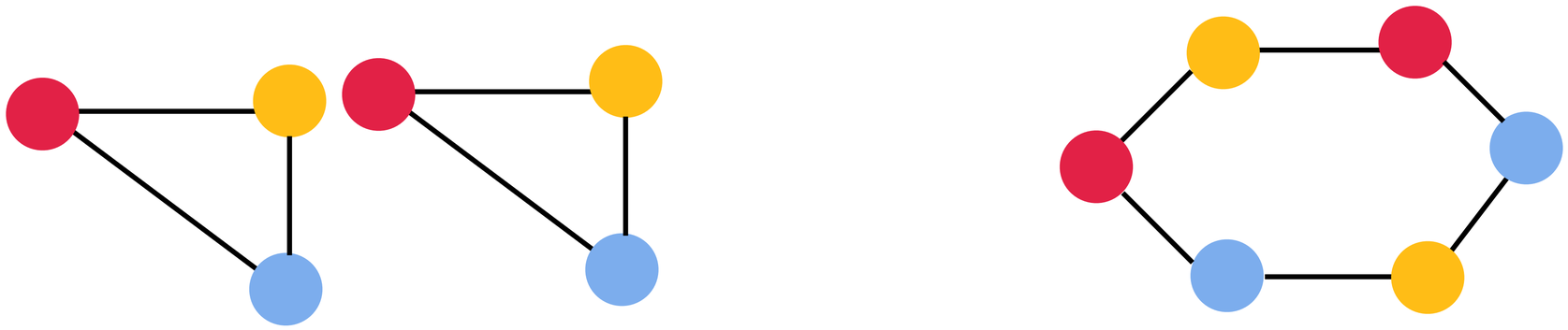

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- The same is true for MPNNs — we can start with any node features.

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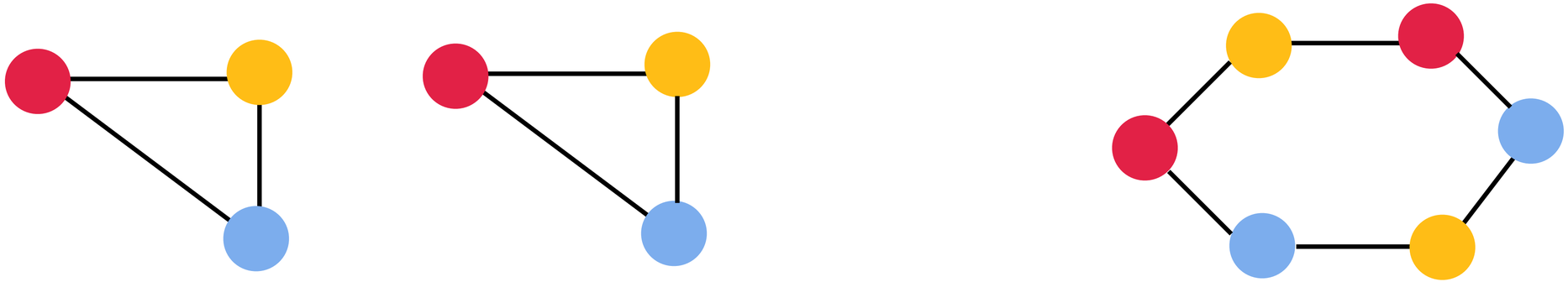

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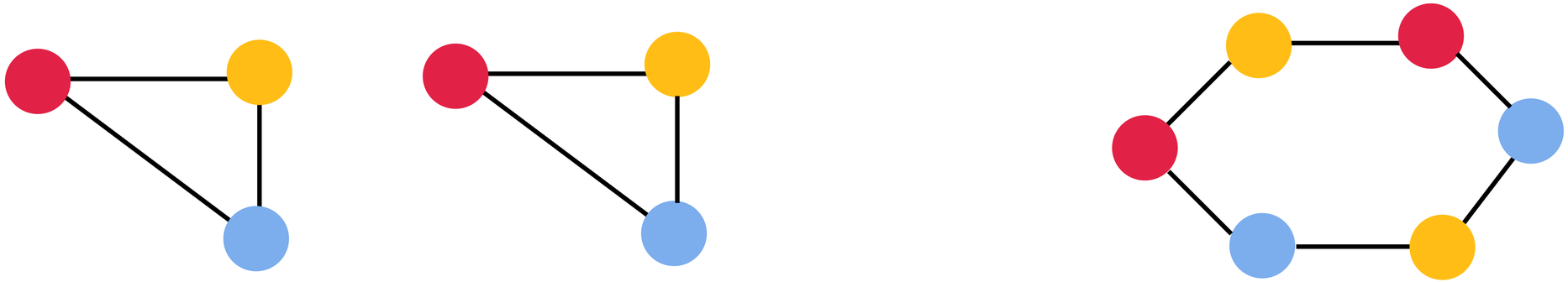

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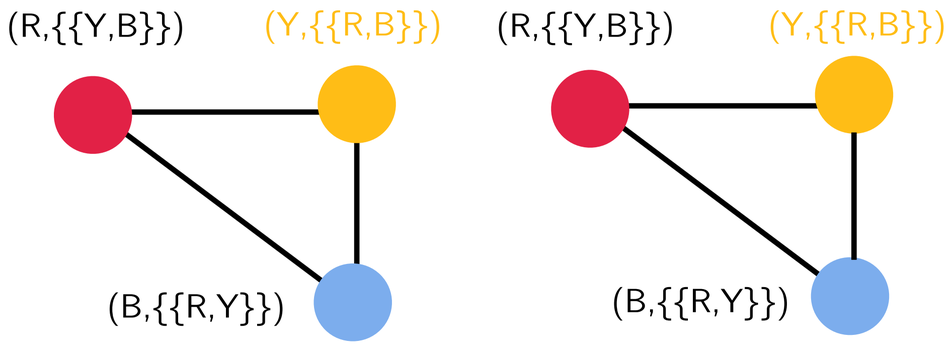

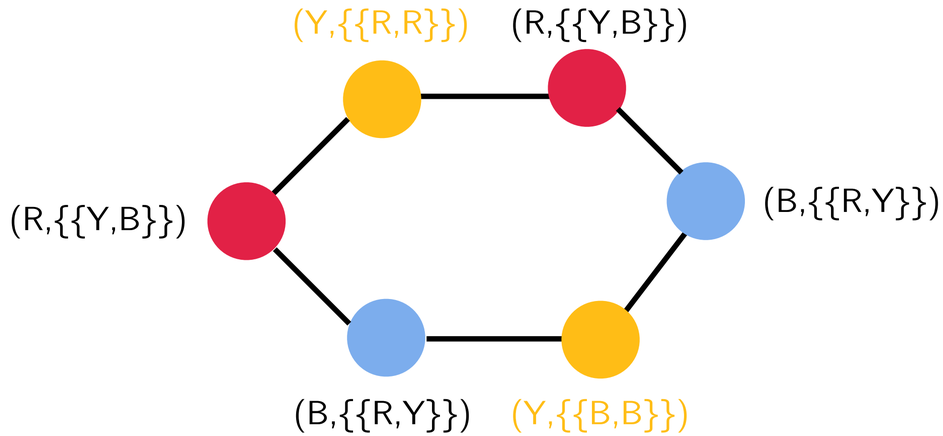

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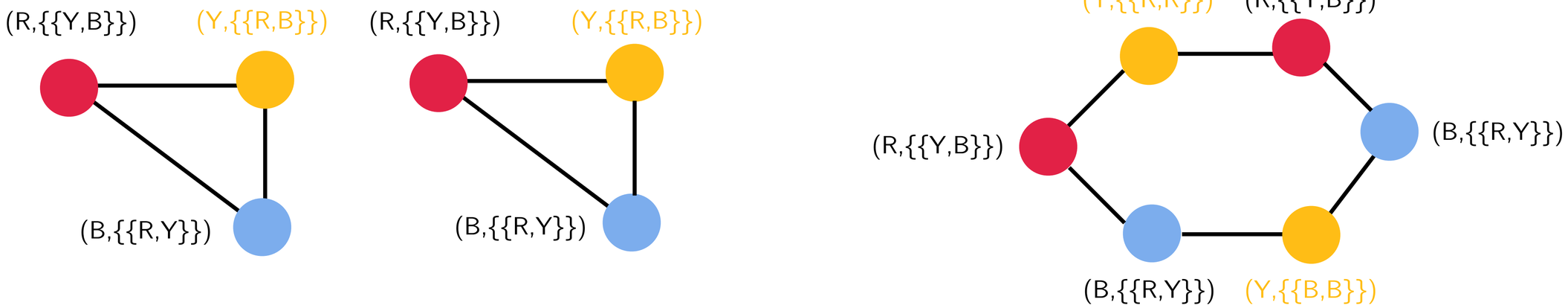

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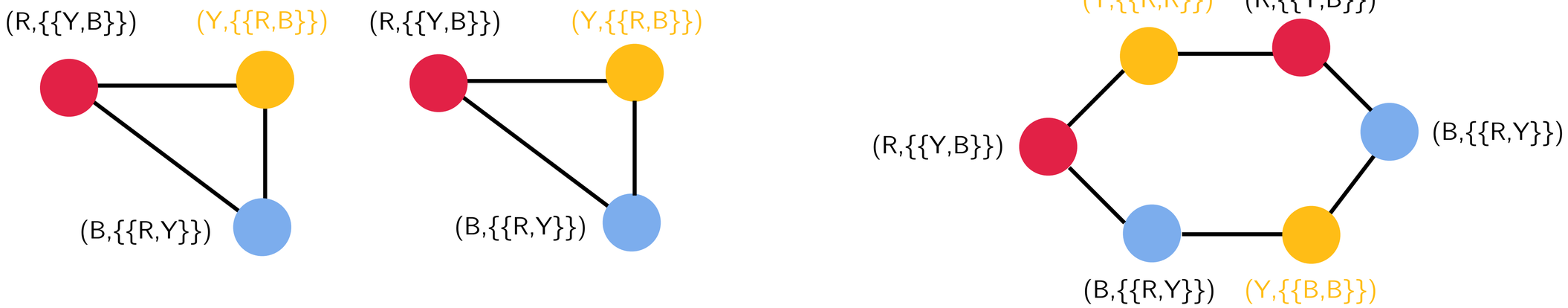

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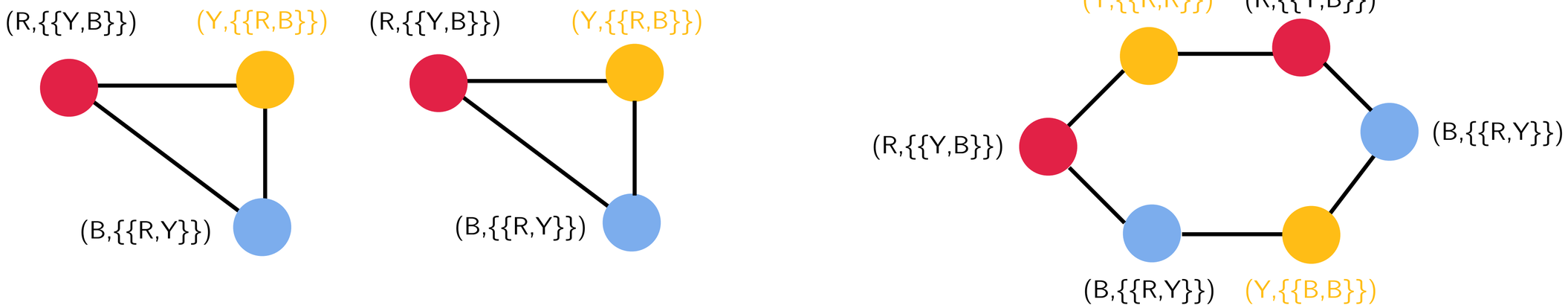

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- After the first iteration of the 1-WL algorithm the graphs are distinguished via the initially yellow nodes.
- After the second iteration the graphs will differ with respect to any node.
- The same is true for MPNNs — if we set the node features accordingly.

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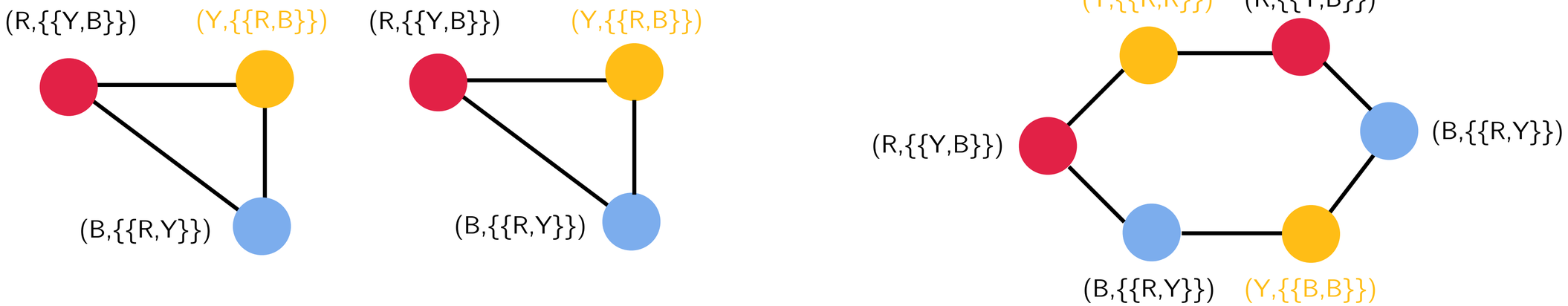

Wouldn't initialising node features in an MPNN to different colours be ideal?

This will yield an expressive model — 1-WL can distinguish any pair of ordered/coloured graphs.

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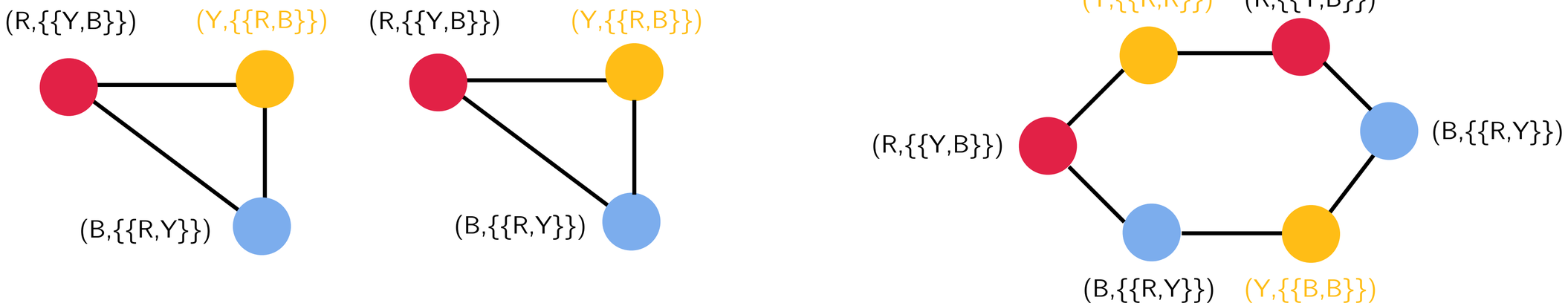
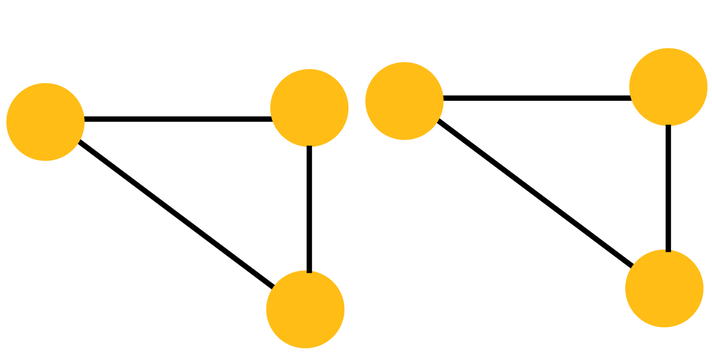


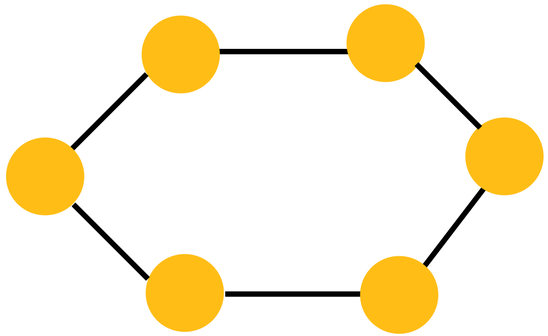
There are **problems** in initialising nodes with such features:

- We assign colours to nodes from a fixed class of colours which do not necessarily have a meaning.
- We change the meaning of the given node features — potentially losing valuable information.
- These features are deterministic and it is hard to generalise over these structures.

MPNNs with Random Features

Random Node Features and Coloured Graphs





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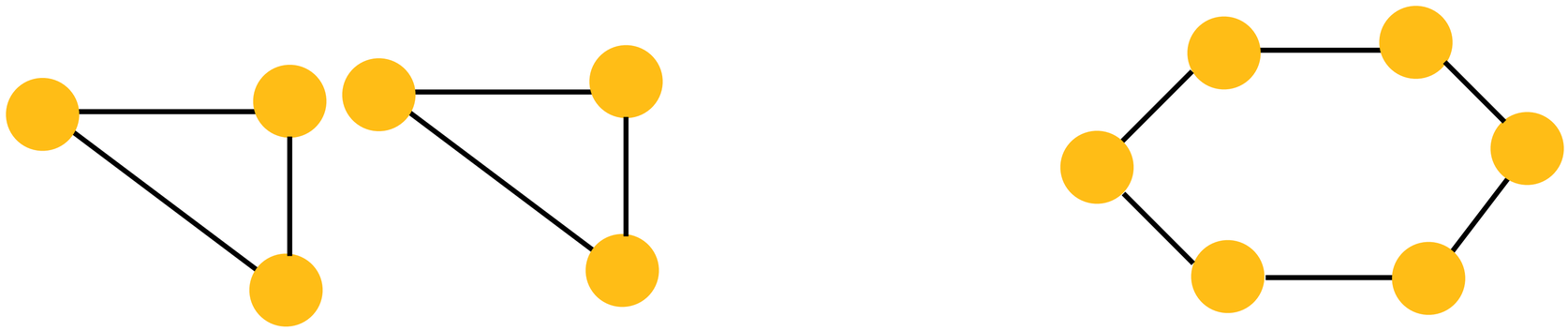

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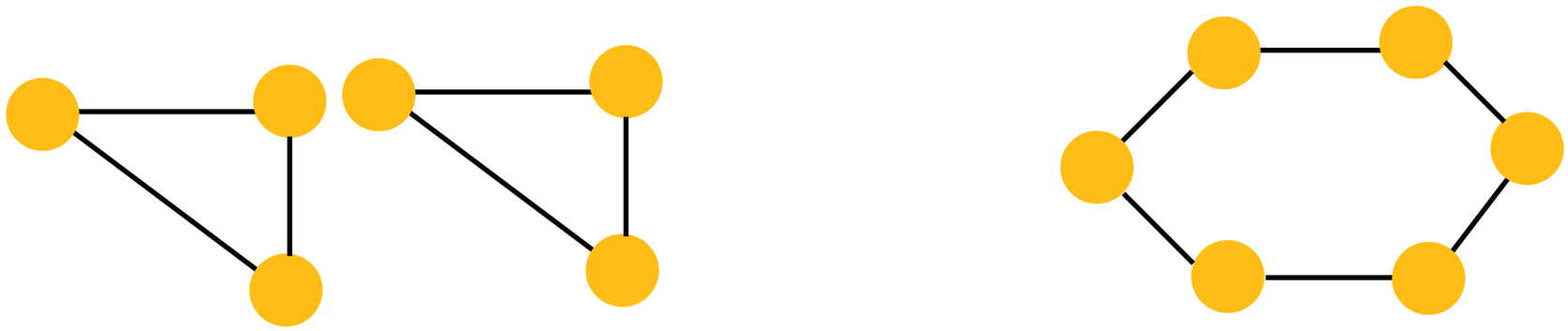

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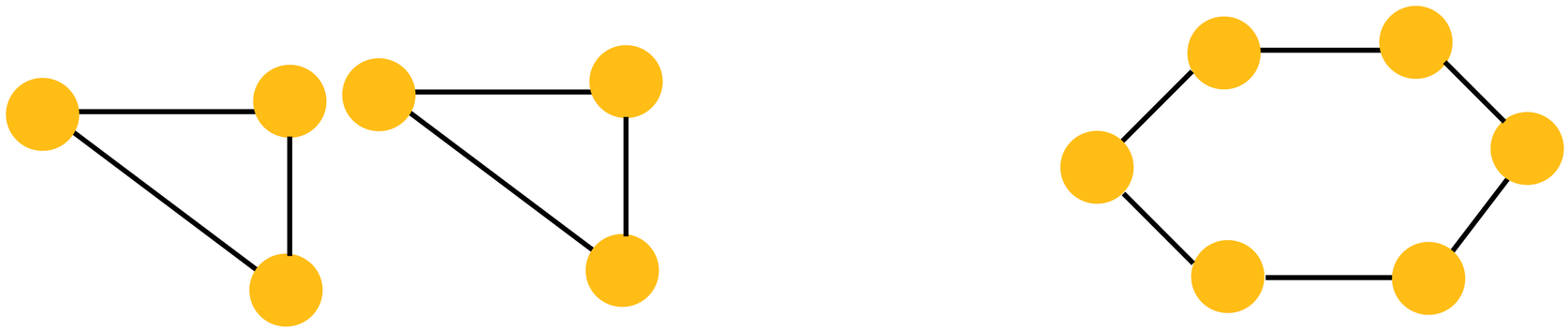

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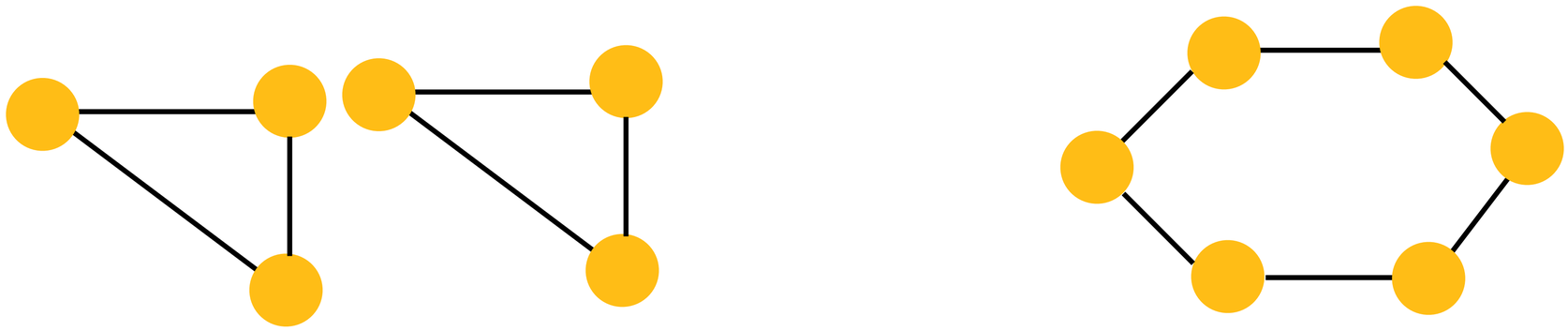

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Intuition: Random features can implicitly induce a colouring, and yield a more expressive model.

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To make the distinction clear, we speak of node features, and hence of random node initialisations here. Note that one can also consider random edge initialisations.

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GIN-RNI models go beyond the capabilities of GINs which cannot determine the existence of a triangle.

Remark: This theorem does not imply universality, as it only asserts distinguishability w.r.t. a fixed structure. This is not the same as being able to approximate any function (which can depend on multiple, interacting structures) over this space.

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- GIN-RNI achieves >90% accuracy and GCN-RNI >85% achieves accuracy on normal and extrapolation datasets.
- Since the test graphs in the extrapolation dataset have more nodes than the training graphs, this shows that MPNN-RNI models can potentially extrapolate to variable size graphs.

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Question: What is the expressive power of MPNN-RNI models, and can these be universal?

Universality of MPNNs with Random Node Initialisation

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Given these, we can pose the following concrete question.

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- We know that we can approximate any Boolean function $g : \mathcal{G}_n \mapsto \mathbb{B}$, by the lemma above.
- To approximate $f : \mathcal{G}_n \mapsto \mathbb{R}$, we can define a function g combining the Boolean functions $g_1, \ldots, g_s$ s.t.:

$$g_i(G) \mapsto 1, \text{ if } f(G) \mapsto y_i, \text{ and } g_i(G) \mapsto 0, \text{ otherwise.}$$

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That is, the graph G satisfies the property specified by Φ if $G \models \Phi$, and we can simply denote this by $\Phi(G)$, viewing $\Phi : V_G \mapsto \mathbb{B}$.

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The main connection comes from the fact that 1-WL can distinguish all ordered structures/graphs and so there is a C^2 sentence that can uniquely (up to isomorphism) identify an ordered graph.

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Coloured graphs: We say a graph is ordered if there is a total order on the nodes of the graph. Observe that colouring the nodes of a graph with distinct colours induces a total order on the nodes of a graph. We can therefore refer to coloured graphs instead, where each node is assigned colours from a finite set of colours.

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Remark: This result holds even with partial node initialisations — even with a single randomised dimension.

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- The broader picture is, however, rather subtle: We can view such a model as computing a random variable (or as generating an output distribution), and this random variable would still be invariant.
- This means that the outcome of the computation of an MPNN-RNI does still not depend on the specific representation of the input graph, which fundamentally maintains invariance.

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Together with the arguments above, MPNN-RNI models, allowing variability, are universal models, and preserve the good inductive bias of MPNNs.

Benchmarking Expressiveness Evaluation

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SAT is combinatorial by its nature and is not local, i.e., the satisfiability of a formula cannot be determined by local properties alone.

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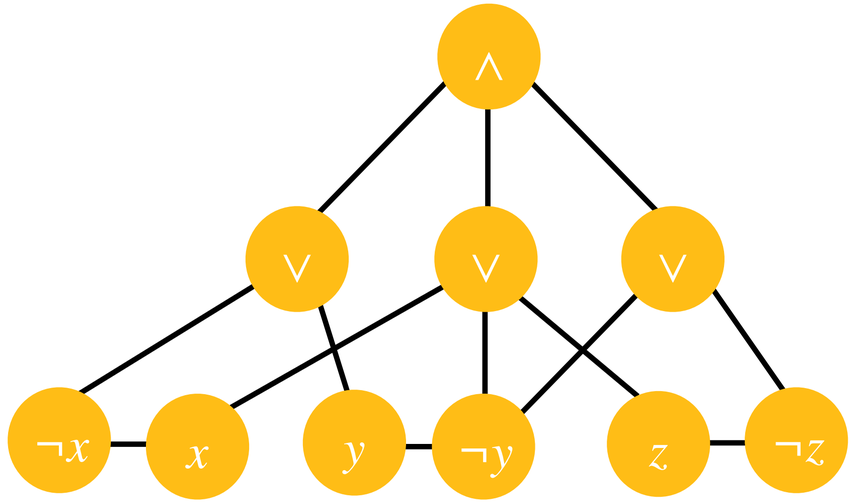

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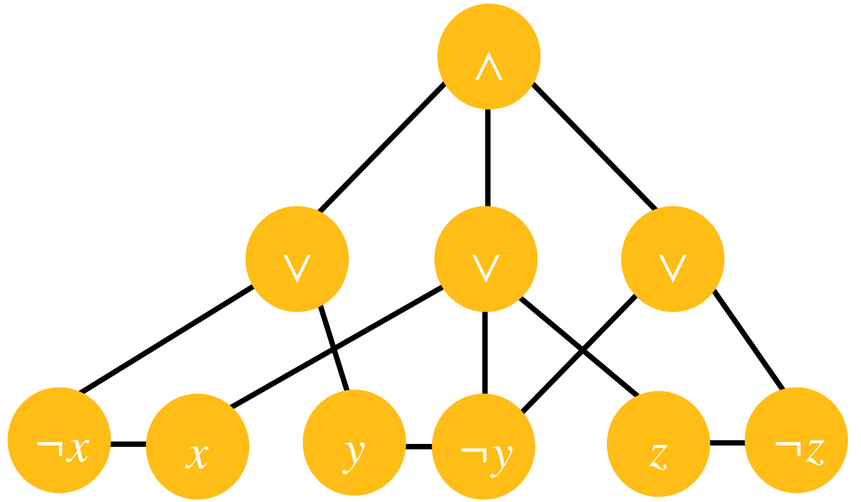

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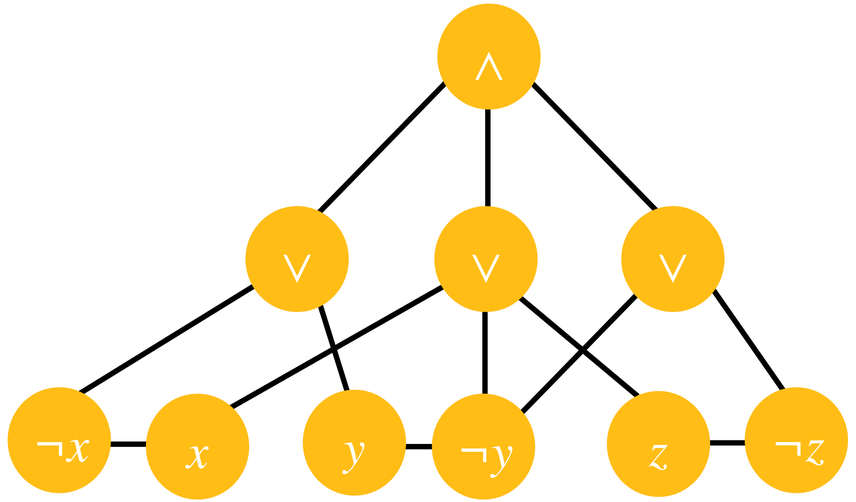

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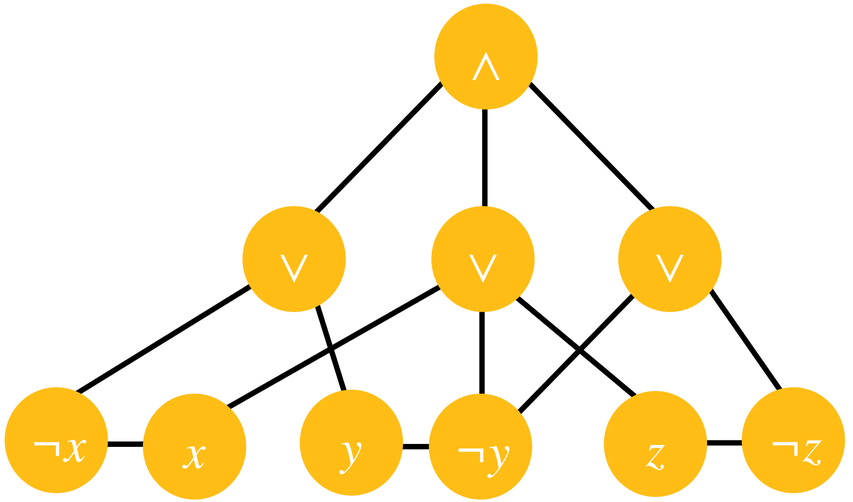
A simple graph encoding of a propositional formula is shown on the right hand side.



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- G_i and H_i are 2-WL distinguishable, so can be classified differently by higher-order GNNs that have 2-WL expressive power.

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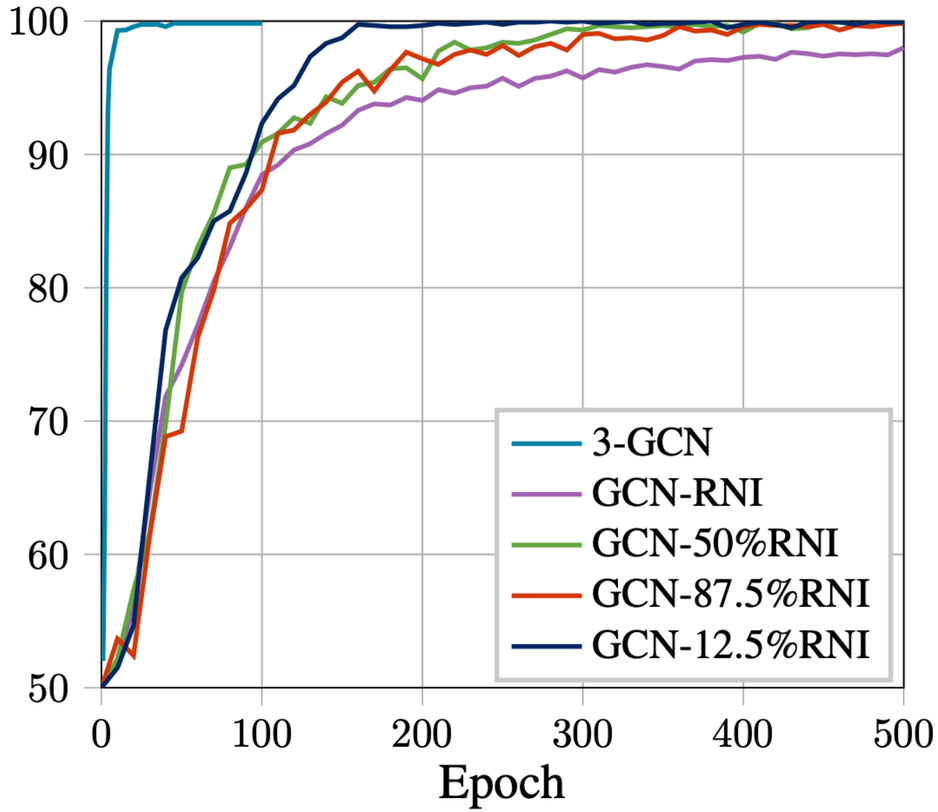

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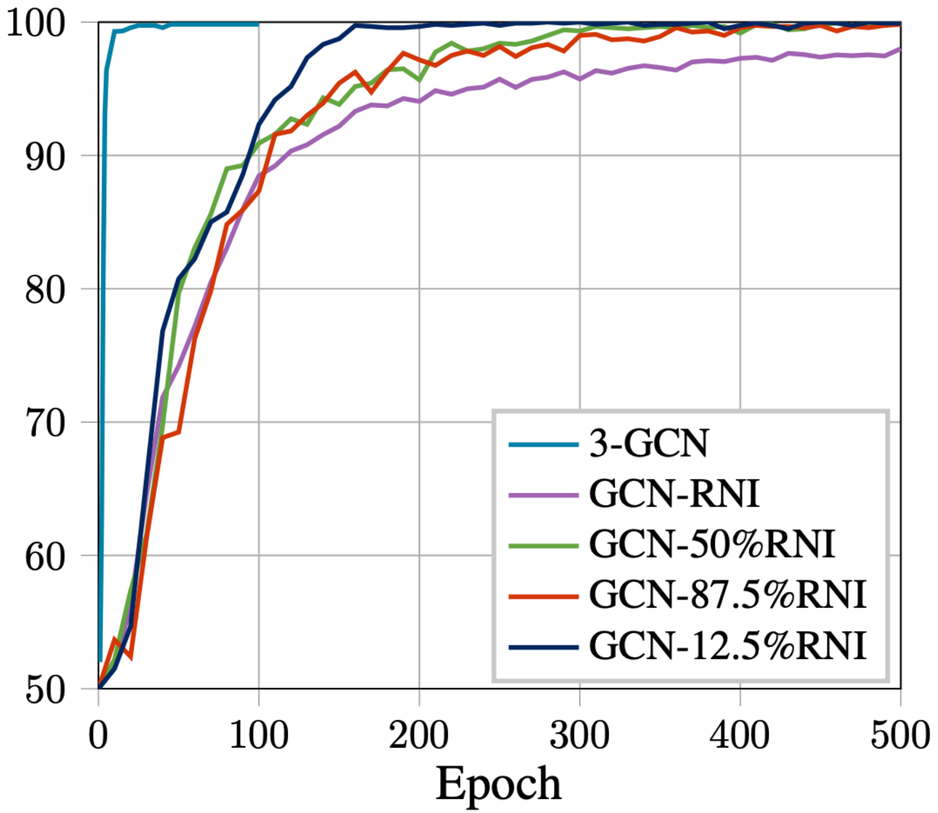

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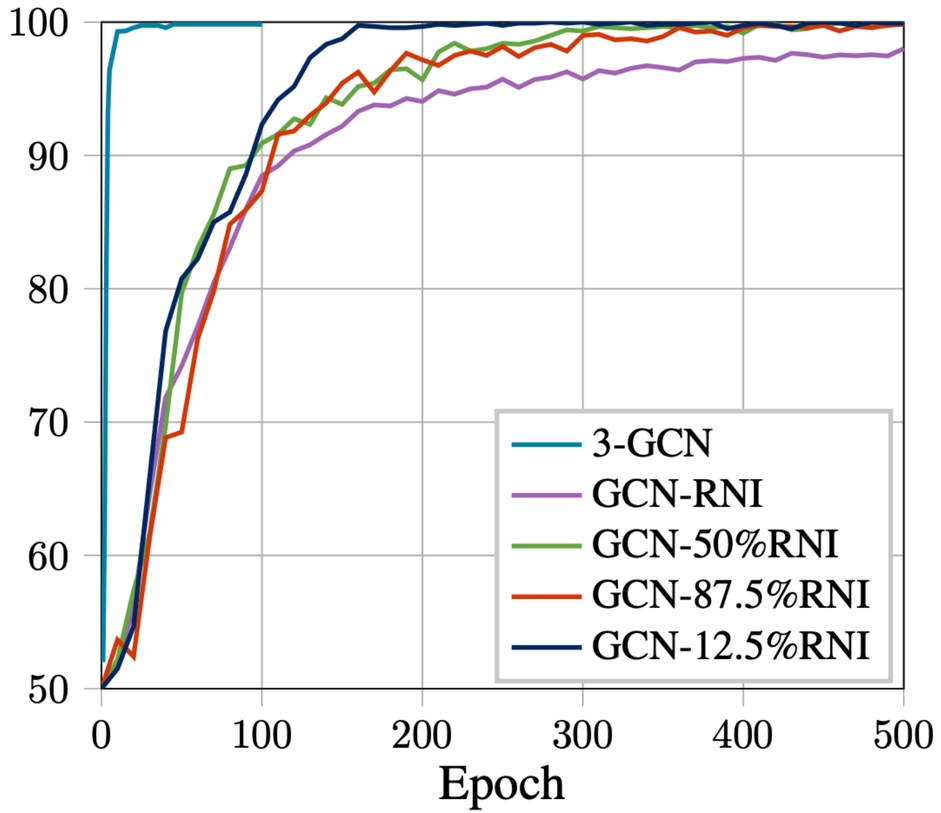

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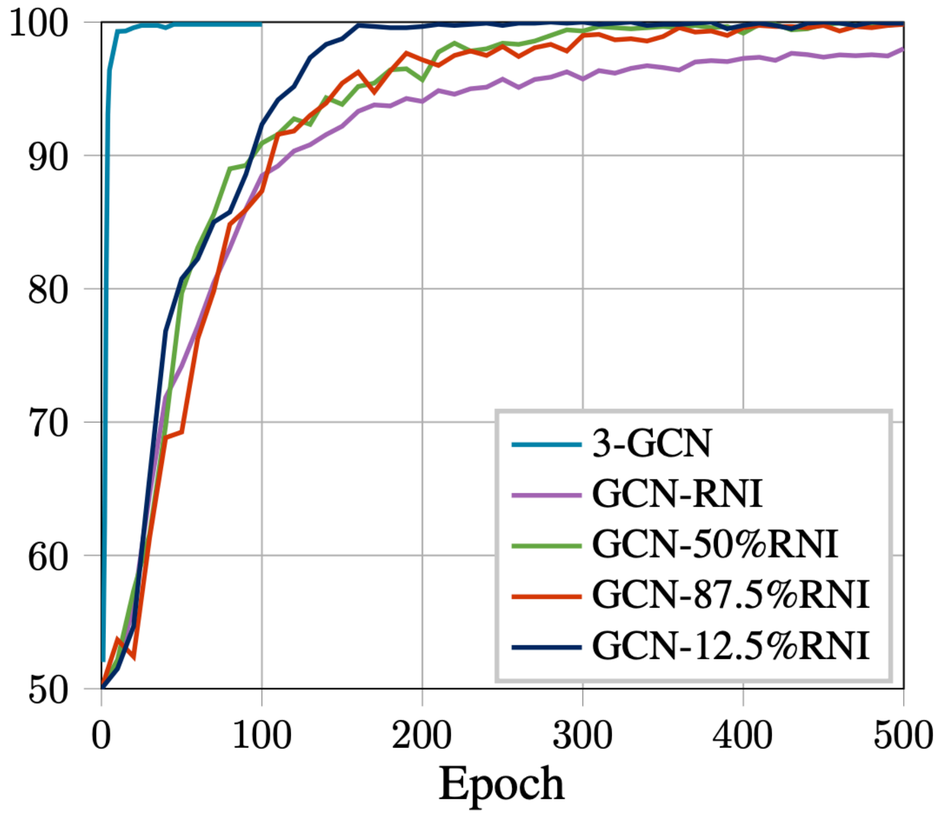

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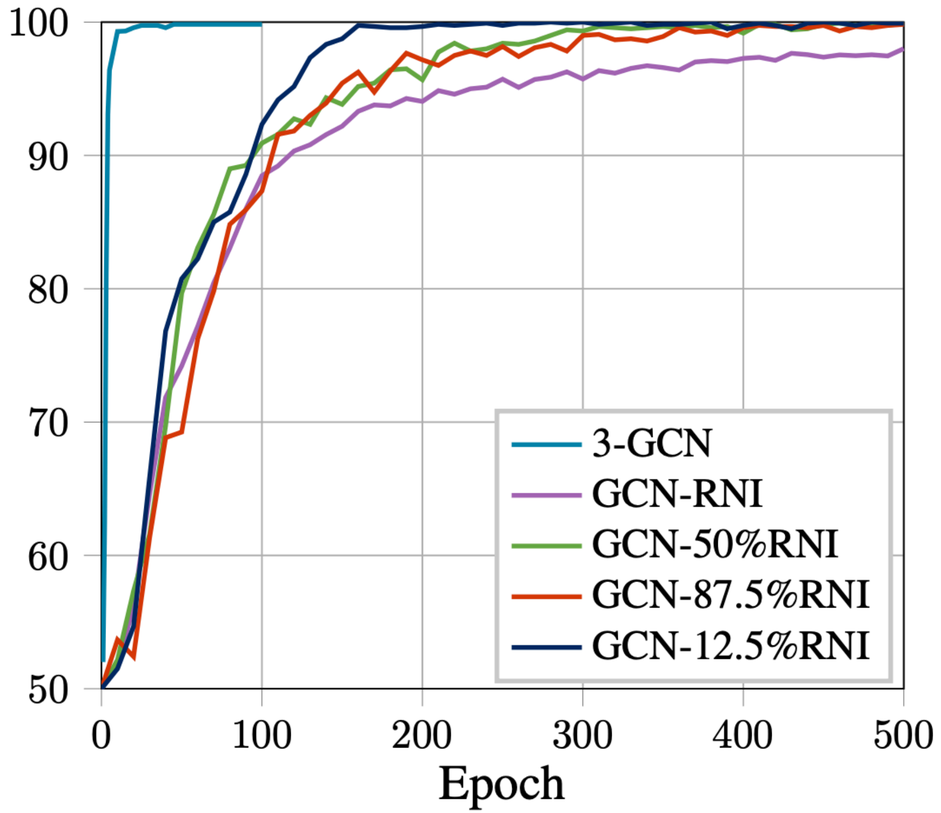

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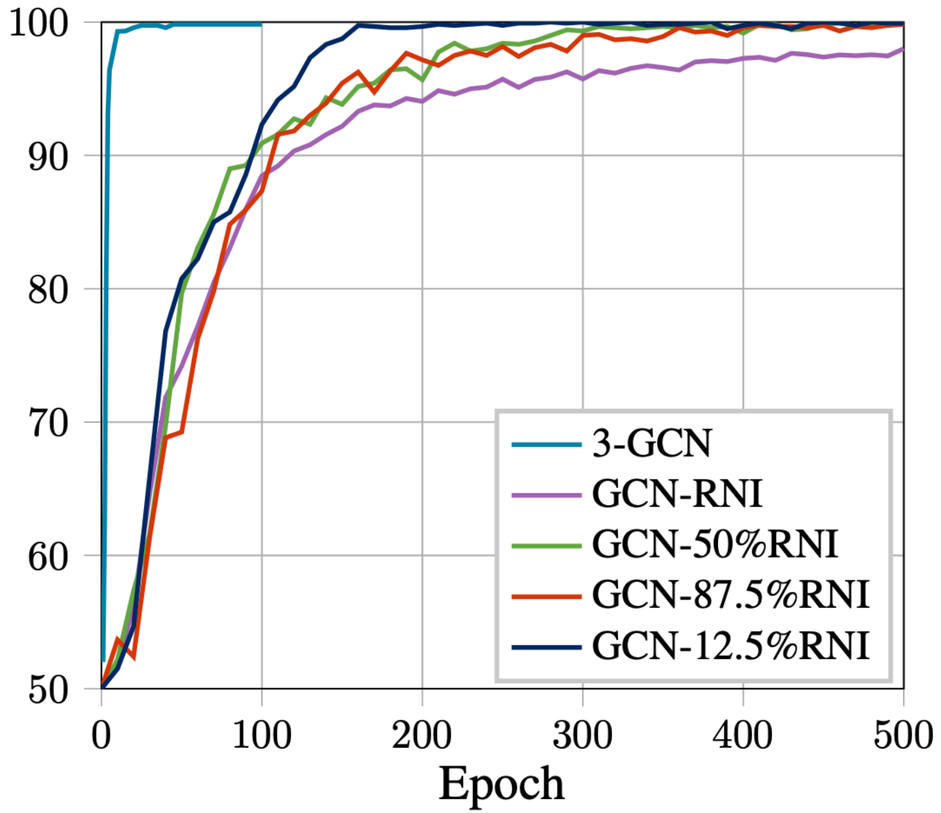

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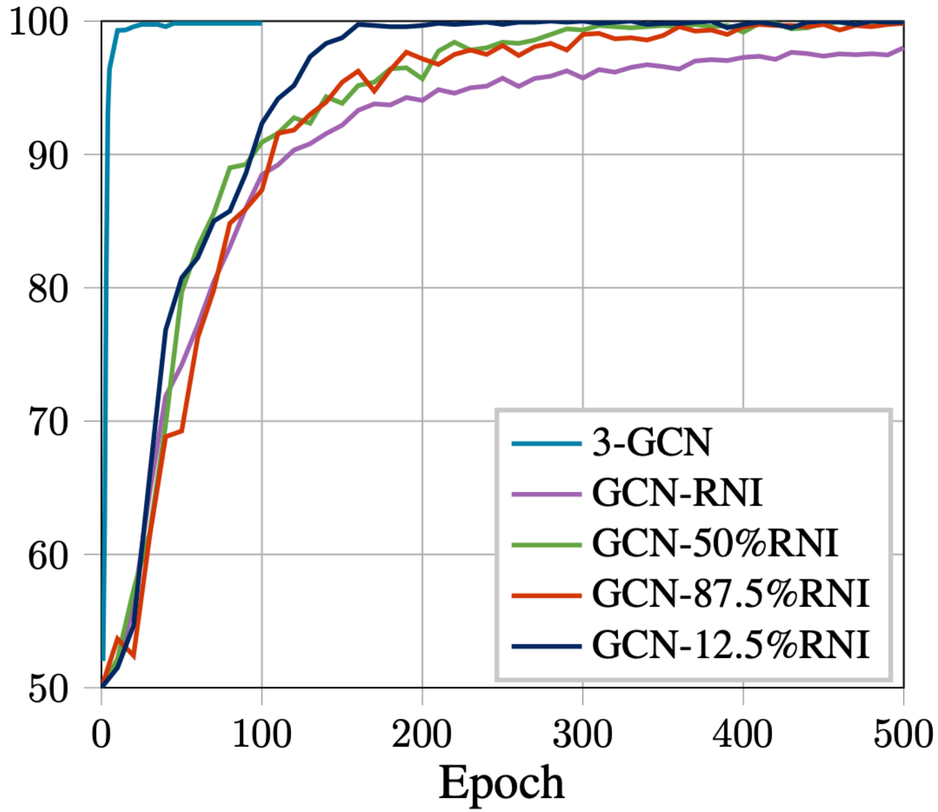

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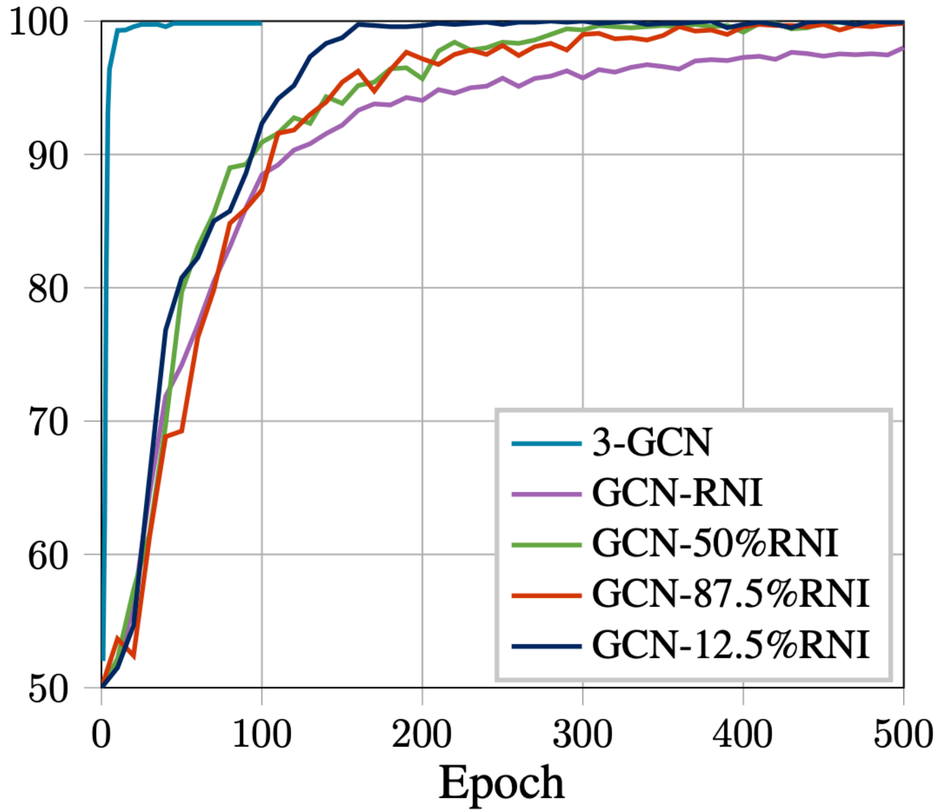

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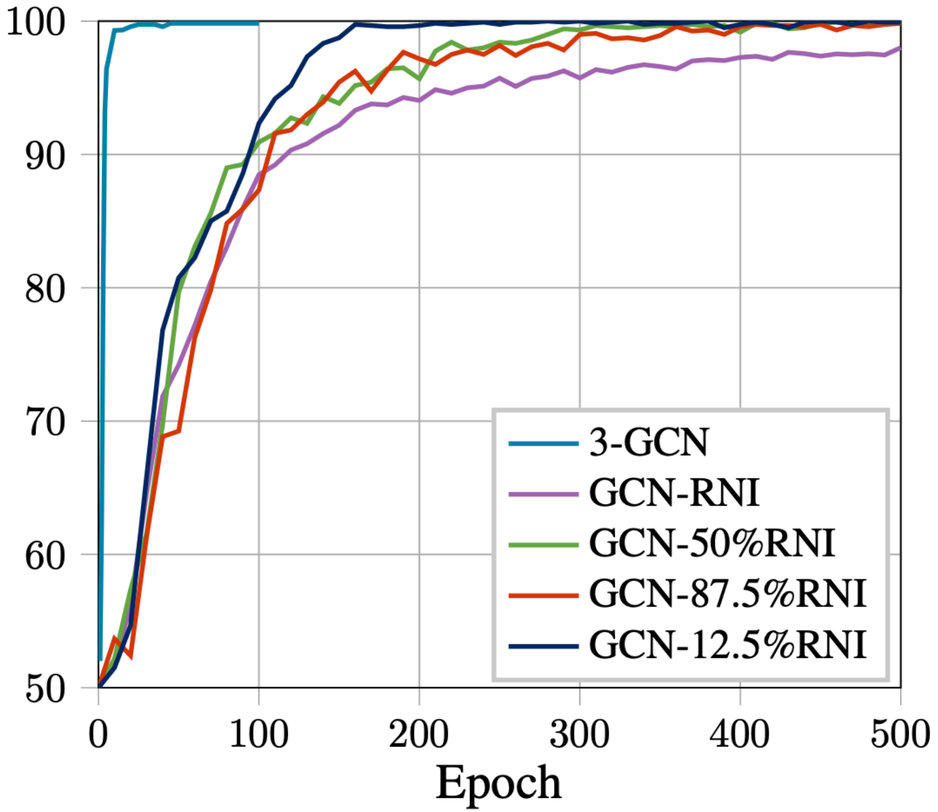

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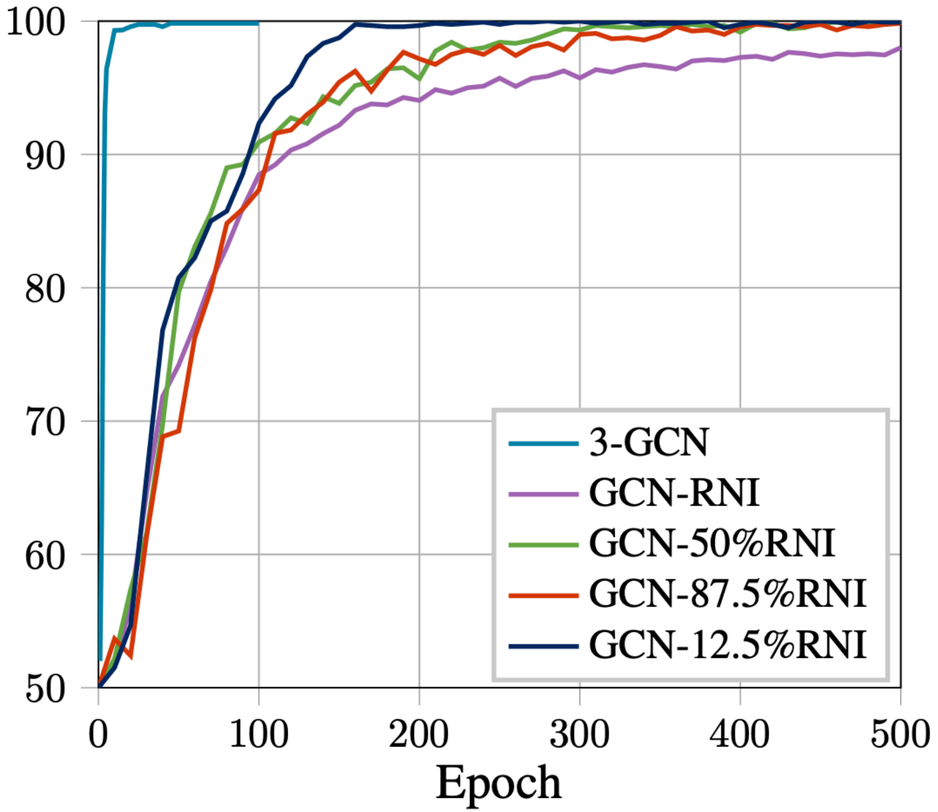

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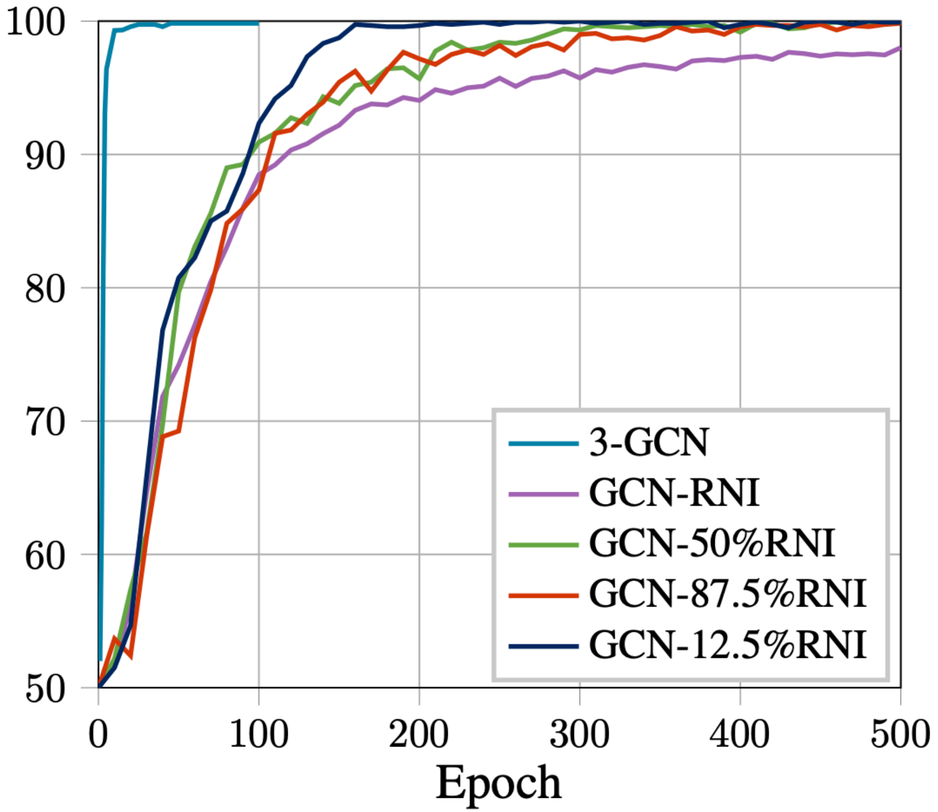
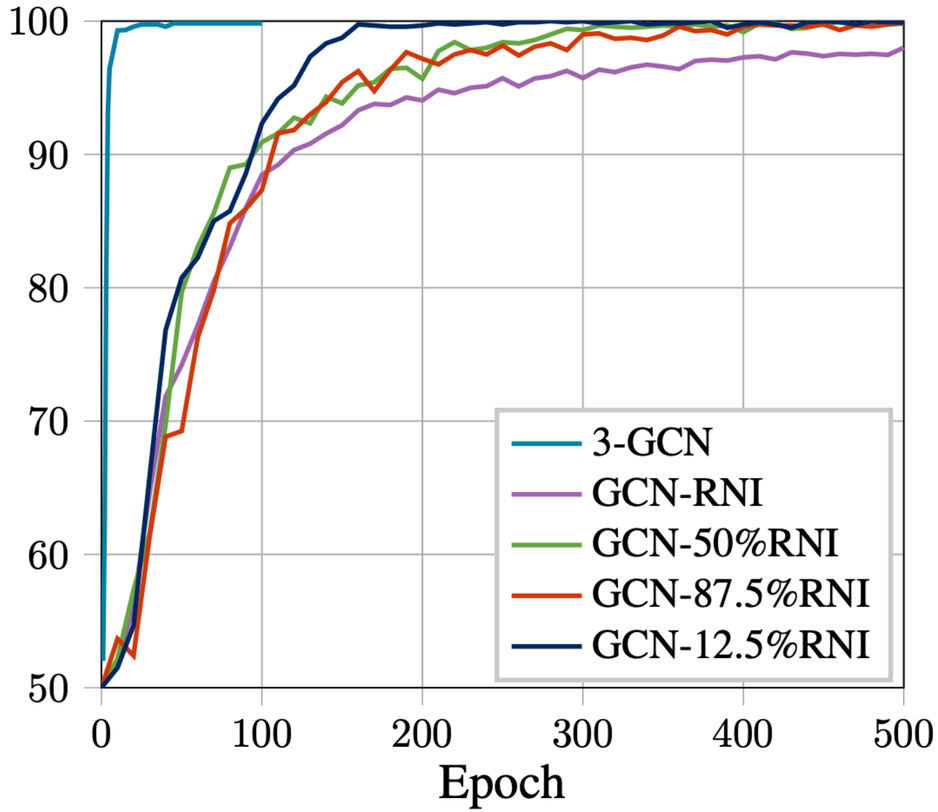
Somewhat surprisingly, GCN-RNI closely matches the performance of 3-GCN, and can easily scale to larger instances that are not within reach for 3-GCN.



Randomised Models Converge Slower



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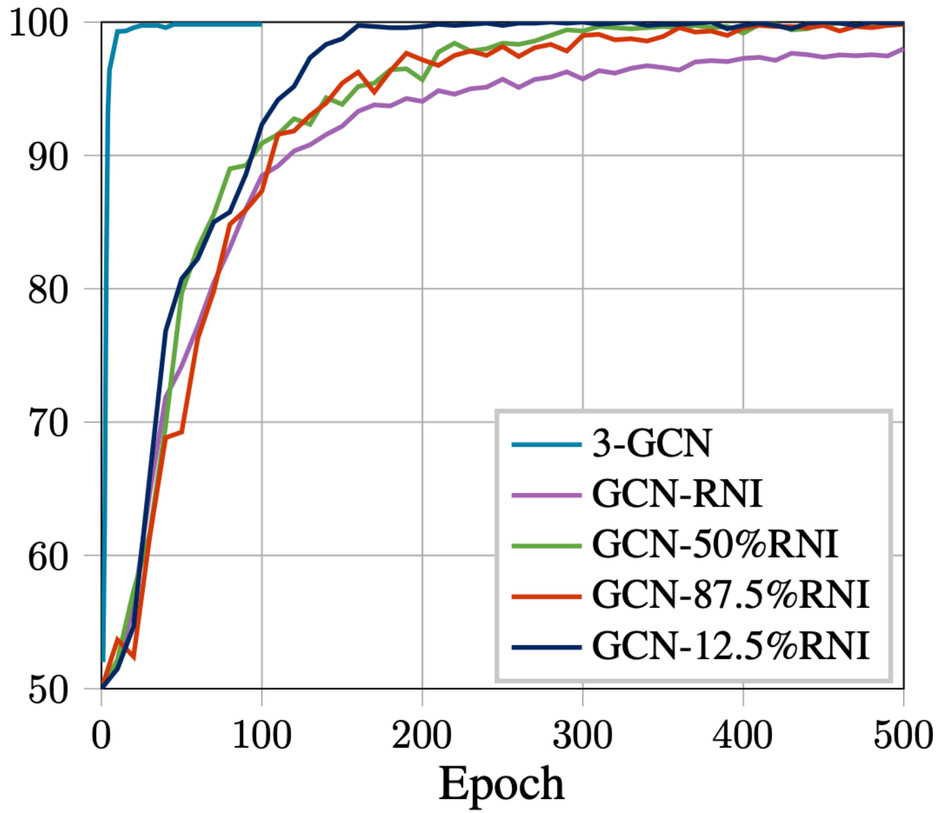

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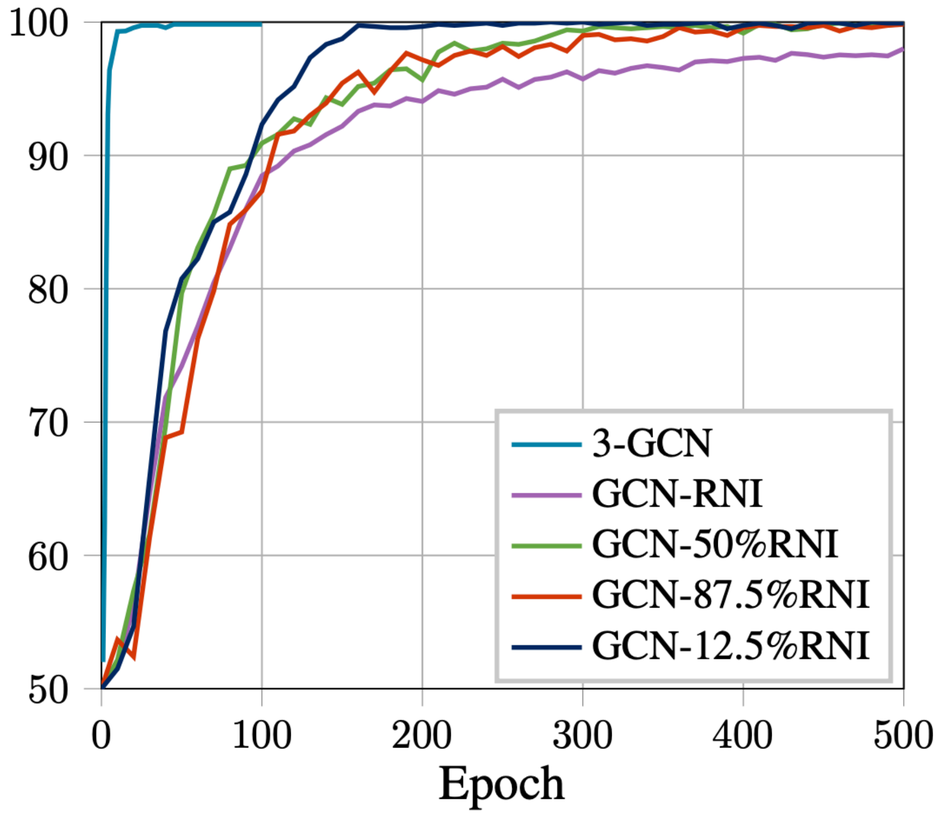
"3-GCN only requires about 10 epochs to achieve its optimal performance, whereas GCN-RNI models all require in excess of 100 epochs. Intuitively, the slower convergence of GCN-RNI can be attributed to a significantly harder learning task compared to 3-GCN: Whereas 3-GCN must learn from a deterministic set of node embeddings, and is naturally capable of discerning between dataset cores, GCN-RNI relies on RNI to discern between data points in EXP, via an artificial node ordering. This in turn implies that GCN-RNI must first leverage RNI to detect structure, then subsequently learn robustness against the variability of RNI, which makes the learning task for GCN-RNI especially challenging."



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- CORRUPT does not require expressiveness, but makes the overall learning task harder due to the structural similarities to EXP instances — Hence, an expressive model that generalises poorly can be identified by poor performance on this dataset.

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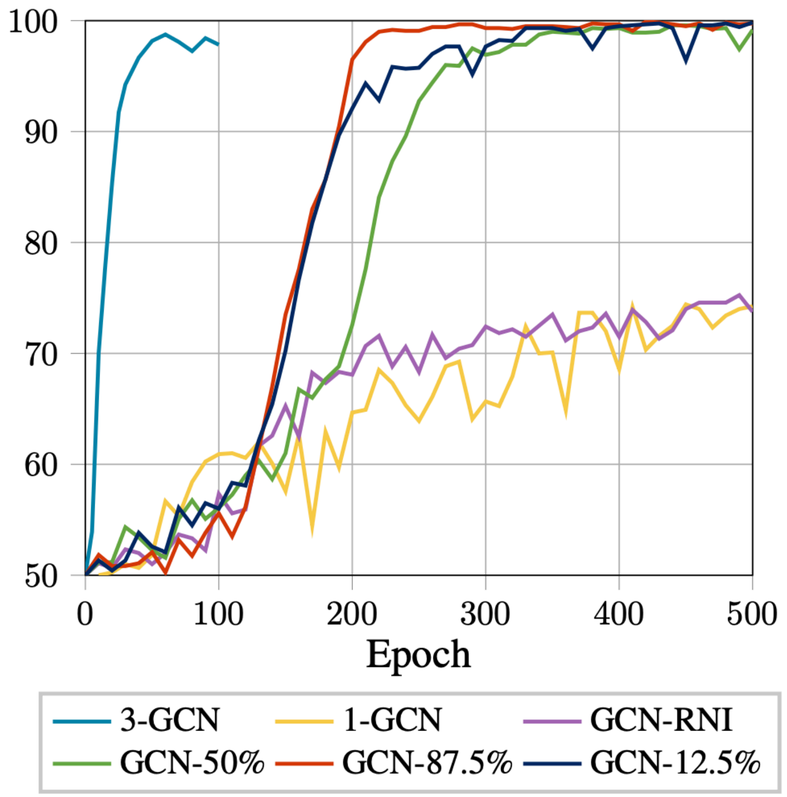

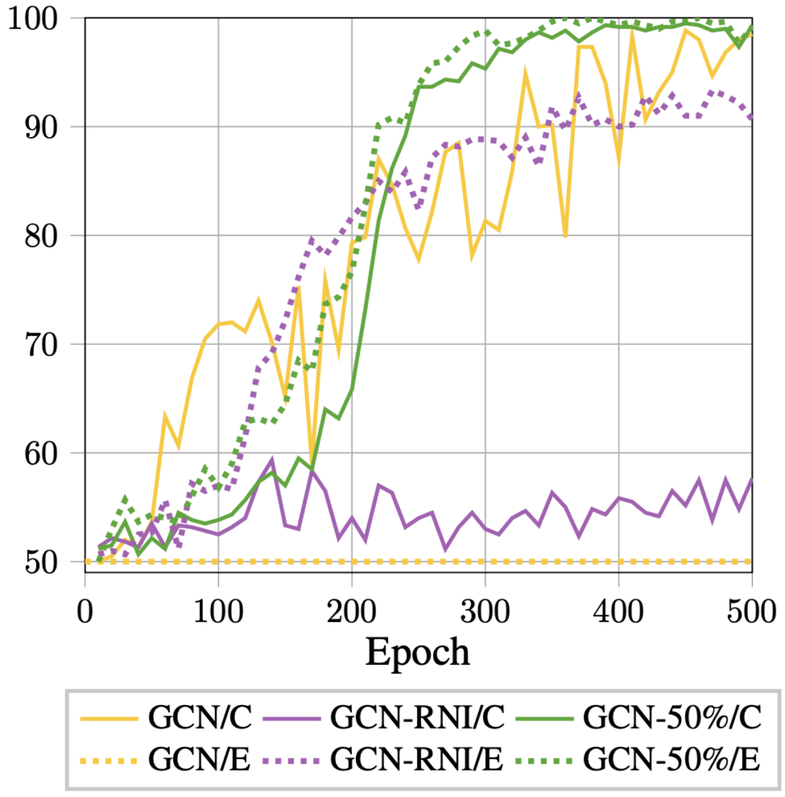

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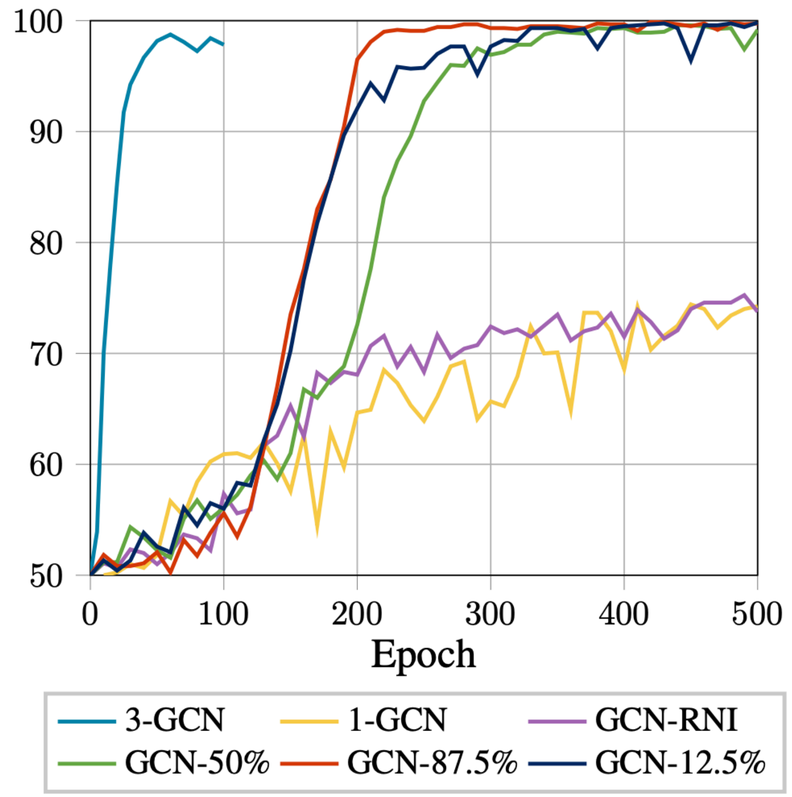

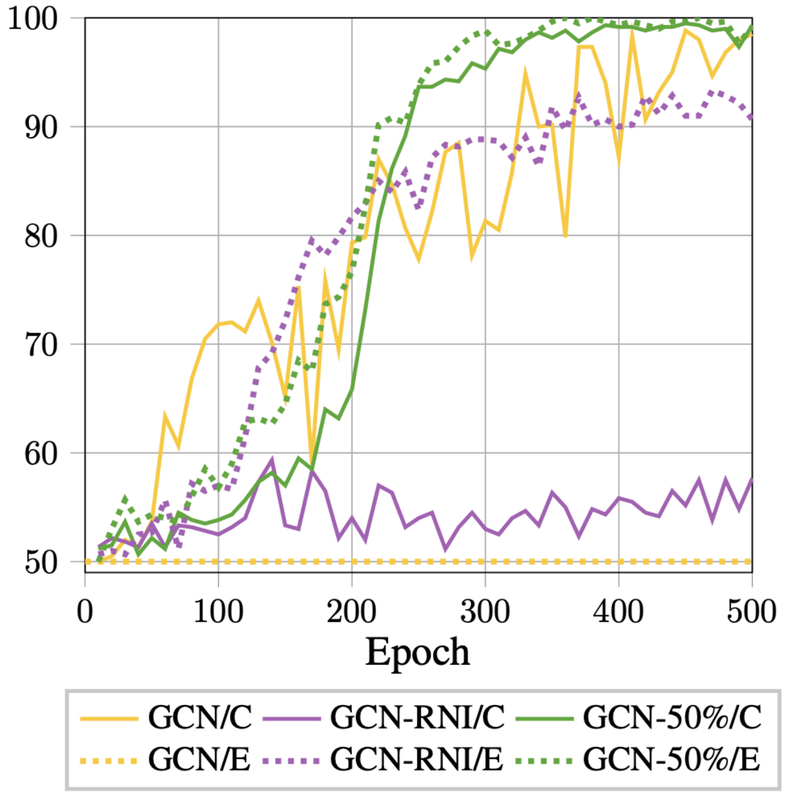

Fully randomised GCN-RNI model achieves $91\,\%$ accuracy on the EXP subset (dotted-purple line on the RHS), but struggles on CORRUPT subset (purple line on the RHS), slightly below $60\,\%$.

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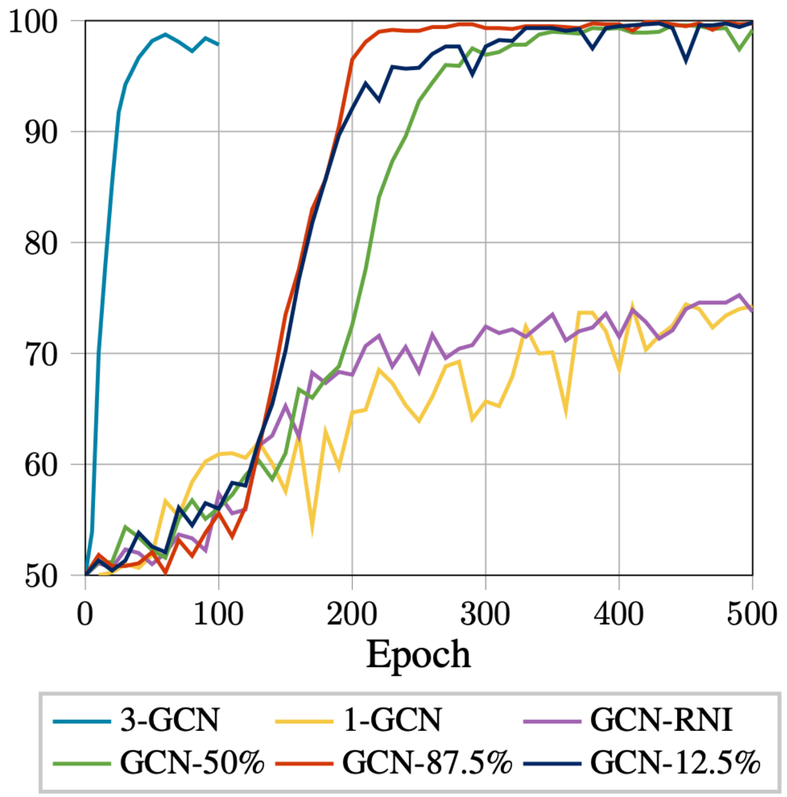

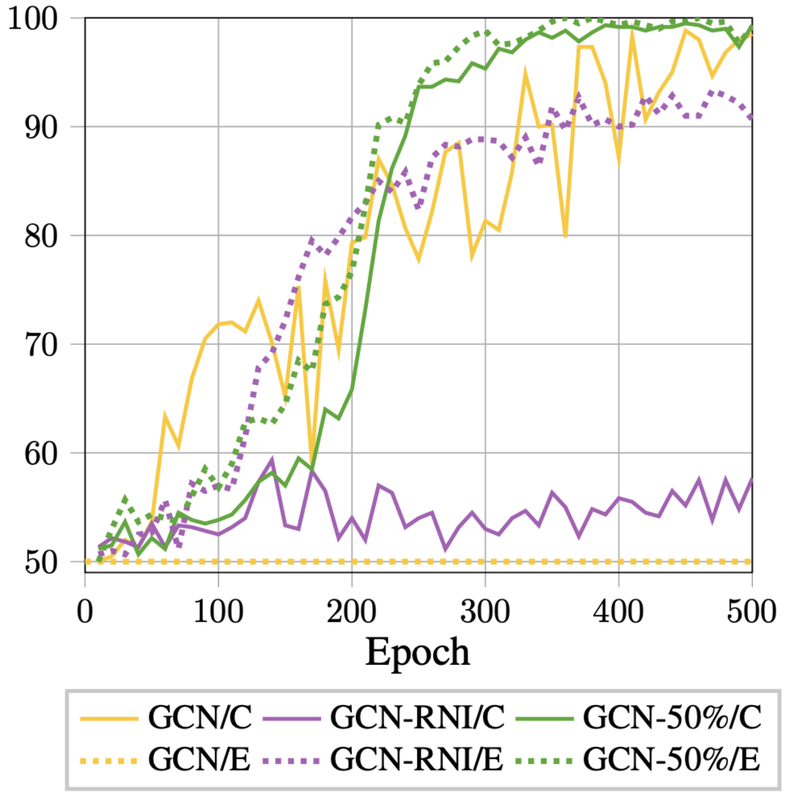

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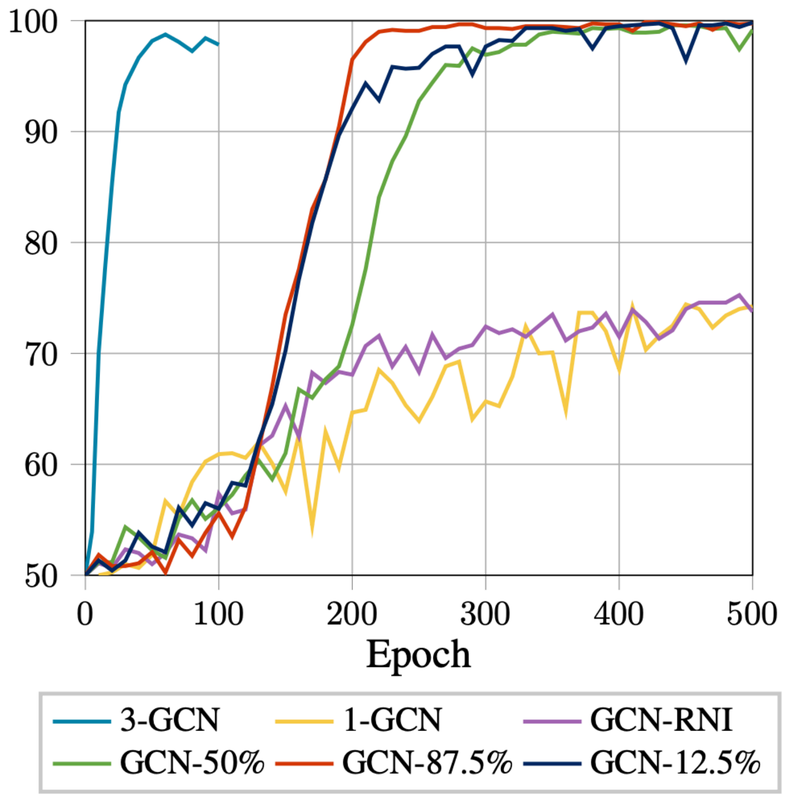

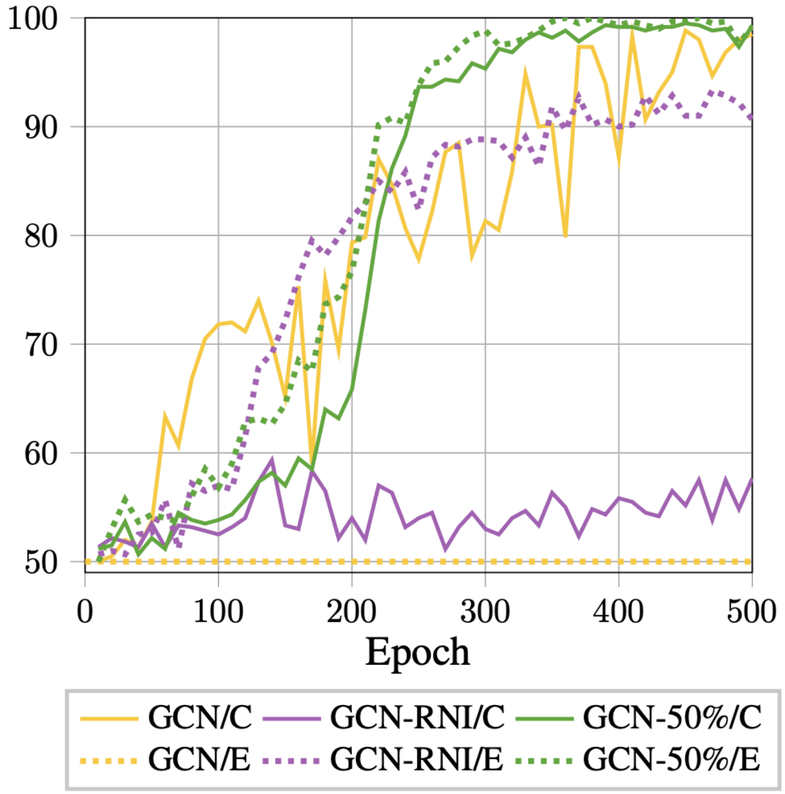

Observation: Fully randomised GCN-RNI loses all node type information, which is valuable for making robust predictions, and therefore struggles on CORRUPT, and converges much slower.

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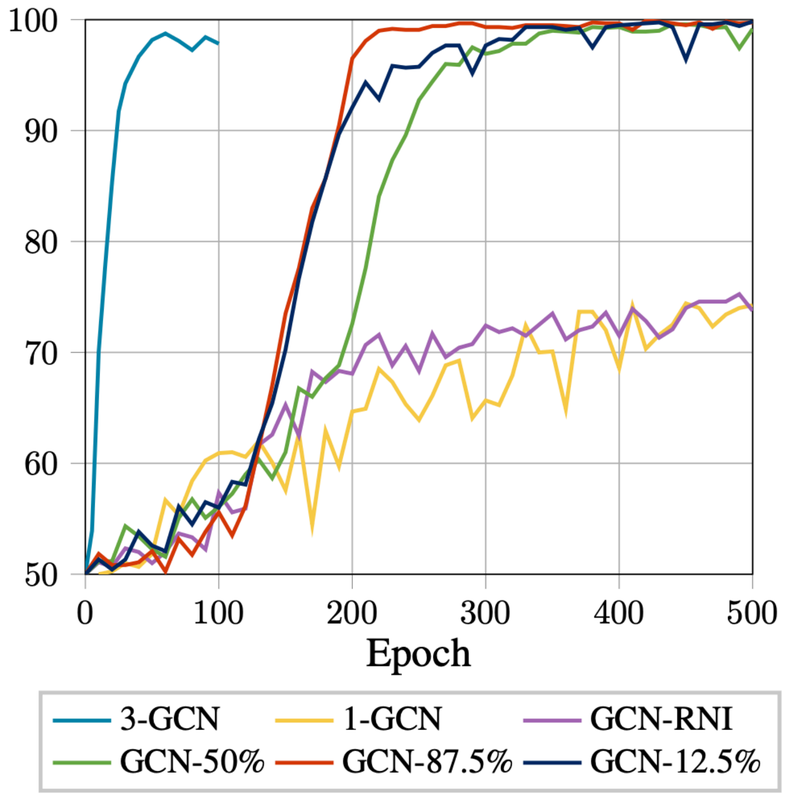

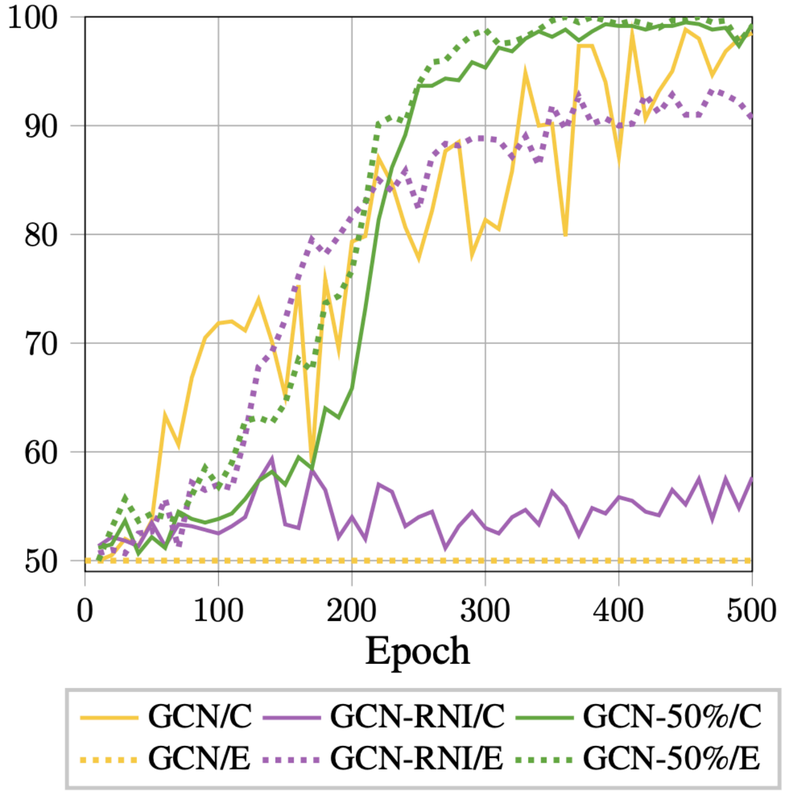

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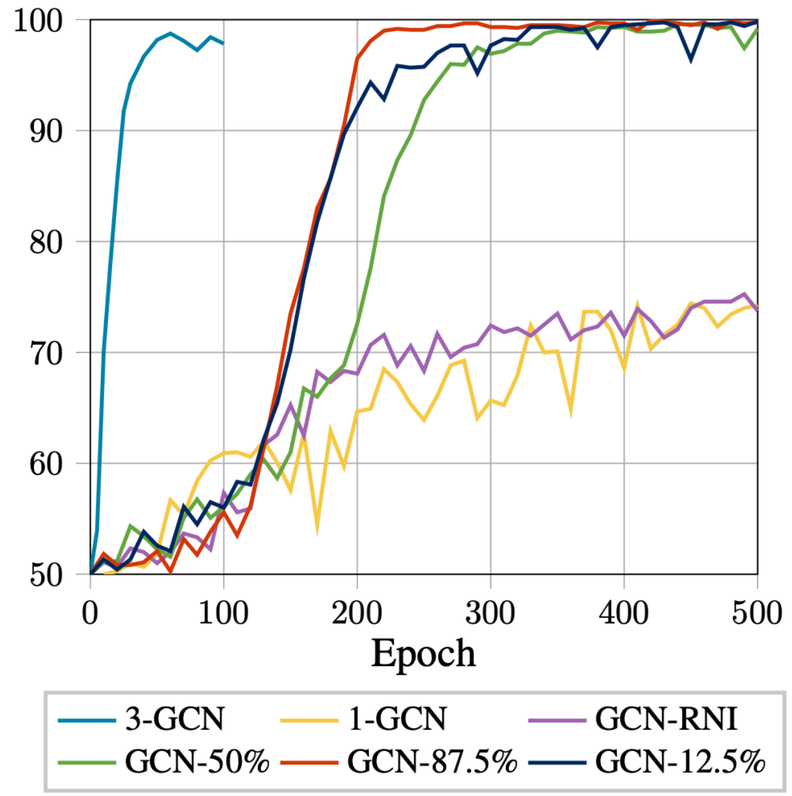
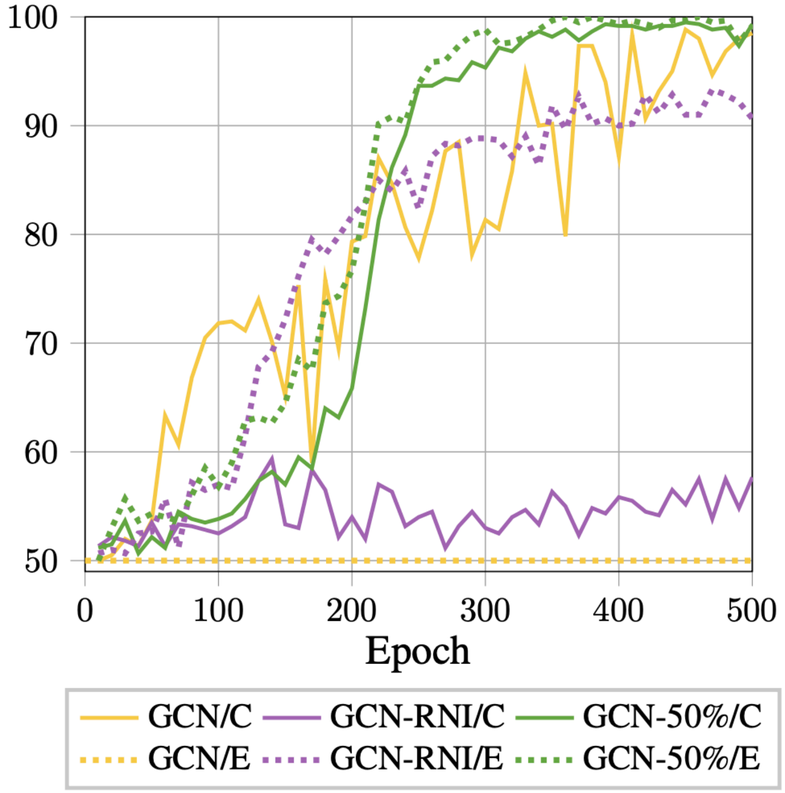
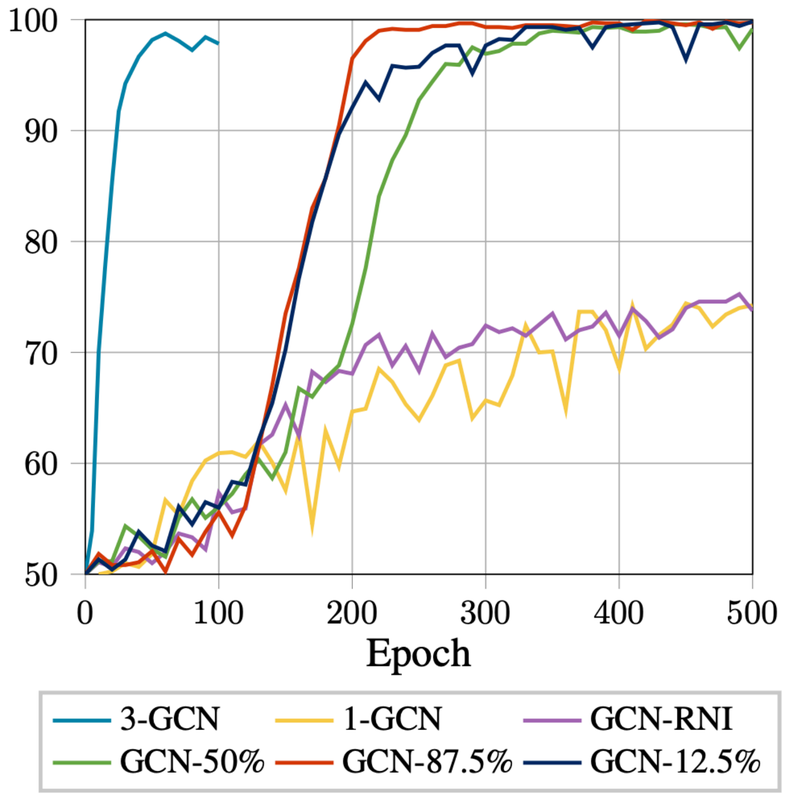
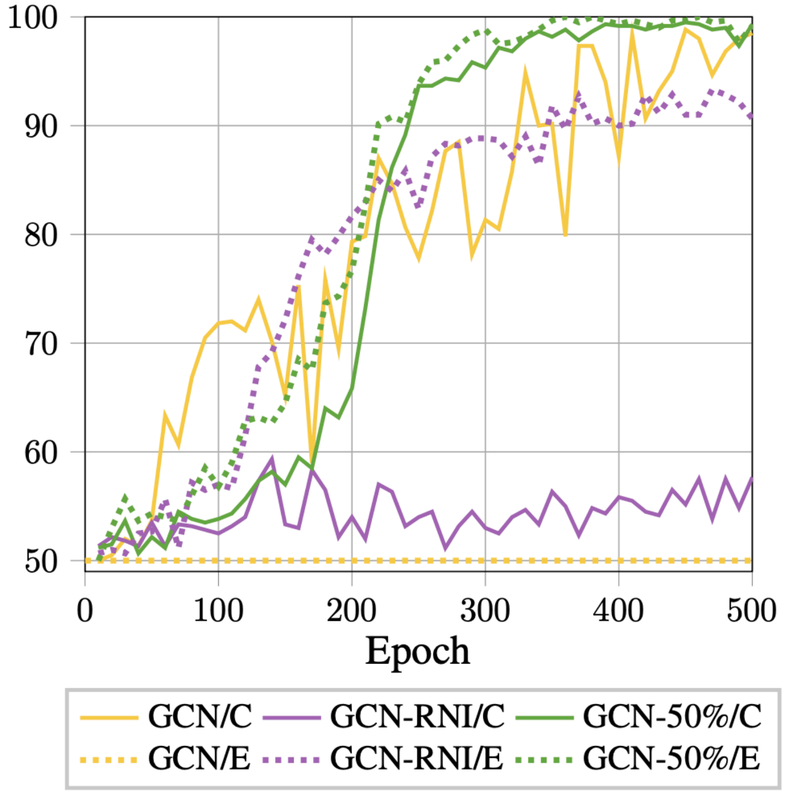




On the other hand, all partially randomised models, perform near-perfect also on this challenging dataset!

A More Variable Dataset





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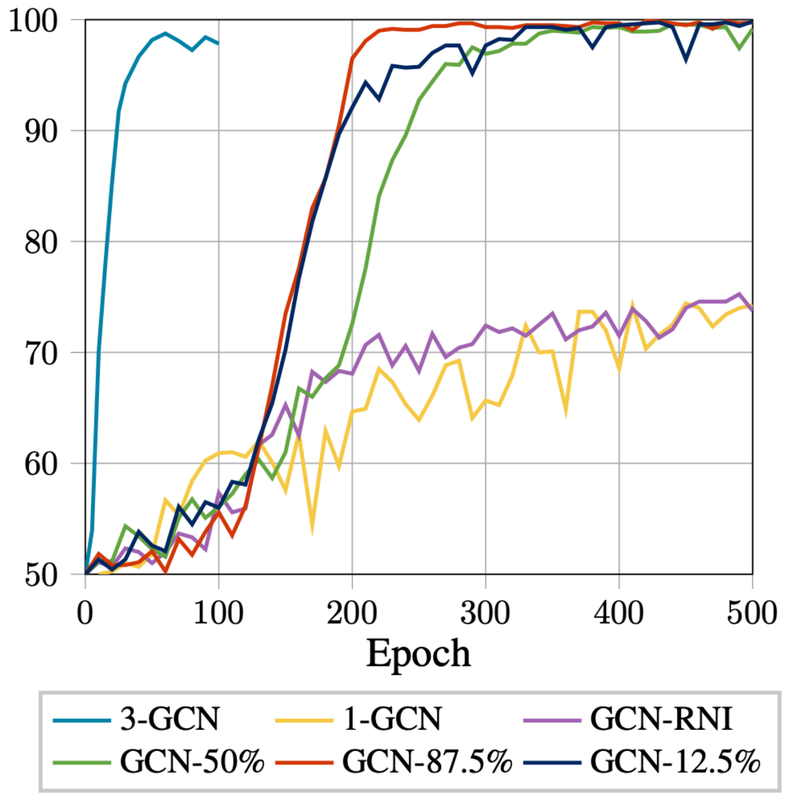

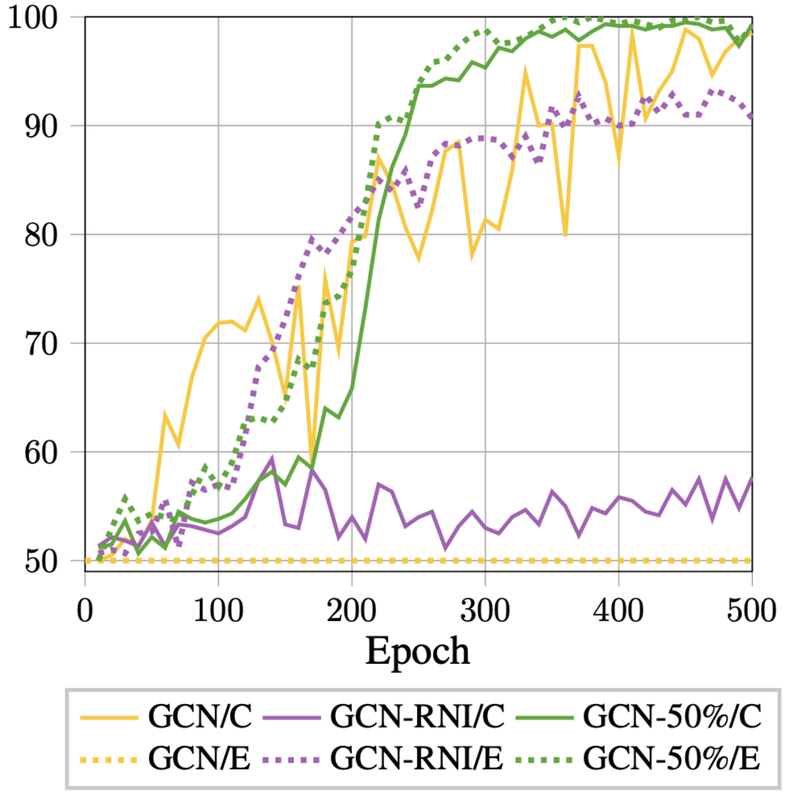

Observation: Partially randomised models achieve the best of both worlds on CEXP, leveraging inductive bias from deterministic node embeddings, while harnessing the power of random embeddings to gain expressiveness.

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- Partially randomised MPNN-RNI models both perform better and converge faster than fully random MPNN-RNI models — attributed to the fact that they combine the best of both worlds.
- Partial RNI is sufficient, and this is more so for real-world datasets that do not require to handle so many edge cases jointly.

Discussions and Outlook

Descriptive Complexity and Network Size

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    - The width of the resulting MPNN depends polynomially on the confidence parameter δ, as this directly determines the dimensions of the state vectors to reach the desired accuracy
- This gives rise to direct bounds on the size of MPNN-RNI models for special classes of functions, and paves the way for a principled and formal analysis of MPNN-RNI models.

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Local vs global: While MPNN-RNI models have the capacity to learn global properties using randomisation, they can behave similar to MPNNs w.r.t other properties we discussed. For example, homophily is likely captured by MPNN-RNI models similarly to MPNNs, as they are still based on local neighbourhood aggregation — and they can flexibly adapt to focus on local properties.

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Full vs partial RNI: Empirical evidence suggests that full randomisation can hurt inductive bias — as the randomness increases, the overall learning task becomes harder, and the presence of deterministic features prove helpful to preserve inductive bias, while gaining expressiveness.

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- With this, we have covered all theoretical and foundational aspects, for practical aspects: Lecture 8.

References

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