How powerful are Graph Neural Networks?

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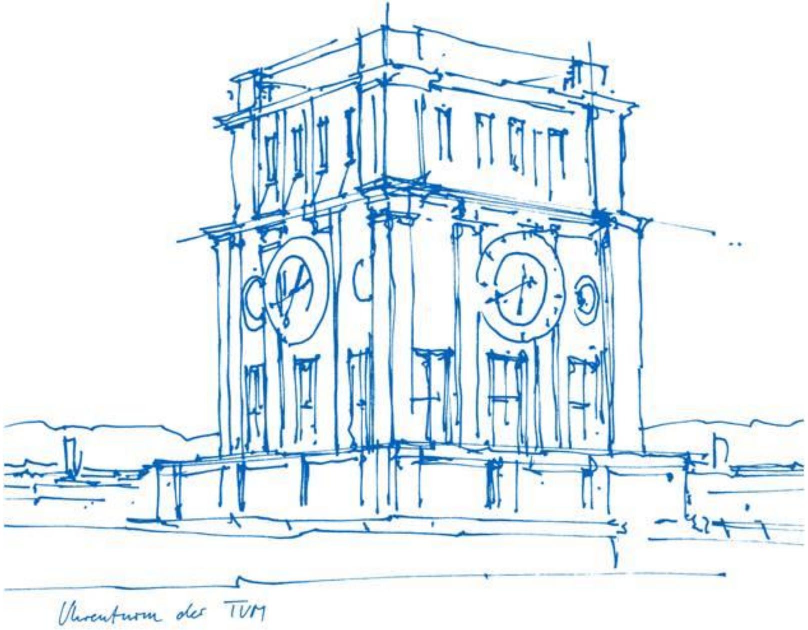

Recap of Graph Neural Networks (GNNs)

State-of-the-art performance in various fields

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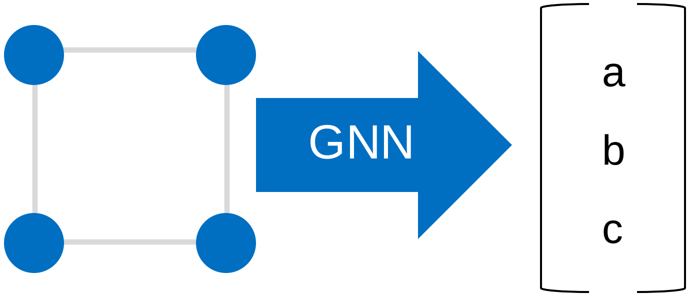
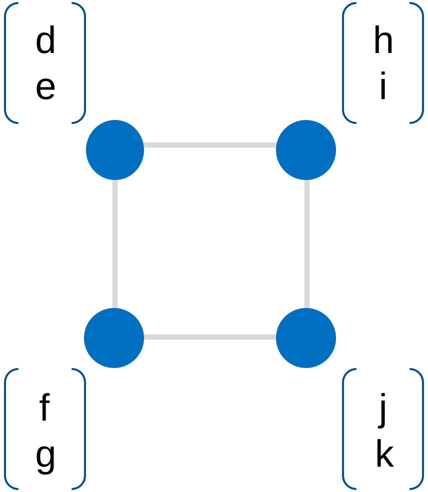


$$\mathcal{G} \to \mathbb{R}^d$$

Recap of Graph Neural Networks (GNNs)



State-of-the-art performance in various fields

A GNN maps a graph to a vector:

- Embed information in numerical vectors (labels)

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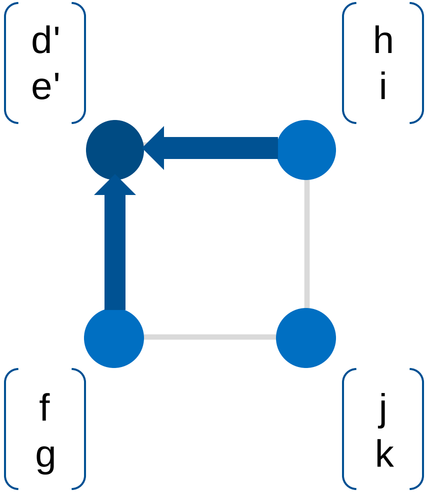

State-of-the-art performance in various fields

A GNN maps a graph to a vector:
- Embed information in numerical vectors (labels)
- Aggregate neighbouring labels for new label

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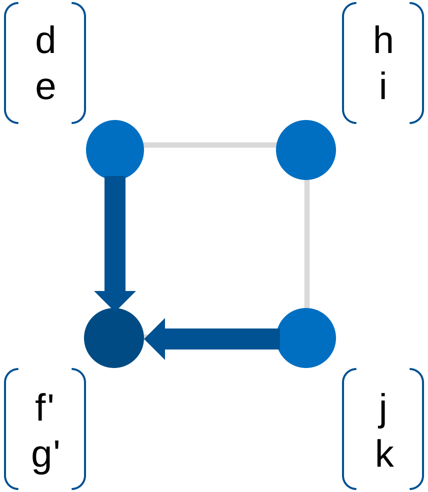

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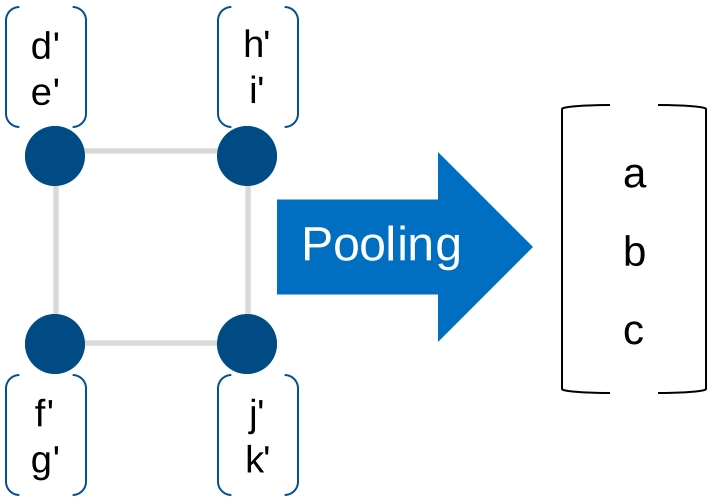
A GNN maps a graph to a vector:

- Embed information in numerical vectors (labels)
- Aggregate neighbouring labels for new label
- Aggregate all node labels to a vector in final layer



How powerful are GNNs?

How powerful can GNNs theoretically be?

What properties determine the expressiveness of a GNN?

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Can GNNs solve the graph isomorphism problem?

Graph Isomorphism Problem

No algorithm with polynomial runtime known

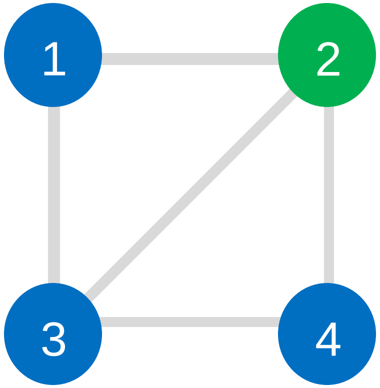
If GNNs could distinguish all graphs, then we would have a polynomial solution!

Weisfeiler-Lehman (WL) Test

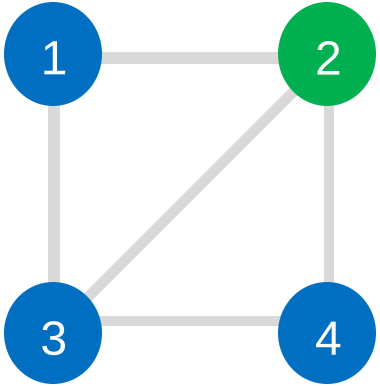
Classical isomorphism test based on labels

Powerful but not capable to distinguish all graphs

WL Test



WL Test



T = 0

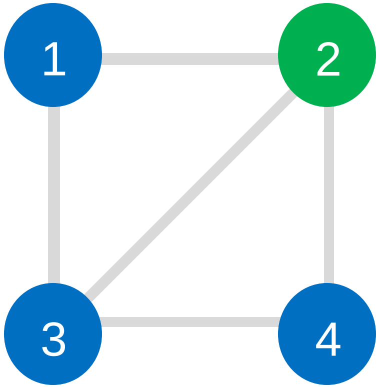
1:{B}

2:{G}

3:{B}

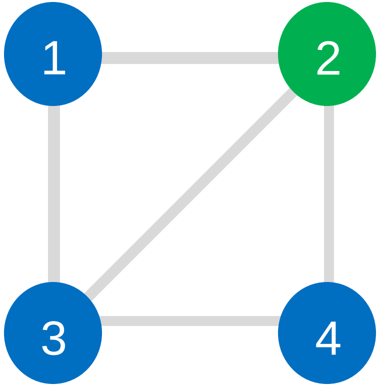
4:{B}

WL Test



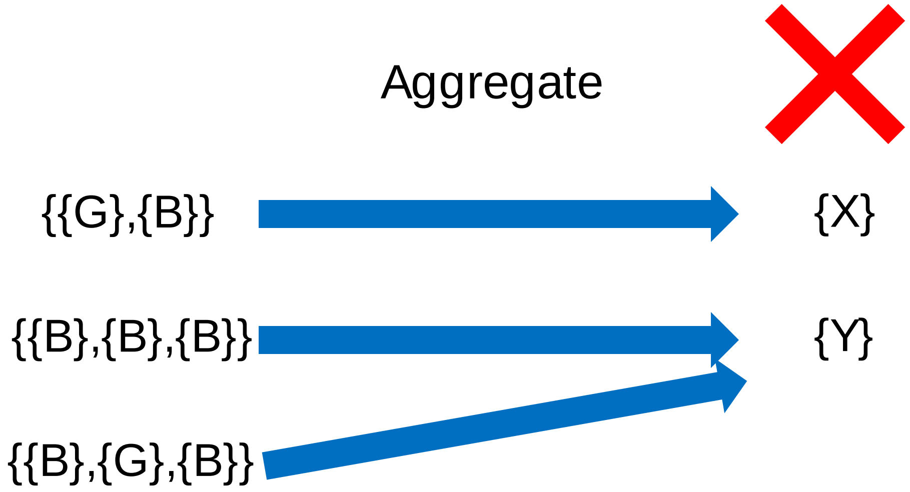
T = 0	T = 1
1:{B}	1:{{G},{B}}
2:{G}	2:{{B},{B},{B}}
3:{B}	3:{{B},{G},{B}}
4:{B}	4:{{G},{B}}

WL Test

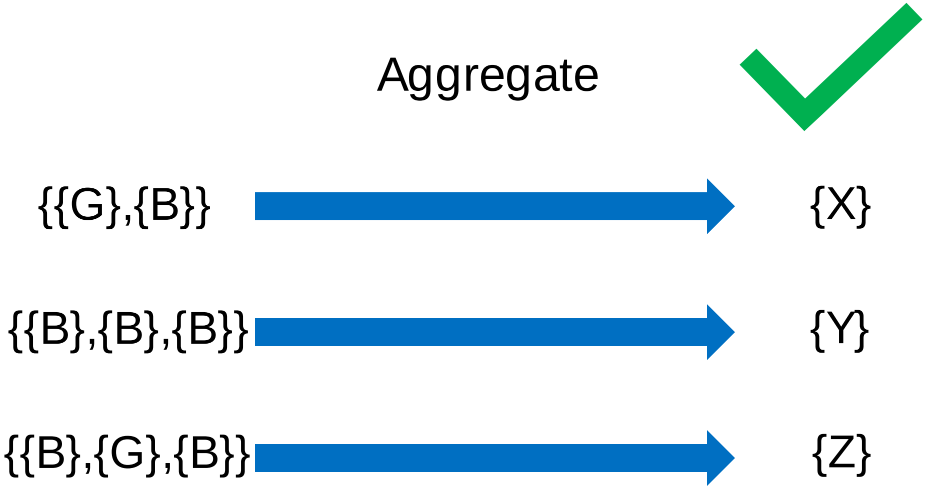


T = 0	T = 1	T = 2
1:{B}	1:{{G},{B}}	1:{{{B},{B},{B}},
2:{G}	2:{{B},{B},{B}}	{{B},{G},{B}}}
3:{B}	3:{{B},{G},{B}}	2: ...
4:{B}	4:{{G},{B}}	...

Can GNNs be as powerful as WL?



Can GNNs be as powerful as WL?



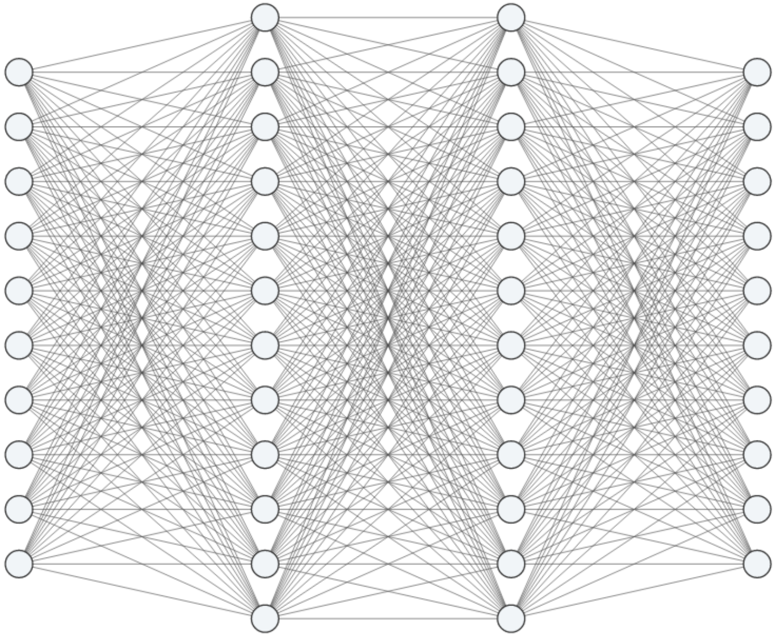
Universal Approximation Theory

Universal approximation theorem
An MLP with a linear output layer and one hidden layer can approximate any continuous function defined over a closed and bounded subset of $\mathbb{R}^D$, under mild assumptions on the activation function ('squashing' activation functions; e.g. sigmoid) and given the number of hidden units is large enough.

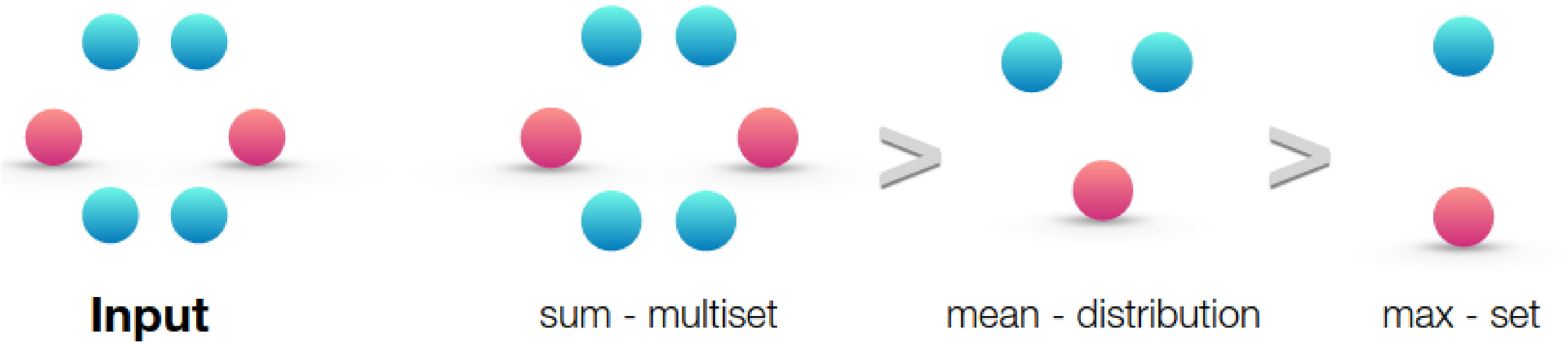
[Cybenko 1989; Funahashi 1989; Hornik et al 1989, 1991; Hartman et al 1990].

Universal Approximation Theory

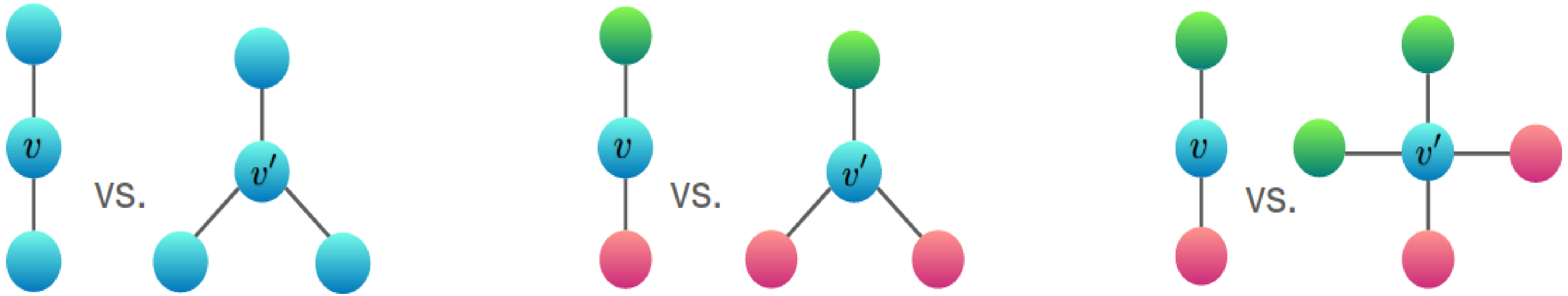
$$f(x) \equiv$$



What properties determine the expressiveness of a GNN?



What properties determine the expressiveness of a GNN?



(a) Mean and Max both fail

$$\begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}1\\0\\0\end{pmatrix} \quad \begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}1\\0\\0\end{pmatrix}$$

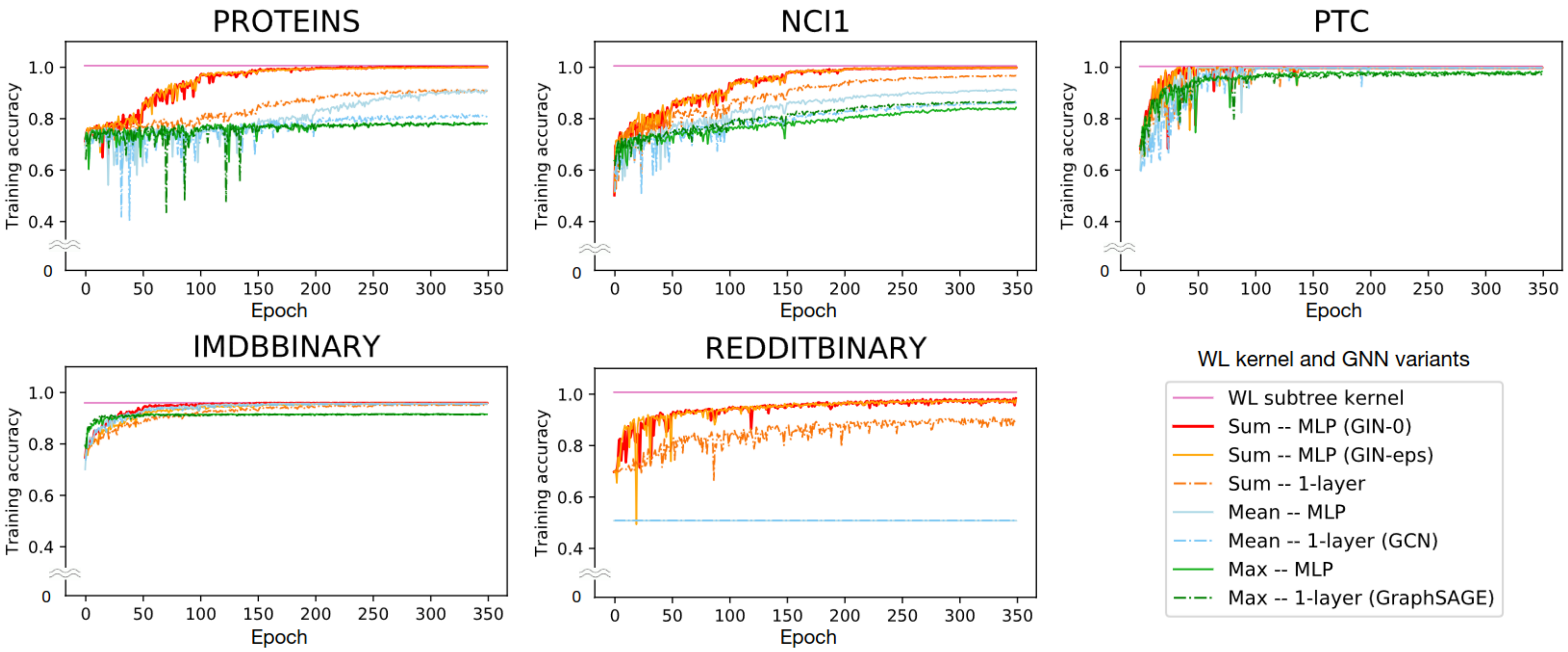
(b) Max fails

$$\begin{pmatrix}0\\1/2\\1/2\end{pmatrix}\begin{pmatrix}0\\1\\1\end{pmatrix} \quad \begin{pmatrix}0\\2/3\\1/3\end{pmatrix}\begin{pmatrix}0\\1\\1\end{pmatrix}$$

(c) Mean and Max both fail

$$\begin{pmatrix}0\\1/2\\1/2\end{pmatrix}\begin{pmatrix}0\\1\\1\end{pmatrix} \quad \begin{pmatrix}0\\2/4\\2/4\end{pmatrix}\begin{pmatrix}0\\1\\1\end{pmatrix}$$

Emperical Verification



How should we address these limitations?

1. Expand and modify GNN architecture
2. Design and test different architectures
3. Increase label information

Summary

1 GNNs can be as powerful as WL Test

2 The information lost by transformations and aggregations determines the capabilities of a GNN

3 Non-injective transformations and aggregations lead to decreased performance

Do you have any questions?

Thank you for your attention