Neural execution of graph algorithms

Implementation by Gbetondji Dovonon

Neural algorithmic reasoning on graphs

WHAT

The paper tries to train neural networks that perform algorithm step by step

HOW

They use an encoder-processor-decoder model that performs a single step

WHY

Benchmarking
Generalization
Multi-task learning

What do we learn to execute

- The model is performed on the input
- It is called on its own output until terminated

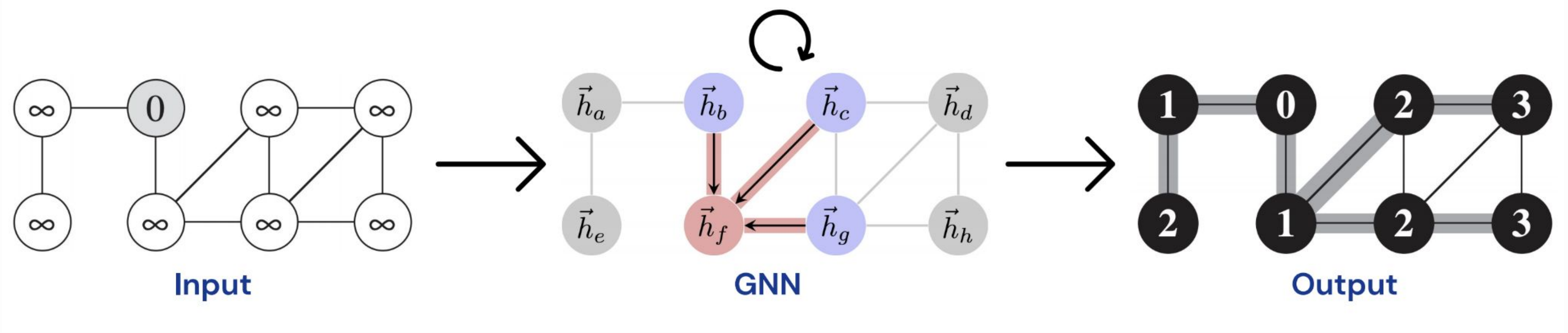


Diagram by Petar Veličković *https://petar-v.com/talks/Algo-WWW.pdf*

How do we learn an algorithm

1. **Input**
   Graph with features [n_nodes, 1]

2. **Encoder**
   Linear transformation to [n_nodes, hidden dimension]

3. **Processor**
   Performs the operations. Most of the modeling is here. Outputs to [n_nodes, hidden dimension]

4. **Decoder**
   Linear transformation to [n_nodes, 1]

   Termination
   Int that predicts if the model is done

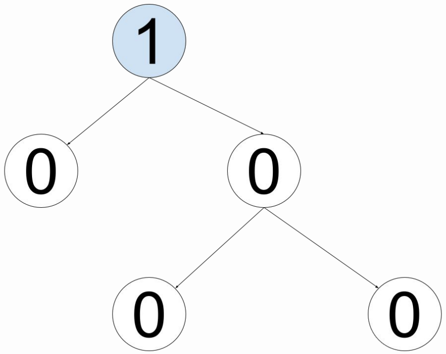
Why do we learn algorithms

- **Better benchmarking**
  Current benchmarks are not reliable. Simplified GCNs achieve strong baselines.
  Algorithms can allow us to generate infinite controlled data with high complexity

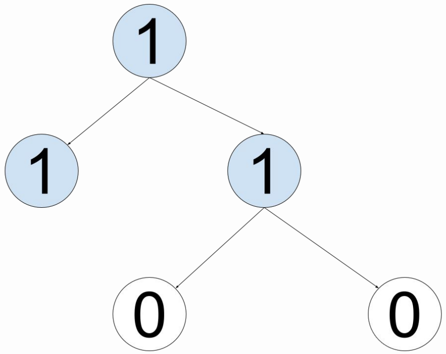
- **Generalization**
  Learning general steps instead of an input/output mapping
  Algorithms generalize trivially

- **Multi task learning**
  Possibility to learn multiple algorithms

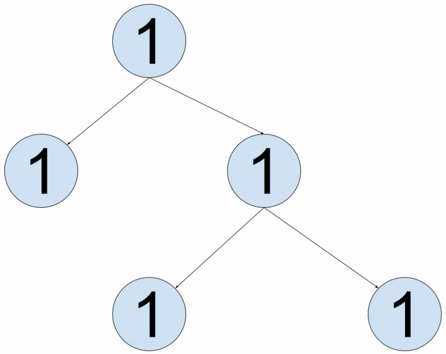
Breadth First Search



input



Step 1



Step 2

Breadth First Search

All models are trained on graphs with 20 nodes and generalize to graphs with more nodes

Mean step by step accuracy / last step accuracy				
Model	20 nodes	50 nodes	100 nodes	1000 nodes
GAT	**100% / 100%**	99.47% / 100 %	99.47% / 99.8%	91% / 99%
MPNN-sum	95% / 100%	96% / 100%	93.64% / 99.96%	76.47% / 86.77%
MPNN-mean	**100% / 100%**	74% / 100%	71.99% / 99.84%	57.96% / 100%
MPNN-max	**100% / 100%**	**100% / 100%**	**100% / 100%**	**100% / 100%**

THANK YOU

Questions?