

DeepMind

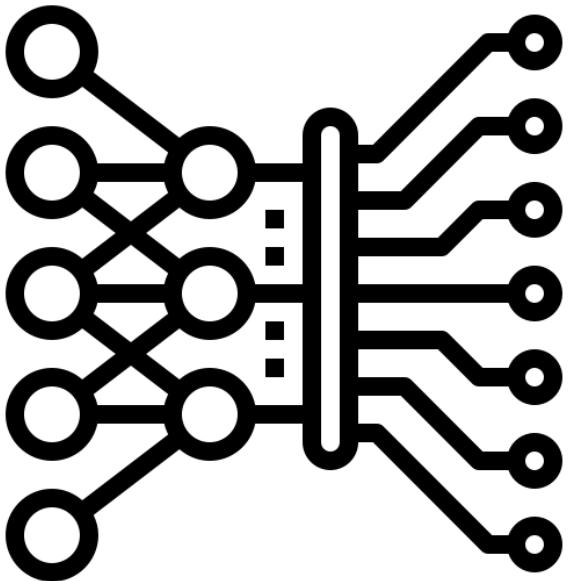
Graph Representation Learning for Algorithmic Reasoning

Petar Veličković

DL4G@WWW2020
21 April 2020



Problem-solving approaches



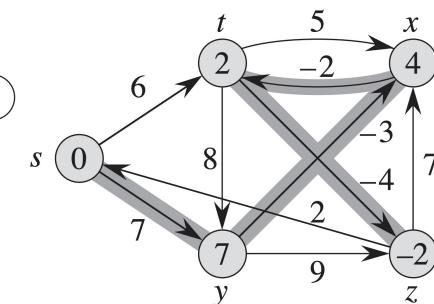
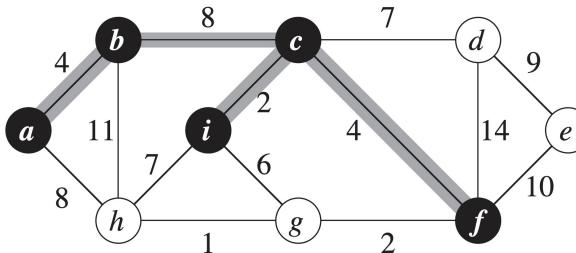
Neural networks

MERGE-SORT(A, p, r)

```

1 if  $p < r$ 
2    $q = \lfloor (p + r)/2 \rfloor$ 
3   MERGE-SORT( $A, p, q$ )
4   MERGE-SORT( $A, q + 1, r$ )
5   MERGE( $A, p, q, r$ )

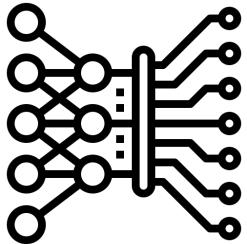
```



Algorithms

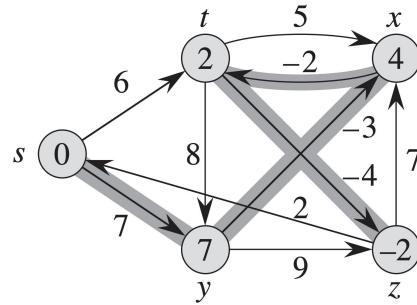


Problem-solving approaches



Neural networks

- + Operate on **raw** inputs
- + Generalise on **noisy** conditions
- + Models **reusable** across tasks
- Require **big data**
- Unreliable when **extrapolating**
- Lack of **interpretability**

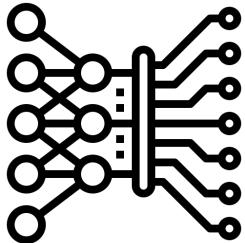


Algorithms

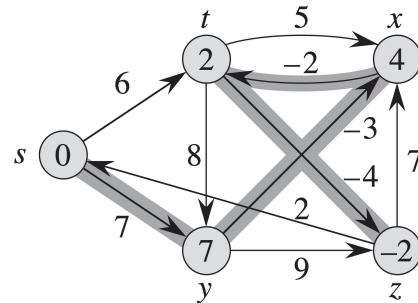
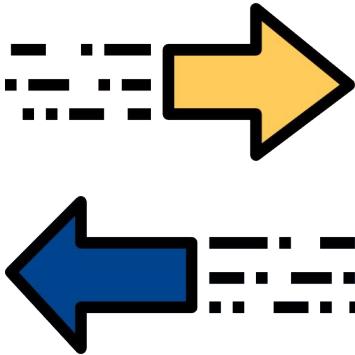
- + Trivially **strongly** generalise
- + **Compositional** (subroutines)
- + Guaranteed **correctness**
- + **Interpretable** operations
- Inputs must match **spec**
- Not **robust** to task variations



Problem-solving approaches



Neural networks



Algorithms

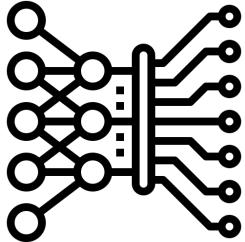
- + Operate on data
- + Generalise
- + Models reality
- Requires training
- Unreliable
- Lack of control

- generalise
- (outlines)
- process
- solutions
- spec
- variations

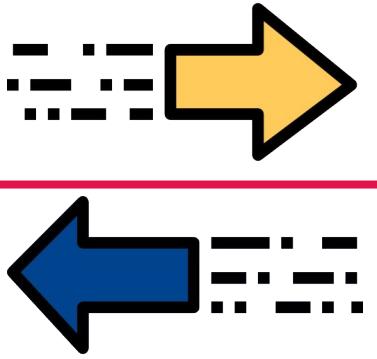
Is it possible to get the best of both worlds?



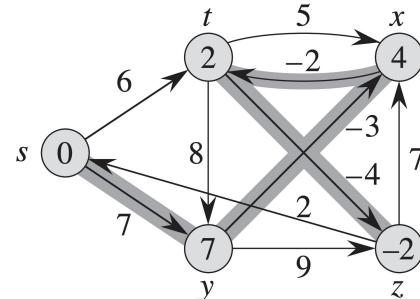
Problem-solving approaches



Neural networks



This talk!



Algorithms

- + Operate
 - + General
 - + Models
 - Requires
 - Unreliab.
 - Lack of

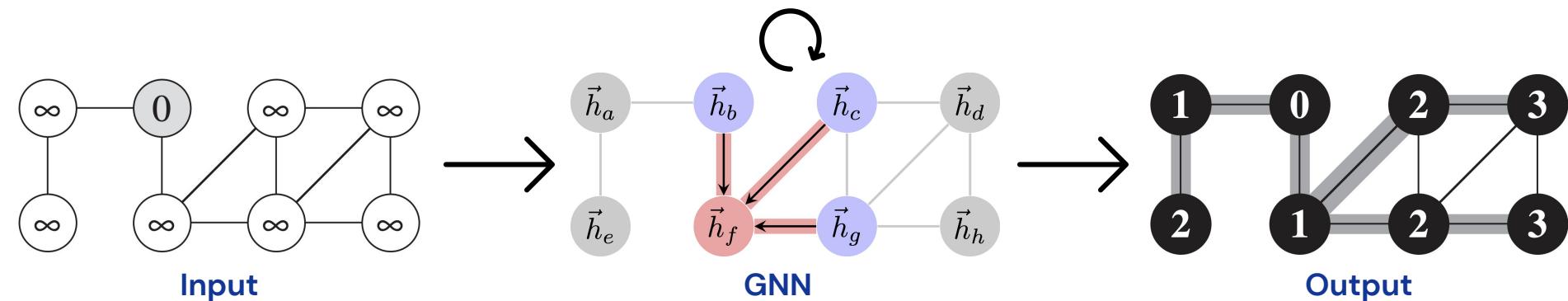
Is it possible to get the best of both worlds?

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Neural Graph-Algorithmic Reasoning

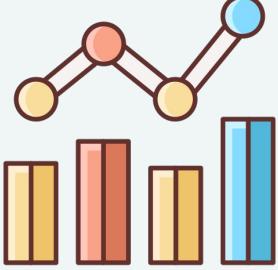
- Can neural nets robustly **reason** like algorithms?
- Algorithms manipulate (un)ordered sets of objects, and their relations.
 - ⇒ They operate over *graphs*.
 - Supervise **graph neural networks** on algorithm execution tasks!



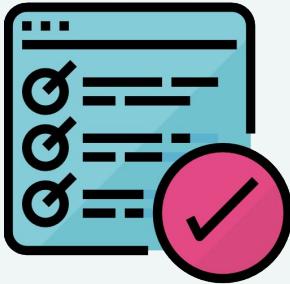
- Call this approach neural graph algorithm execution.



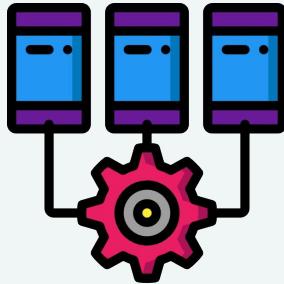
Why?



Benchmarking
graph neural nets



Strong
generalisation



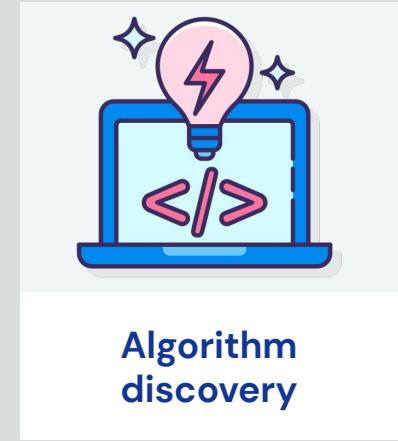
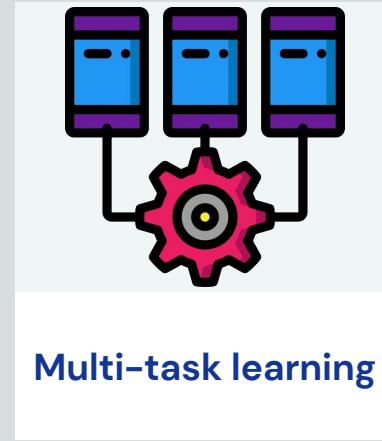
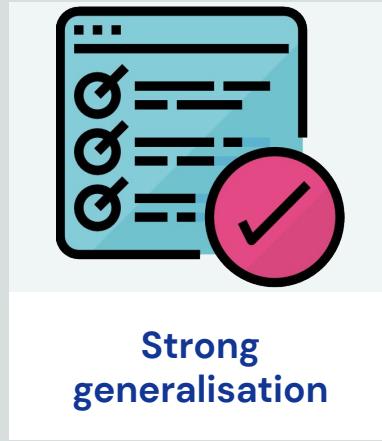
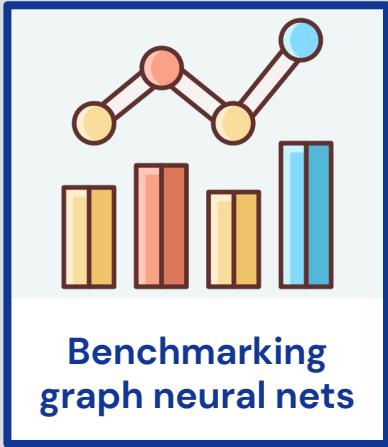
Multi-task learning



Algorithm
discovery



Why?



Benchmarking GNNs

- Popular GNN benchmark datasets often **unreliable**

Pitfalls of Graph Neural Network Evaluation

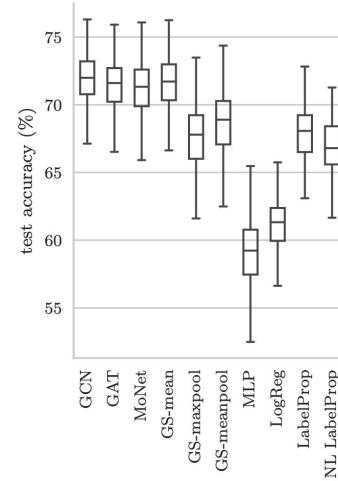
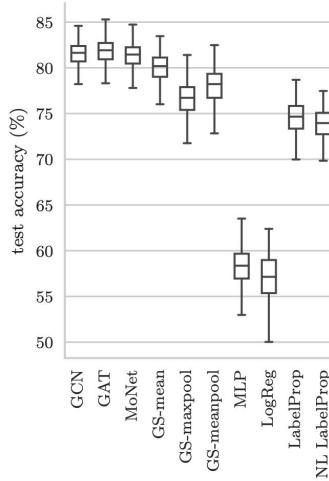
Oleksandr Shchur*, Maximilian Mumme*, Aleksandar Bojchevski, Stephan Günnemann

Technical University of Munich, Germany

{shchur,mumme,a.bojchevski,guennemann}@in.tum.de

On Graph Classification Networks, Datasets and Baselines

Enxhell Luzhnica^{*1} Ben Day^{*1} Pietro Lio¹



MODEL	DATASETS			
	REDDIT ⁵	DD	COLLAB	PROT.
PATCHYSAN	41.32	76.27	72.60	75.00
GRAPH SAGE	42.24	75.42	68.25	70.48
ECC	41.73	74.10	67.79	72.65
SET2SET	43.49	78.12	71.75	74.29
SORTPOOL	41.82	79.37	73.76	75.54
DIFFPOOL-DET	46.18	75.47	82.13	75.62
DIFFPOOL-NOLP	46.65	79.98	75.63	77.42
DIFFPOOL	47.08	81.15	75.50	78.10
GU-NET/SHGC	-	78.59	74.54	75.46
MLP	40.96	80.22	74.00	75.74
GCN(R)-MLP	36.15	78.61	75.38	76.28
GCN-MLP	45.01	79.29	76.50	75.64
JK-SUM	47.16	79.02	77.00	75.82
JK-SUM-DECAY	43.87	79.11	74.14	75.82
JK-SUM-REINIT	46.77	75.97	77.20	75.46

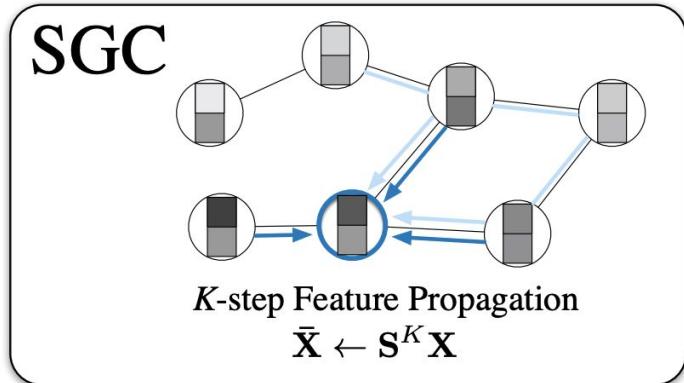


Benchmarking GNNs

- Popular GNN benchmark datasets often unreliable
 - Complexity not very high

Simplifying Graph Convolutional Networks

Felix Wu^{*1} Tianyi Zhang^{*1} Amauri Holanda de Souza Jr.^{*12} Christopher Fifty¹ Tao Yu¹
Kilian Q. Weinberger¹



$$\hat{\mathbf{Y}}_{\text{SGC}} = \text{softmax} (\mathbf{S}^K \mathbf{X} \Theta)$$

Our experiments:

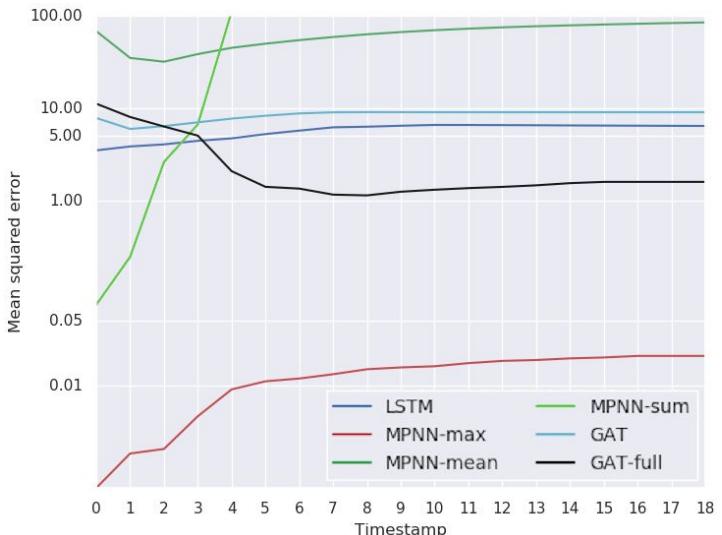
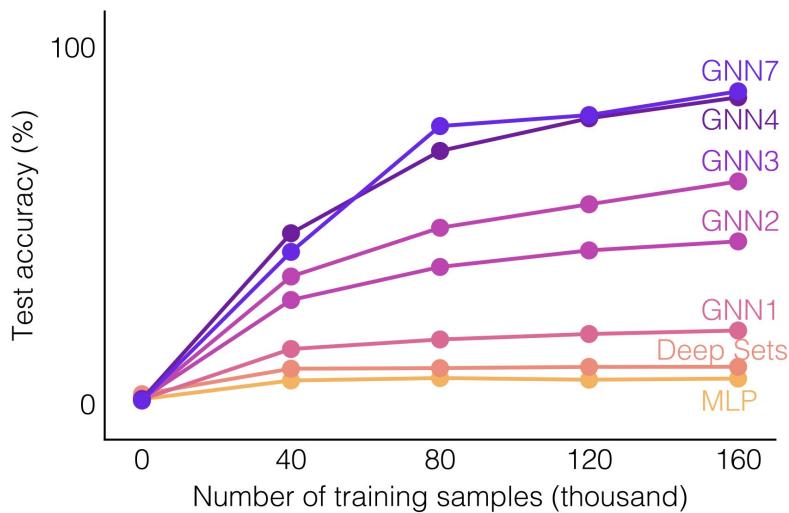
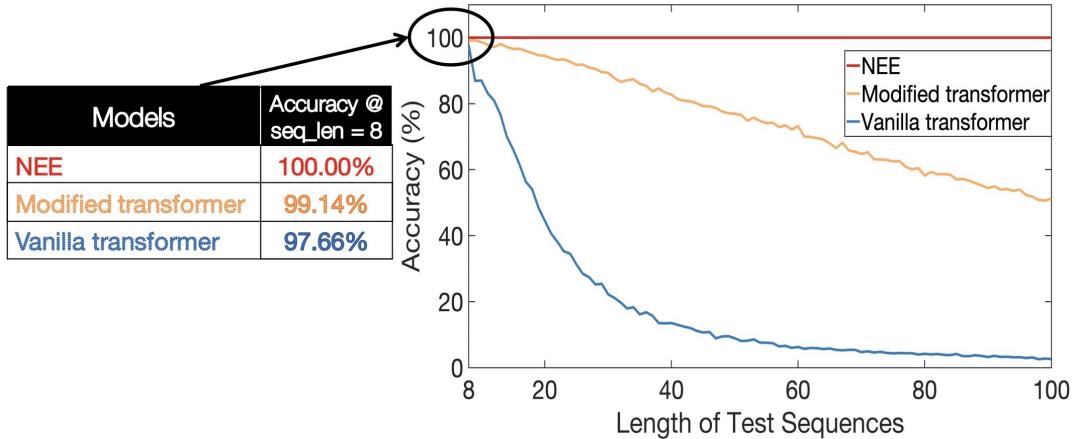
GCN	81.4 ± 0.4	70.9 ± 0.5	79.0 ± 0.4
GAT	83.3 ± 0.7	72.6 ± 0.6	78.5 ± 0.3
FastGCN	79.8 ± 0.3	68.8 ± 0.6	77.4 ± 0.3
GIN	77.6 ± 1.1	66.1 ± 0.9	77.0 ± 1.2
LNet	$80.2 \pm 3.0^\dagger$	67.3 ± 0.5	$78.3 \pm 0.6^\dagger$
AdaLNet	$81.9 \pm 1.9^\dagger$	$70.6 \pm 0.8^\dagger$	$77.8 \pm 0.7^\dagger$
DGI	82.5 ± 0.7	71.6 ± 0.7	78.4 ± 0.7
SGC	81.0 ± 0.0	71.9 ± 0.1	78.9 ± 0.0

Setting	Model	Test F1
Supervised	GaN	96.4
	SAGE-mean	95.0
	SAGE-LSTM	95.4
	SAGE-GCN	93.0
	FastGCN	93.7
	GCN	OOM
Unsupervised	SAGE-mean	89.7
	SAGE-LSTM	90.7
	SAGE-GCN	90.8
	DGI	94.0
No Learning	Random-Init DGI	93.3
	SGC	94.9



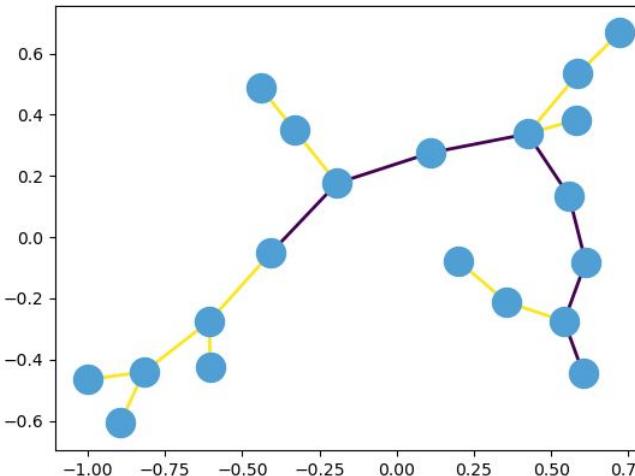
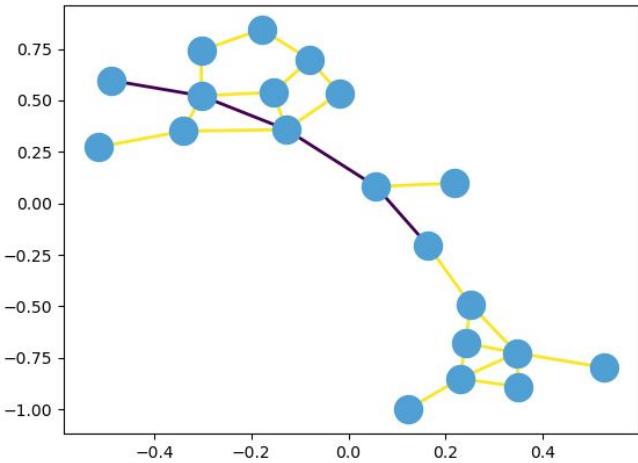
Benchmarking GNNs

- Popular GNN benchmark datasets often **unreliable**
 - Complexity not very high
- Algorithms prove very **favourable**
 - Infinite data
 - Complex data manipulation
 - A clear **hierarchy** of models emerges!



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- A clearly specified **generating** function
 - No **noise** in the data
 - Enabling rigorous **credit assignment**

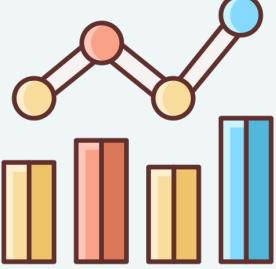


Benchmarking GNNs

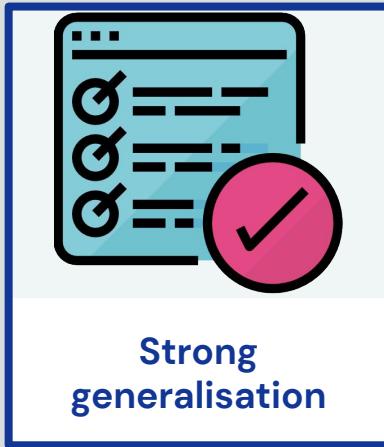
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 - A clear **hierarchy** of models emerges!
- A clearly specified **generating** function
 - No **noise** in the data
 - Enabling rigorous **credit assignment**
- The world is propped-up on *polynomial-time algorithms*
 - Applicable to NP-hard problems (see e.g. Joshi, Laurent and Bresson, NeurIPS'19 GRL)



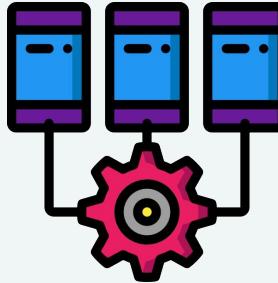
Why?



Benchmarking
graph neural nets



Strong
generalisation



Multi-task learning

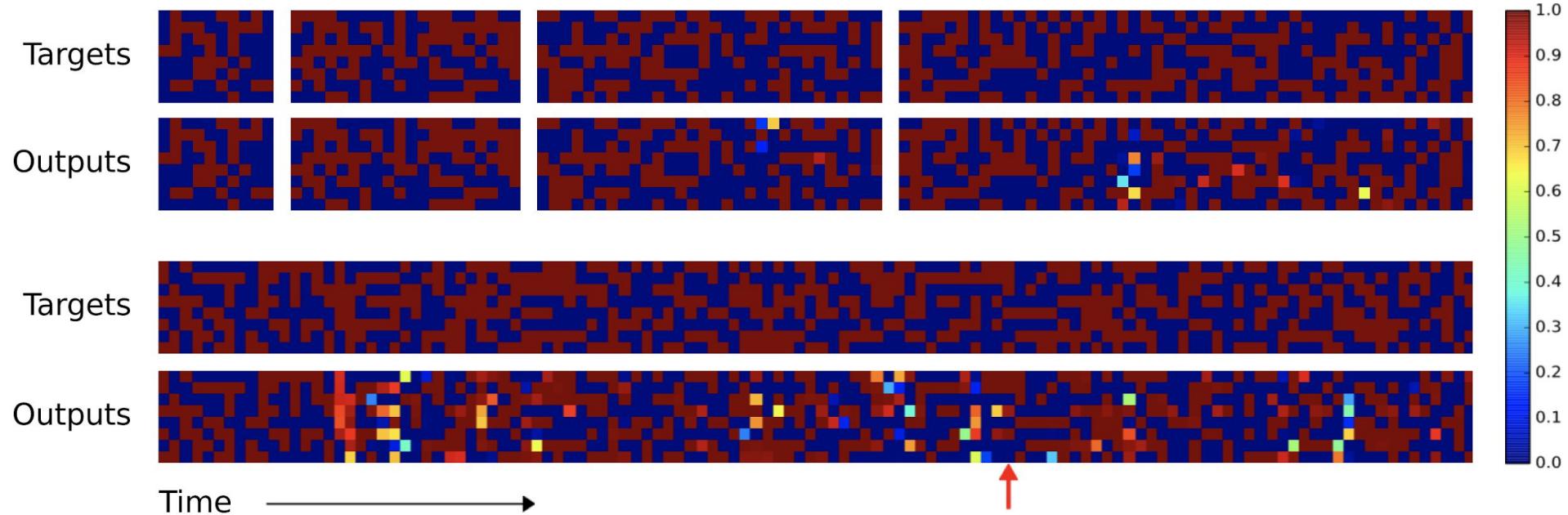


Algorithm
discovery



Strong generalisation

- Learning an *algorithm* is **not** learning input-output *mapping*!



(Graves et al., 2014)

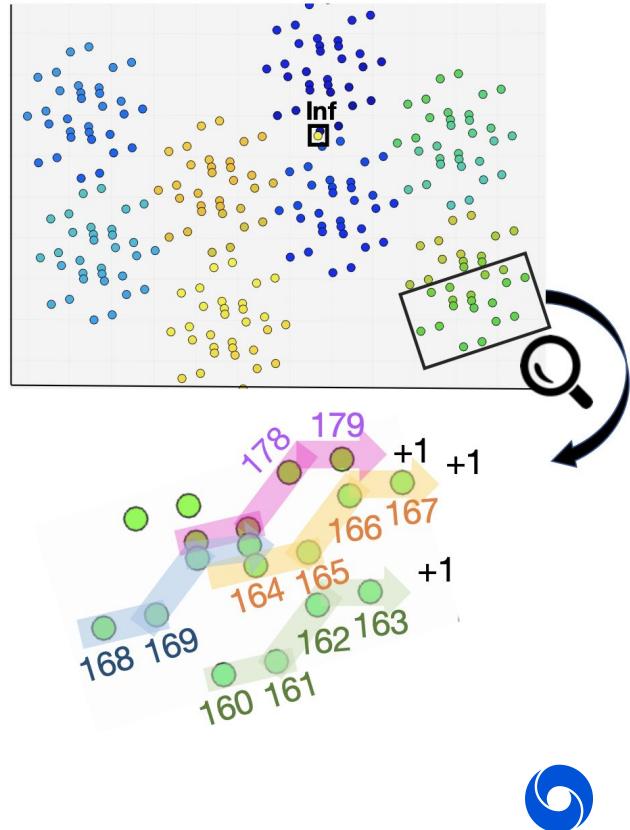


Strong generalisation

- Learning an *algorithm* is **not** learning input-output *mapping*!
- Imitating individual *operations* enables **strong** generalisation.
 - Consider how humans devise algorithms “by hand”.
 - Scales to much larger test graph sizes.

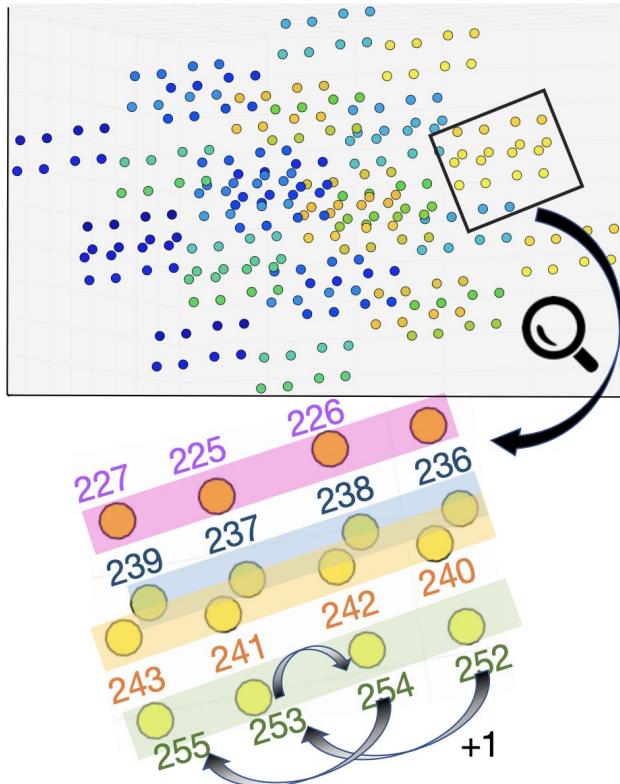
Table 1. Performance of different tasks on variable sizes of test examples (trained with examples of size 8)

Accuracy \ Sizes	25	50	75	100
Selection sort	100.00	100.00	100.00	100.00
Merge sort	100.00	100.00	100.00	100.00
Shortest paths	100.00	100.00	100.00	100.00*

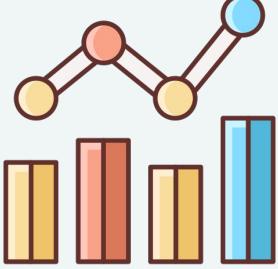


Strong generalisation

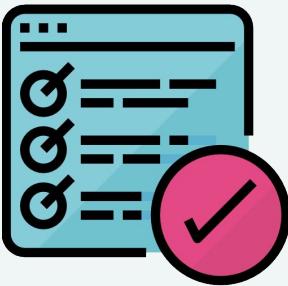
- Learning an *algorithm* is **not** learning input-output *mapping*!
- Imitating individual *operations* enables **strong** generalisation.
 - Consider how humans devise algorithms “by hand”.
 - Scales to much larger test graph sizes.
- **Grounds** the GNN in the underlying algorithmic reasoning
 - Deep learning is about learning representations
 - Learn representations of **manipulations**!



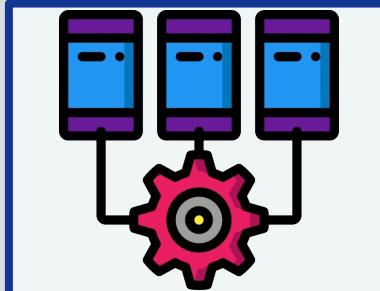
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graph neural nets



Strong
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Multi-task learning



Algorithm
discovery



Multi-task learning

- Learning representations of **manipulations**
 - ⇒ lots of potential for representational reuse.
 - Many algorithms share **subroutines**.

MST-PRIM(G, w, s)

```
1  for each  $u \in G.V$ 
2     $u.key = \infty$ 
3     $u.\pi = \text{NIL}$ 
4     $s.key = 0$ 
5     $Q = G.V$ 
6    while  $Q \neq \emptyset$ 
7       $u = \text{EXTRACT-MIN}(Q)$ 
8      for each  $v \in G.Adj[u]$ 
9        if  $v \in Q$  and  $w(u, v) < v.key$ 
10          DECREASE-KEY( $Q, v, w(u, v)$ )
11           $v.\pi = u$ 
```

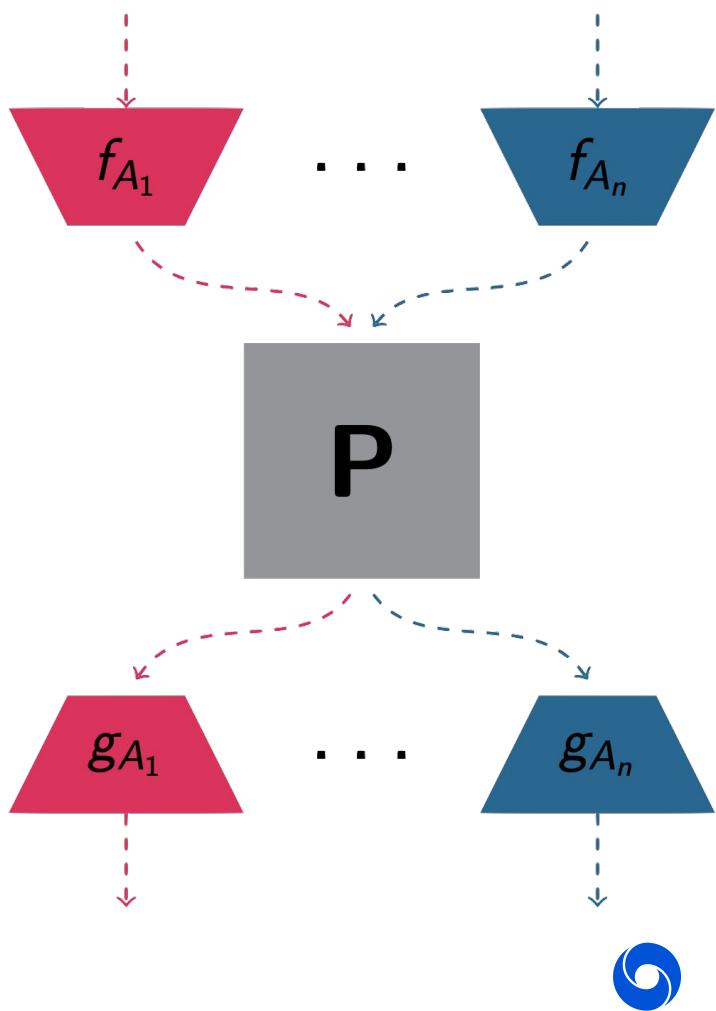
DIJKSTRA(G, w, s)

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8      for each  $v \in G.Adj[u]$ 
9        if  $u.key + w(u, v) < v.key$ 
10          DECREASE-KEY( $Q, v, u.key + w(u, v)$ )
11           $v.\pi = u$ 
```



Multi-task learning

- Learning representations of **manipulations**
 - ⇒ lots of potential for representational reuse.
 - Many algorithms share **subroutines**.
 - Representations can positively **reinforce** one another!
 - **Meta-representation** of algorithms.
 - Plentiful opportunity for:
 - *Multi-task learning*
 - *Meta-learning*
 - *Continual learning*
- with clearly defined task relations!

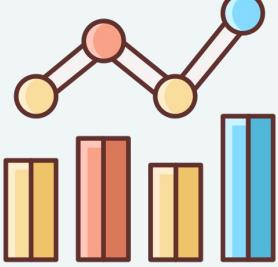


Multi-task learning

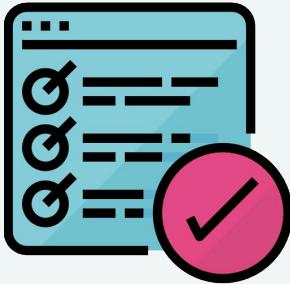
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 - with clearly defined task relations!
- Output of *easier* algorithm can be used as *input* for a harder one.



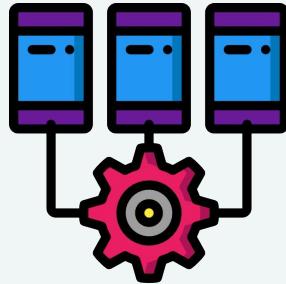
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Benchmarking
graph neural nets



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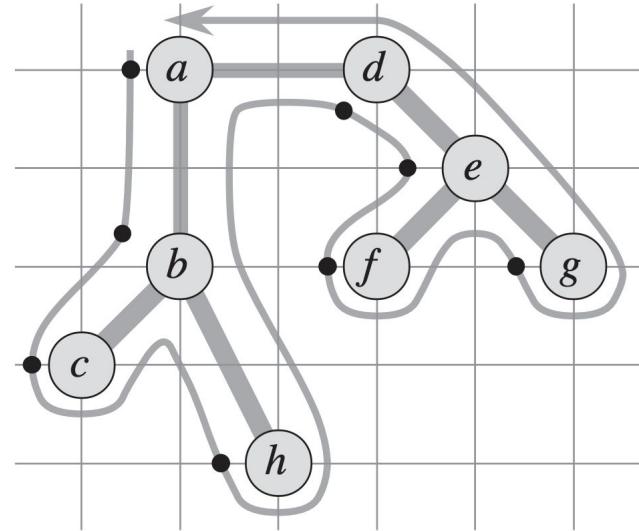
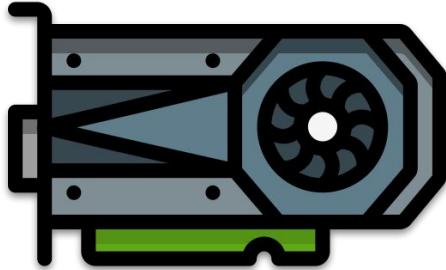


Algorithm
discovery



Algorithm discovery

- Inspecting intermediate outputs of an algorithm can **decode** its behaviour!
- Opportunity for deriving **novel** algorithms, e.g.
 - Improved heuristics for *intractable* problems.
 - Optimising for GNN executors (e.g. GPU/TPU).



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- Machine learning ← **Competitive programming!**
 - My way into computer science :)

Sphere online judge
 **CODEFORCES**



Algorithm discovery

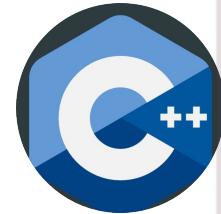
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- Machine learning ← **Competitive programming!**
 - My way into computer science :)
- Conjecture: Can perform **soft subroutine reuse** from polynomial-time algorithms.



Programming language hierarchy



High level



Middle level

10101
01011
10101

Low level



GNN-Algorithmic hierarchy

(Xu, Li, Zhang, Du, Kawarabayashi and Jegelka. ICLR 2020)

WHAT CAN NEURAL NETWORKS REASON ABOUT? **Algo-level**

(Veličković, Ying, Padovano, Hadsell and Blundell. ICLR 2020)

NEURAL EXECUTION OF GRAPH ALGORITHMS **Step-level**

(Yan, Swersky, Koutra, Ranganathan and Hashemi. 2020)

NEURAL EXECUTION ENGINES **Unit-level**



GNN-Algorithmic hierarchy

(Xu, Li, Zhang, Du, Kawarabayashi and Jegelka. ICLR 2020)

- Learns an **algorithm** end-to-end only
- Strong theoretical link between **generalisation power** and **algorithmic alignment**
- GNNs align well with *dynamic programming!*

Algo-level

(Veličković, Ying, Padovano, Hadsell and Blundell. ICLR 2020)

- Supervises on atomic **steps** of an algorithm
- Out-of-distribution testing of various GNNs
- *Multi-task learning + maximisation aggregators generalise stronger!*

Step-level

(Yan, Swersky, Koutra, Ranganathan and Hashemi. 2020)

- Learns to execute tiny **operations**, then composes them
- Binary encoding and conditional masking
- Achieves *perfect strong generalisation!*

Unit-level



GNN-Algorithmic hierarchy

(Xu, Li, Zhang, Du, Kawarabayashi and Jegelka. ICLR 2020)

WHAT CAN NEURAL NETWORKS REASON ABOUT?

Algo-level

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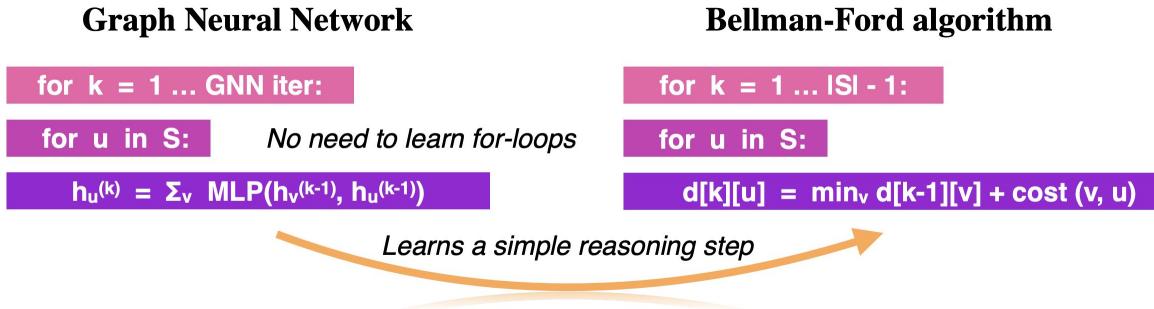
(Yan, Swersky, Koutra, Ranganathan and Hashemi. 2020)

NEURAL EXECUTION ENGINES Unit-level



What Can Neural Networks Reason About?

- Which networks are best suited for certain types of **reasoning**?
 - **Theorem:** better structural alignment implies better generalisation!
 - GNNs ~ dynamic programming

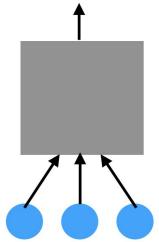


$$\text{Answer}[k][i] = \text{DP-Update}(\{\text{Answer}[k-1][j], j = 1 \dots n\})$$

$$h_s^{(k)} = \sum_{t \in S} \text{MLP}_1^{(k)} \left(h_s^{(k-1)}, h_t^{(k-1)} \right)$$



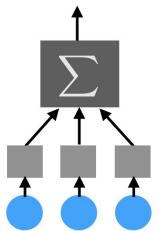
Architectures under study



MLPs

~ feature extraction

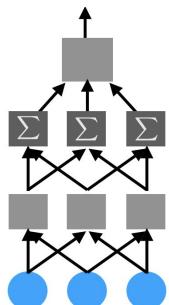
$$y = \text{MLP}(\|_{s \in S} X_s)$$



Deep Sets (Zaheer et al., NeurIPS 2017)

~ summary statistics

$$y = \text{MLP}_2 \left(\sum_{s \in S} \text{MLP}_1(X_s) \right)$$



GNNs

~ (pairwise) relations

$$h_s^{(k)} = \sum_{t \in S} \text{MLP}_1^{(k)} \left(h_s^{(k-1)}, h_t^{(k-1)} \right)$$

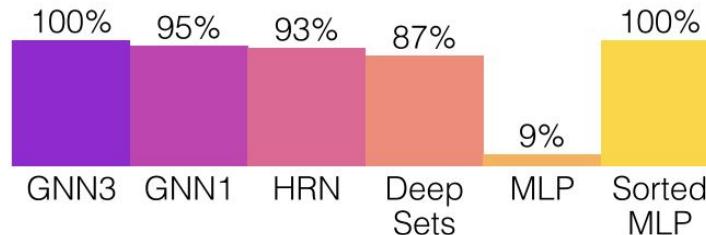
$$y = \text{MLP}_2 \left(\sum_{s \in S} h_s^{(K)} \right)$$



Empirical results

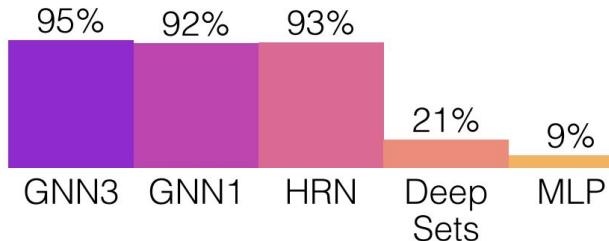
Summary statistics

What is the maximum value difference among treasures?



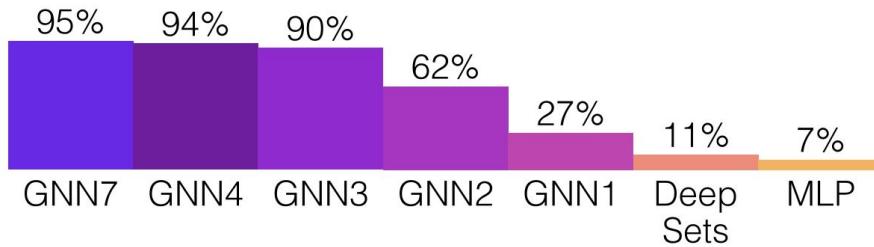
Relational argmax

What are the colors of the furthest pair of objects?



Dynamic programming

What is the cost to defeat monster X by following the optimal path?



GNN-Algorithmic hierarchy

(Xu, Li, Zhang, Du, Kawarabayashi and Jegelka. ICLR 2020)

WHAT CAN NEURAL NETWORKS REASON ABOUT? **Algo-level**

(Veličković, Ying, Padovano, Hadsell and Blundell. ICLR 2020)

NEURAL EXECUTION OF GRAPH ALGORITHMS **Step-level**

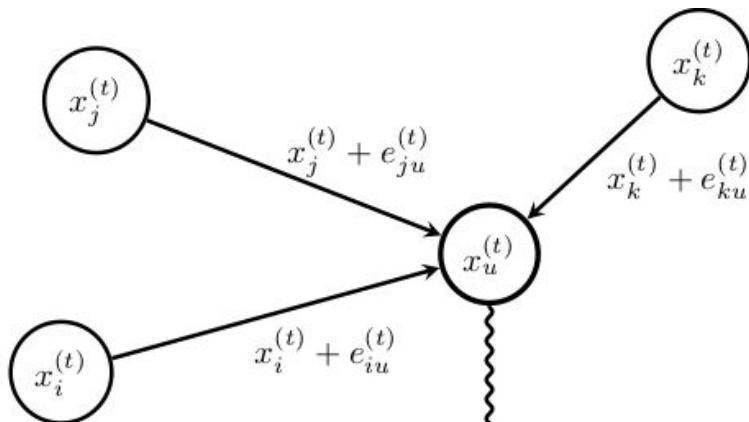
(Yan, Swersky, Koutra, Ranganathan and Hashemi. 2020)

NEURAL EXECUTION ENGINES **Unit-level**

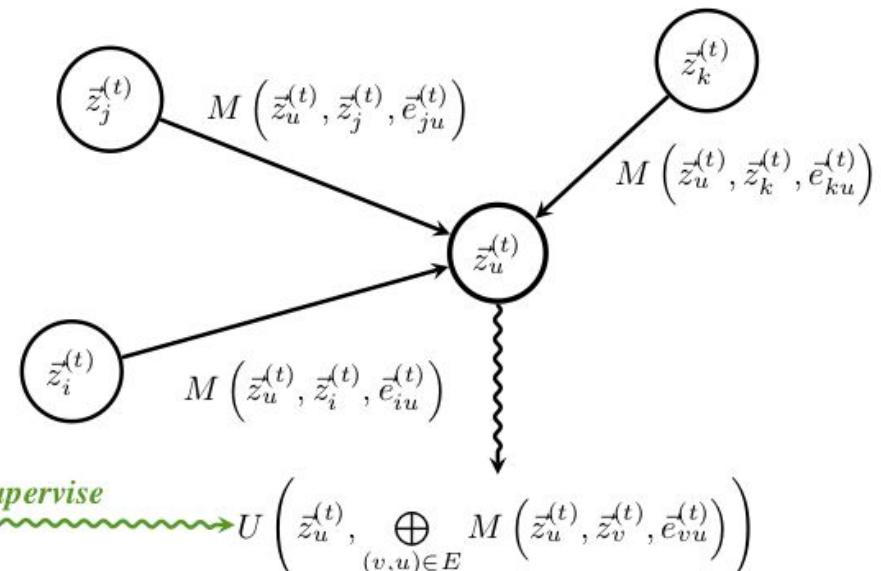


Neural Execution of Graph Algorithms

Supervise on appropriate output values **at every step**.



Bellman-Ford algorithm



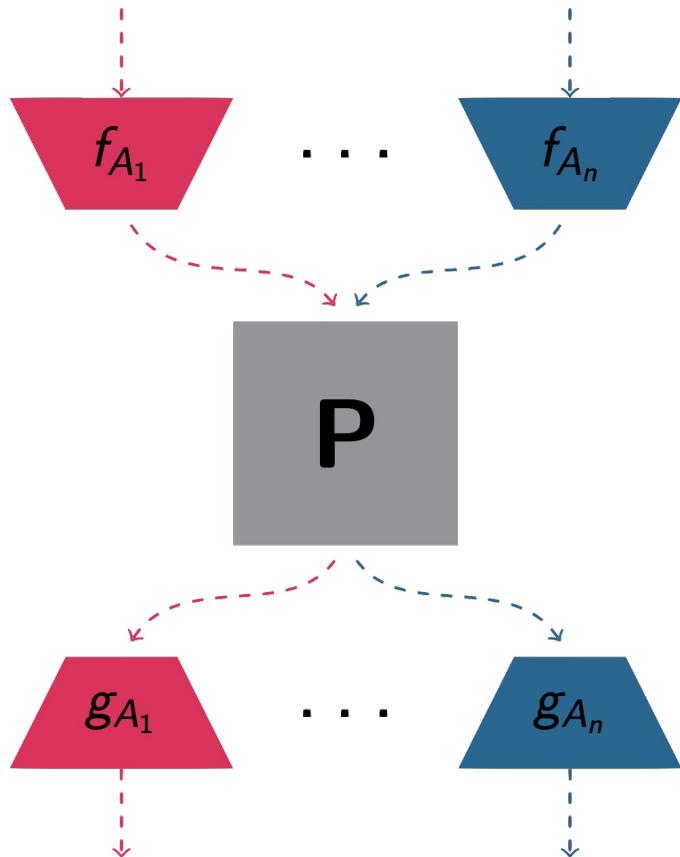
Message-passing neural network



Components of the executor

- **Encoder network*** $\vec{z}_i^{(t)} = f_A(\vec{x}_i^{(t)}, \vec{h}_i^{(t-1)})$
- **Processor network** $\mathbf{H}^{(t)} = P(\mathbf{Z}^{(t)}, \mathbf{E}^{(t)})$
- **Decoder network*** $\vec{y}_i^{(t)} = g_A(\vec{z}_i^{(t)}, \vec{h}_i^{(t)})$
- **Termination network*** $\tau^{(t)} = \sigma(T_A(\mathbf{H}^{(t)}))$
- **Repeat as long as** $\tau^{(t)} > 0.5$

*algorithm-specific



- Hypothesis: **MPNN-max** is a highly suitable processor



Evaluation

- Evaluate on *parallel* and *sequential* algorithms.
 - Parallel: *Reachability (BFS)*, *Shortest paths (Bellman-Ford)*
 - Sequential: *Minimal spanning trees (Prim)*
 - Explicit inductive bias on sequentiality (learnable mask!)
- Generate **graphs** from a wide variety of distributions:
 - Ladder, Grid, Tree, 4-Caveman, 4-Community, Erdős-Rényi, Barabási-Albert
 - Attach random-valued weights to each edge
- Study the “human-programmer” perspective: test generalisation from small graphs (20 nodes) to larger graphs (50/100 nodes).
- Learn to execute BFS and Bellman-Ford with **same** processor!



Evaluation: Shortest paths (+ Reachability)

Model	Predecessor (mean step accuracy / last-step accuracy)		
	20 nodes	50 nodes	100 nodes
LSTM (Hochreiter & Schmidhuber, 1997)	47.20% / 47.04%	36.34% / 35.24%	27.59% / 27.31%
GAT* (Veličković et al., 2018)	64.77% / 60.37%	52.20% / 49.71%	47.23% / 44.90%
GAT-full* (Vaswani et al., 2017)	67.31% / 63.99%	50.54% / 48.51%	43.12% / 41.80%
MPNN-mean (Gilmer et al., 2017)	93.83% / 93.20%	58.60% / 58.02%	44.24% / 43.93%
MPNN-sum (Gilmer et al., 2017)	82.46% / 80.49%	54.78% / 52.06%	37.97% / 37.32%
MPNN-max (Gilmer et al., 2017)	97.13% / 96.84%	94.71% / 93.88%	90.91% / 88.79%
MPNN-max (<i>curriculum</i>)	95.88% / 95.54%	91.00% / 88.74%	84.18% / 83.16%
MPNN-max (<i>no-reach</i>)	82.40% / 78.29%	78.79% / 77.53%	81.04% / 81.06%
MPNN-max (<i>no-algo</i>)	78.97% / 95.56%	83.82% / 85.87%	79.77% / 78.84%

Trained on 20-node graphs!

Trained without reachability objective

Trained without step-wise supervision



Evaluation: Sequential execution

Model	Accuracy (next MST node / MST predecessor)		
	20 nodes	50 nodes	100 nodes
LSTM (Hochreiter & Schmidhuber, 1997)	11.29% / 52.81%	3.54% / 47.74%	2.66% / 40.89%
GAT* (Veličković et al., 2018)	27.94% / 61.74%	22.11% / 58.66%	10.97% / 53.80%
GAT-full* (Vaswani et al., 2017)	29.94% / 64.27%	18.91% / 53.34%	14.83% / 51.49%
MPNN-mean (Gilmer et al., 2017)	90.56% / 93.63%	52.23% / 88.97%	20.63% / 80.50%
MPNN-sum (Gilmer et al., 2017)	48.05% / 77.41%	24.40% / 61.83%	31.60% / 43.98%
MPNN-max (Gilmer et al., 2017)	87.85% / 93.23%	63.89% / 91.14%	41.37% / 90.02%
MPNN-max (<i>no-algo</i>)	— / 71.02%	— / 49.83%	— / 23.61%

The sequential inductive bias is very **helpful!**



GNN-Algorithmic hierarchy

(Xu, Li, Zhang, Du, Kawarabayashi and Jegelka. ICLR 2020)

WHAT CAN NEURAL NETWORKS REASON ABOUT? **Algo-level**

(Veličković, Ying, Padovano, Hadsell and Blundell. ICLR 2020)

NEURAL EXECUTION OF GRAPH ALGORITHMS **Step-level**

(Yan, Swersky, Koutra, Ranganathan and Hashemi. 2020)

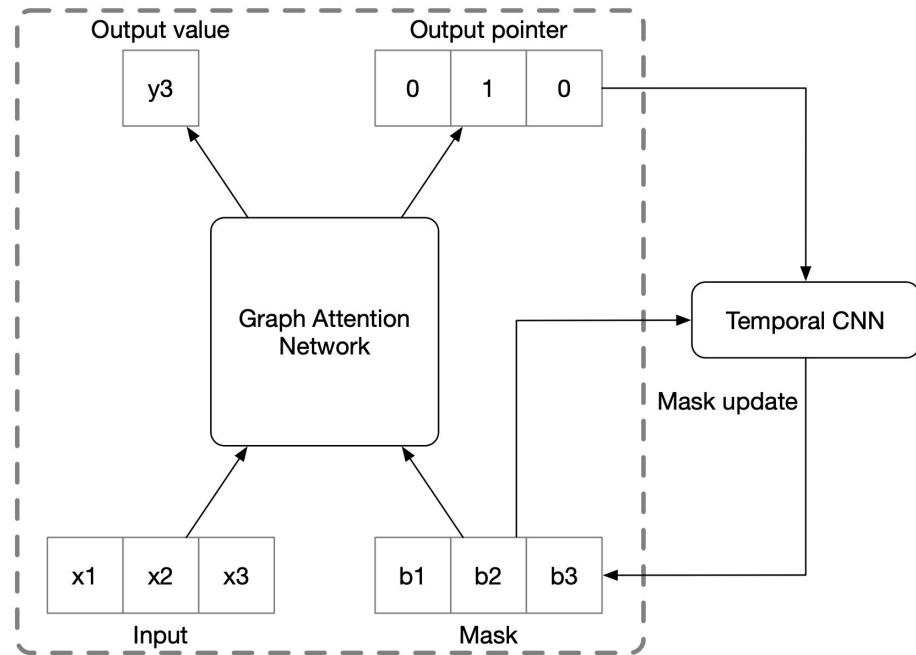
NEURAL EXECUTION ENGINES

Unit-level



Neural Execution Engines

- Teach a neural net to **strongly** perform *tiny* tasks (e.g. sum, product, argmin)
 - Compose** tasks to specify algorithms
 - The building blocks must stay robust with long/OOD rollouts!
- Key components:
 - Bitwise embeddings
 - Transformers
 - Conditional masking



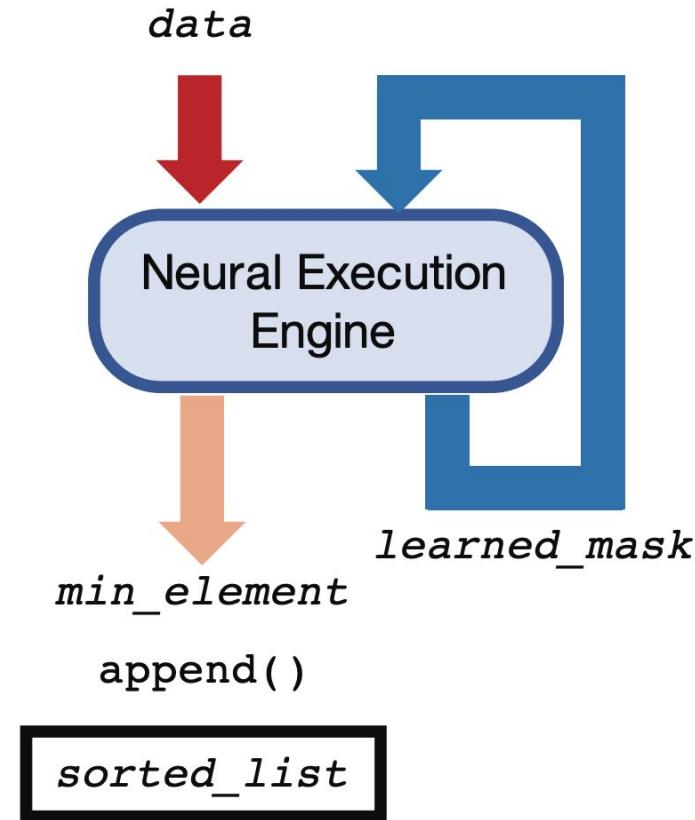
Learning to selection sort by composing argmin

```

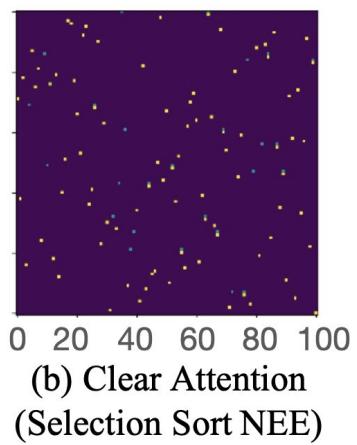
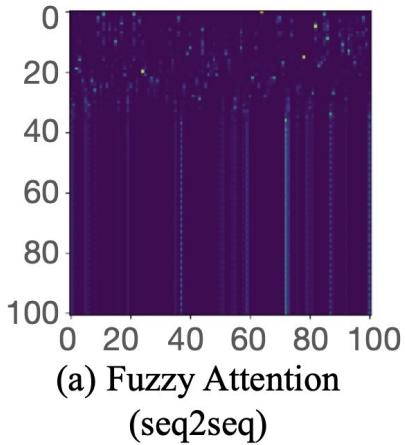
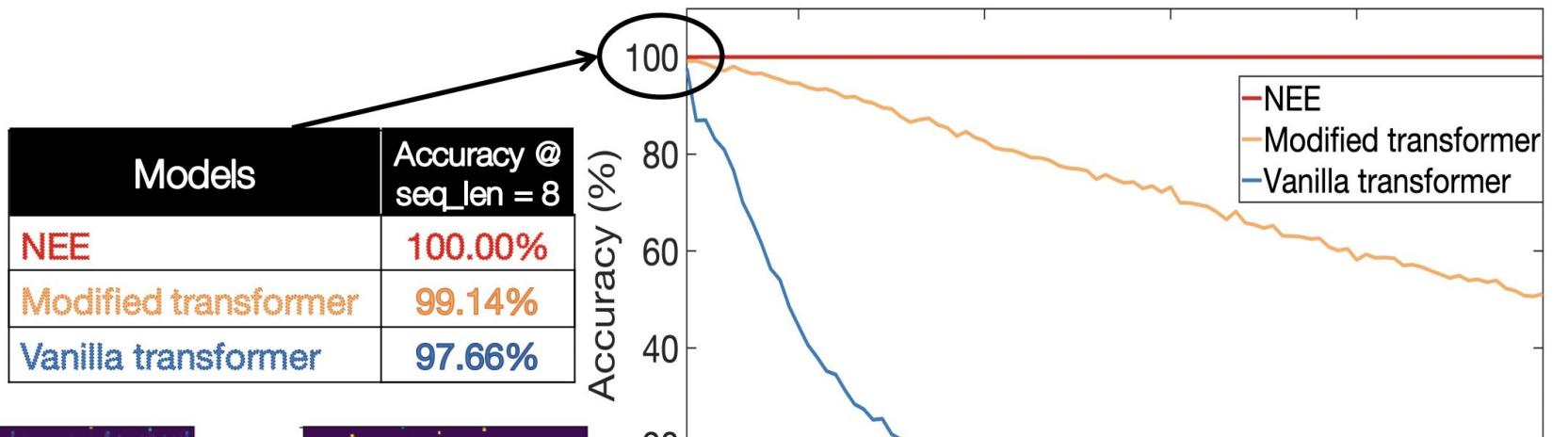
selection_sort(data):
    sorted_list = []
    while (len(data) > 0):
        min_index, min_element = find_min(data)
        data.delete(min_index)
        sorted_list.append(min_element)
    return sorted_list

find_min(data):
    min_element = -1
    min_index = -1
    for index, element in enumerate(data):
        if (element < min_element):
            min_element = element
            min_index = index
    return [min_index, min_element]

```



Learning to selection sort by composing argmin



Composing subroutines (Dijkstra)

```
shortest_path(graph, source_node, shortest_path):
```

```
    dists = []

```

```
    nodes = []

```

```
    anchor_node = source_node
```

```
    node_list = graph.get_nodes()
```

```
while node_list:
```

```
    possible_paths = sum(graph.adj(anchor_node),  
                         shortest_path(anchor_node))
```

```
    shortest_path = min(possible_paths, shortest_path)
```

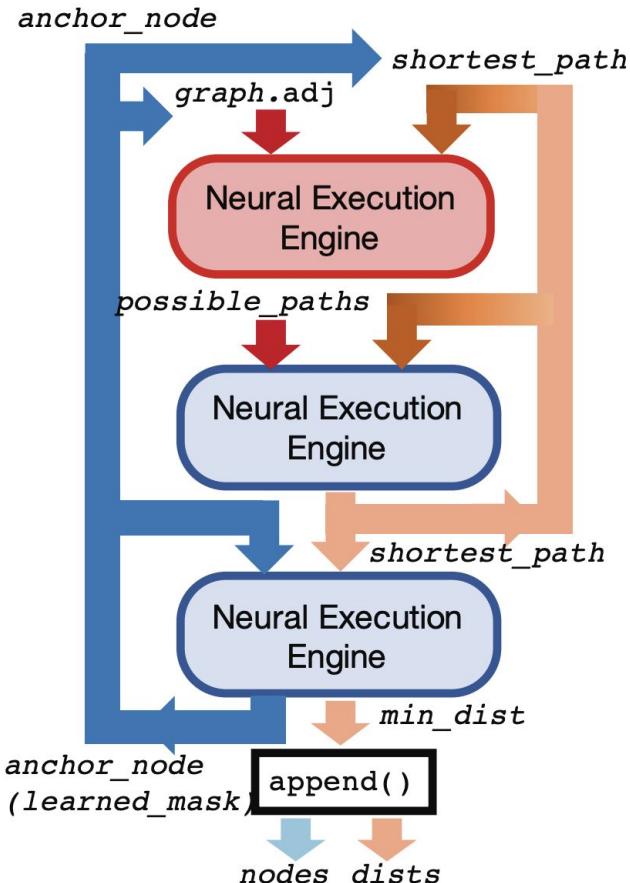
```
    anchor_node, min_dist = min(shortest_path)
```

```
    node_list.delete(anchor_node)
```

```
    nodes.append(anchor_node)
```

```
    dists.append(min_dist)
```

```
return dists, nodes
```



Recursive subroutines (Merge sort)

merge_sort(*data, start, end*):

if (*start < end*):

mid = (*start + end*) / 2

merge_sort(*data, start, mid*)

merge_sort(*data, mid+1, end*)

merge(*data, start, mid, end*)

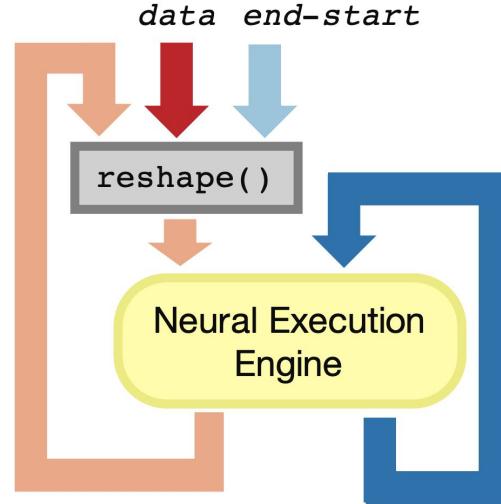


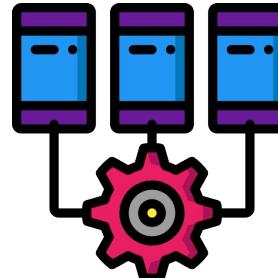
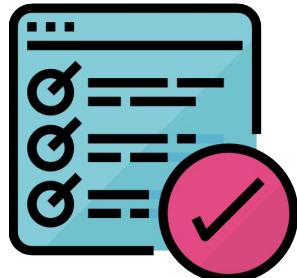
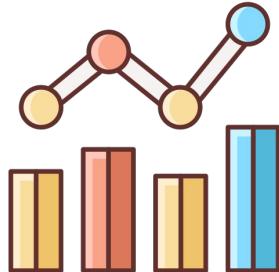
Table 1. Performance of different tasks on variable sizes of test examples (trained with examples of size 8)

Accuracy \ Sizes	25	50	75	100
Selection sort	100.00	100.00	100.00	100.00
Merge sort	100.00	100.00	100.00	100.00
Shortest paths	100.00	100.00	100.00	100.00*



Conclusions

- **Algorithmic reasoning** is an exciting novel area for **graph representation learning!**
 - Three concurrent works explore it at different levels:
 - Algo-level (*Xu, Li, Zhang, Du, Kawarabayashi and Jegelka. ICLR 2020*)
 - Step-level (*Veličković, Ying, Padovano, Hadsell and Blundell. ICLR 2020*)
 - Unit-level (*Yan, Swersky, Koutra, Raganathan and Hashemi. 2020*)
- Many questions left to be answered, at *all* levels of the hierarchy!
 - <Your contribution here/>



DeepMind

Thank you!

Questions?

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In collaboration with Charles Blundell, Raia Hadsell, Rex Ying, Matilde Padovano,
Lars Buesing, Matt Overlan, Razvan Pascanu and Oriol Vinyals

