Algorithmic Execution via Graph Representation Learning

ScAi Lab Reading Group Report

Zhiping (Patricia) Xiao

University of California, Los Angeles

October 13, 2021

Outline

Introduction

References

Petar's work:

- Neural Execution of Graph Algorithms (ICLR'20)
- Pointer Graph Networks (NeurIPS'20)

Author's Presentations:

- `https://slideslive.com/38938392/algorithmic-reasoning-in-the-real-world` [1]
- `https://petar-v.com/talks/Algo-WWW.pdf`
- (and more: `https://petar-v.com/communications.html`)

[1] Special thanks to Ziniu.

Motivation

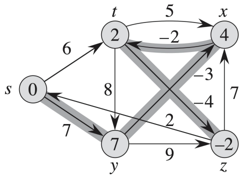


Figure: Algorithms

- - Inputs must match spec
- - Not robust to task variations
- + Interpretable operations
- + Trivially strongly generalise
- + Small data is fine

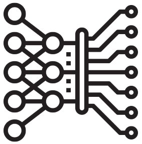


Figure: Neural Networks

- + Operate on raw inputs
- + Models are reusable across tasks
- - Lack of interpretability
- - Unreliable when extrapolating
- - Require big data

Observation on Classical Algorithms

Scenario 1: Parallel Algorithm
Many algorithms share subroutines. e.g.:

- Shortest-Path Computation via Bellman-Ford Algorithm
- Reachability Computation via Breadth-First Search

both enumerates sets of edges adjacent to a particular node.

Scenario 2: Sequential Algorithm
Some Algorithms focus on one node at a time (different than ↑).
e.g.:

- Minimum Spanning Trees generation via Prim's Algorithm

Idea

So far, researchers have studied: use *ground-truth* algorithmic solution (algorithm) to drive learning (neural networks).

Petar's works: use neural networks (**graph** neural networks) to execute classical algorithms (on **graph**s).

They name it as **Neural Graph Algorithm Execution**.

Neural Graph Algorithm Execution

The approach that:

- Learn several algorithms simultaneously
- Provide a supervision signal
    - signal: driven by prior knowledge on how classical algorithms' behaviors

and thus transfer knowledge between different algorithms.

Neural Execution of Graph Algorithms

Graph Component

Two roles:

- Part of the problem provided;
- Inputs to a GNN.

The graph $G = (V, E)$ consists of:

- V: the set of nodes / vertices;
- E: the set of edges / node-pairs.

GNN receives a sequence of T graph-structured inputs (index $t \in \{1, \ldots t)$,

- Each node $i \in V$ has features $\mathbf{x}_i^{(t)} \in \mathbb{R}^{N_x}$
- Eech edge $(i, j) \in E$ has features $\mathbf{e}_{ij}^{(t)} \in \mathbb{R}^{N_e}$
- Each step *node-level* output $\mathbf{y}_i^{(t)} \in \mathbb{R}^{N_y}$

Encoder-Process-Decoder Architecture [2]

Consisting of three components:

- an *encoder* network f_A for **each** algorithm A
  - inputs: node feature $\mathbf{x}$, (previous) latent feature $\mathbf{h}$
  - output: encoded input $\mathbf{z}$
- a *processor* network P shared among all algorithms
  - inputs: edge feature $\mathbf{e}$, encoded input $\mathbf{z}$
  - output: latent feature $\mathbf{h}$
- a *decoder* network g_A for **each** algorithm A
  - inputs: encoded input $\mathbf{z}$, latent feature $\mathbf{h}$
  - output: node-level outputs $\mathbf{y}$

[2] Follows Hamrick et al. 2018

Visualization of the Idea

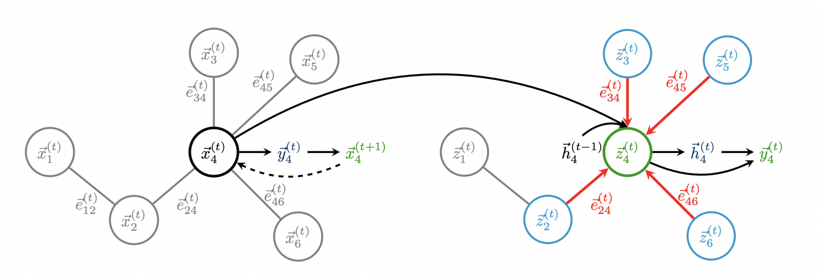
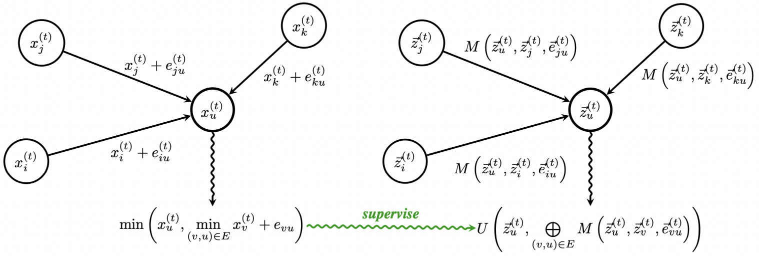


Figure: Relation between local computation of graph algorithm (**left**) and the neural graph algorithm executor (**right**).
Node values $\mathbf{y}_i^{(t)}$ (e.g. reachability, shortest-path distance, etc.) are updated at every step of execution.
Analogously, node values are predicted by the neural executor from hidden rep $\mathbf{h}_i^{(t)}$ via message-passing.
(Figure 1 of the paper.)

Visualization of the Idea



$x_j^{(t)}$
$x_k^{(t)}$
$x_u^{(t)}$
$x_i^{(t)}$
$x_j^{(t)} + e_{ju}^{(t)}$
$x_k^{(t)} + e_{ku}^{(t)}$
$x_i^{(t)} + e_{iu}^{(t)}$
$\min\left(x_u^{(t)}, \min_{(v,u)\in E} x_v^{(t)} + e_{vu}\right)$
supervise
$\vec{z}_j^{(t)}$
$\vec{z}_k^{(t)}$
$\vec{z}_u^{(t)}$
$\vec{z}_i^{(t)}$
$M\left(\vec{z}_u^{(t)}, \vec{z}_j^{(t)}, \vec{e}_{ju}^{(t)}\right)$
$M\left(\vec{z}_u^{(t)}, \vec{z}_k^{(t)}, \vec{e}_{ku}^{(t)}\right)$
$M\left(\vec{z}_u^{(t)}, \vec{z}_i^{(t)}, \vec{e}_{iu}^{(t)}\right)$
$U\left(\vec{z}_u^{(t)}, \bigoplus_{(v,u)\in E} M\left(\vec{z}_u^{(t)}, \vec{z}_v^{(t)}, \vec{e}_{vu}^{(t)}\right)\right)$

Figure: An example. Illustrating the alignment of one step of the Bellman-Ford algorithm (**left**) with one step of a message passing neural network (**right**), and the supervision signal used for the algorithm learner.
(Figure 2 of the paper.)

Encoder Network f_A

From features to encoded inputs:

- $\mathbf{x}_i^{(t)}$: node feature of node i at step t
- $\mathbf{h}_i^{(t-1)}$: *previous* latent feature of node i
- $\mathbf{z}_i^{(t)}$: encoded input of node i at step t

$$\mathbf{z}_i^{(t)} = f_A(\mathbf{x}_i^{(t)}, \mathbf{h}_i^{(t-1)}), \qquad \mathbf{h}_i^{(0)} = 0$$

Process Network P

From encoded inputs to latent representation:

- $\mathbf{E}^{(t)} = \{\mathbf{e}_{ij}^{(t)}\}_{(i,j)\in E}$: all edge features at step t
- $\mathbf{Z}^{(t)} = \{\mathbf{z}_{i}^{(t)}\}_{i\in V}$: all encoded inputs at step t
- $\mathbf{H}^{(t)} = \{h_i^t \in \mathbb{R}^K\}_{i\in V}$: all latent features at step t

$$\mathbf{H}^{(t)} = P(\mathbf{Z}^{(t)}, \mathbf{E}^{(t)})$$

Note that:

1. Parameters of P are **shared** among all algorithms being learnt.
2. P make decision on when to terminate the algorithm, handled by an *algorithm-specific* termination network T_A

Process Network P: Termination Network T_A

T_A is specific to algorithm A:

- $\mathbf{H}^{(t)} = \{h_i^t \in \mathbb{R}^K\}_{i \in V}$: all latent features at step t
- $\overline{\mathbf{H}^{(t)}} = \frac{1}{|V|} \sum_{i \in V} \mathbf{h}_i^{(t)}$: the average node embedding at step t
- σ: the logistic sigmoid activation
- $\tau^{(t)}$: the probability of termination

$$\tau^{(t)} = \sigma(T_A(\mathbf{H}^{(t)}, \overline{\mathbf{H}^{(t)}}))$$

Only when $\tau^{(t)}$ is below some threshold (e.g. 0.5) we will move on to the next step $(t + 1)$.

Decoder Network g_A

From (algorithm-specific) encoded inputs, and shared latent features, to algorithm-specific outputs:

- $\mathbf{z}_i^{(t)}$: encoded input of node i at step t
- $\mathbf{h}_i^{(t)}$: latent feature of node i at step t
- $\mathbf{y}_i^{(t)}$: algorithm-specific output of node i at step t

$$\mathbf{y}_i^{(t)} = g_A(\mathbf{z}_i^{(t)}, \mathbf{h}_i^{(t)})$$

If the algorithm hasn't been terminated ($\tau^{(t)}$ is big enough), parts of $\mathbf{y}_i^{(t)}$ might be reused in $\mathbf{x}_i^{(t+1)}$ (next step node feature).

High-Level Design Decisions

All algorithms need to be executed simultaneously.

- Make processor network P algorithm-agnostic.

The majority of the representational power should be placed in the processor network P.

- All the algorithm-dependent networks f_A, g_A, T_A are simply linear projections.

Most algorithms require making *discrete decisions* over neighborhoods (e.g. “which edge to take”).

- *Message-passing neural network* with a *maximization aggregator* is naturally suitable.

Message-Passing Neural Networks (MPNNs)

GATs (Graph Attention Networks):

$$\mathbf{h}_i^{(t)} = \mathrm{ReLU}\Big(\sum_{(j,i)\in E} \alpha\big(\mathbf{z}_i^{(t)}, \mathbf{z}_j^{(t)}, \mathbf{e}_{ij}^{(t)}\big) \mathbf{W} \mathbf{z}_j^{(t)} \Big) ,$$

where W is learnable projection matrix, α is the attention mechanism producing *scalar coefficients*.

MPNNs (Message-Passing Neural Networks):

$$\mathbf{h}_i^{(t)} = U\Big(\mathbf{z}_i^{(t)}, \bigoplus_{(j,i)\in E} M\big(\mathbf{z}_i^{(t)}, \mathbf{z}_j^{(t)}, \mathbf{e}_{ij}^{(t)}\big) \Big) ,$$

where M, U are neural networks producing *vector messages*. $\bigoplus$ represents an element-wise aggregation operator, could be maximization, summation, averaging, etc.

Detailed Design Decisions

Employ a GNN layer as P, using MPNNs:

$$\mathbf{h}_i^{(t)} = U\left(\mathbf{z}_i^{(t)}, \bigoplus_{(j,i)\in E} M\left(\mathbf{z}_i^{(t)}, \mathbf{z}_j^{(t)}, \mathbf{e}_{ij}^{(t)}\right)\right),$$

- Inserting a self-edge to every node, to make retention of self-information easier.
- M, U: linear projections
- $\bigoplus$: try mean, sum, max
- Compare to GATs baselines

Data Sets

Graphs are generated. [3]

For each edge, $\mathbf{e}_{ij}^{(t)} \in \mathbb{R}$ is simply a real-value weight, drawn uniformly from range $[0.2, 1]$.

- Benefit: randomly-sampled edge weights guarantees the uniqueness of the recovery solution, simplifying downstream evaluation.

[3]Follows You et al. 2018, 2019.

Parallel Algorithm: e.g. BFS v.s. B-F

Both algorithms:

1. Initialize by randomly select a source node s
2. Input $x_i^{(1)}$ is initialized according to $i = s$ or $i \neq s$
3. Aggregate neighborhood information to update
4. Requires discrete decisions (which edge to select)
   - For the baselines e.g. GAT, coefficients are thus *sharpened*.

Parallel Algorithm: e.g. BFS v.s. B-F

BFS (Breadth-First Search) for reachability:

$$x_i^{(1)} = \begin{cases} 1 & i = s \\ 0 & i \neq s \end{cases}$$

$$x_i^{(t+1)} = \begin{cases} 1 & x_i^{(t)} = 1 \\ 1 & \exists j.(j,i) \in E \wedge x_j^{(t)} = 1 \\ 0 & \text{otherwise} \end{cases}$$

$x_i^{(t)}$: is i reachable from s in $\leq t$ hops?

Bellman-Ford for Shortest Paths:

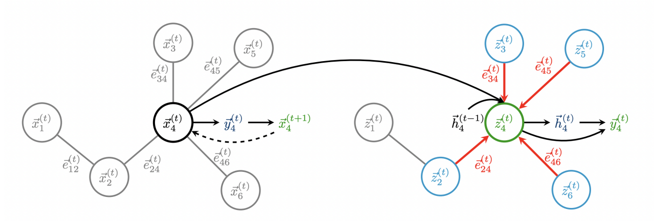
$$x_i^{(1)} = \begin{cases} 0 & i = s \\ +\infty & i \neq s \end{cases}$$

$$x_i^{(t+1)} = \min\left(x_i^{(t)}, \min_{(j,i)\in E} x_j^{(t)} + e_{ji}^{(t)}\right)$$

$x_i^{(t)}$: shortest distance from s to i (using $\leq t$ hops)

Parallel Algorithm: e.g. BFS v.s. B-F

Recall:



For BFS, no additional information is being computed, thus node-level output $y_i^{(t)} = x_i^{(t+1)}$

For Bellman-Ford, one have to remember the *predecessor* so as to reconstruct the path. Therefore, $y_i^{(t)} = p_i^{(t)}||x_i^{(t+1)}$ where

$$\text{predecessor } p_i^t = \begin{cases} i & i = s \\ \arg\min_{j;(j,i)\in E} x_j^{(t)} + e_{ji}^{(t)} & i \neq s \end{cases}$$

Sequential Algorithm: e.g. Prim's Algorithm

Prim's Algorithm for Minimum Spanning Trees (MST):

$$x_i^{(1)} = \begin{cases} 1 & i = s \\ 0 & i \neq s \end{cases}$$

$$x_i^{(t+1)} = \begin{cases} 1 & x_i^{(t)} = 1 \\ 1 & i = \arg\min_{j \ s.t. x_j^{(t)}=0} \min_{k \ s.t. x_k^{(t)}=1} e_{jk}^{(t)} \\ 0 & \text{otherwise} \end{cases}$$

$x_i^{(t)}$: is i in the partial MST tree built from s after t steps?

Similar to Bellman-Ford, the *predecessor* has to be recorded.
Keeping $p_i^{(t)}$ — the predecessor of i in the partial MST.

Experimental Results

Trained on a graph of 20 nodes, performing well on graphs with more nodes.

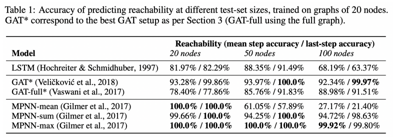


Table 1: Accuracy of predicting reachability at different test-set sizes, trained on graphs of 20 nodes. GAT* correspond to the best GAT setup as per Section 3 (GAT-full using the full graph).

	Reachability (mean step accuracy / last-step accuracy)		
Model	*20 nodes*	*50 nodes*	*100 nodes*
LSTM (Hochreiter & Schmidhuber, 1997)	81.97% / 82.29%	88.35% / 91.49%	68.19% / 63.37%
GAT* (Veličković et al., 2018)	93.28% / 99.86%	93.97% / **100.0%**	92.34% / **99.97%**
GAT-full* (Vaswani et al., 2017)	78.40% / 77.86%	85.76% / 91.83%	88.98% / 91.51%
MPNN-mean (Gilmer et al., 2017)	**100.0% / 100.0%**	61.05% / 57.89%	27.17% / 21.40%
MPNN-sum (Gilmer et al., 2017)	99.66% / **100.0%**	94.25% / **100.0%**	94.72% / 98.63%
MPNN-max (Gilmer et al., 2017)	**100.0% / 100.0%**	**100.0% / 100.0%**	**99.92%** / 99.80%

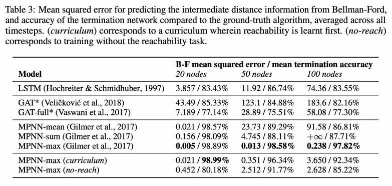


Table 3: Mean squared error for predicting the intermediate distance information from Bellman-Ford, and accuracy of the termination network compared to the ground-truth algorithm, averaged across all timesteps. (*curriculum*) corresponds to a curriculum wherein reachability is learnt first. (*no-reach*) corresponds to training without the reachability task.

	B-F mean squared error / mean termination accuracy		
Model	*20 nodes*	*50 nodes*	*100 nodes*
LSTM (Hochreiter & Schmidhuber, 1997)	3.857 / 83.43%	11.92 / 86.74%	74.36 / 83.55%
GAT* (Veličković et al., 2018)	43.49 / 85.33%	123.1 / 84.88%	183.6 / 82.16%
GAT-full* (Vaswani et al., 2017)	7.189 / 77.14%	28.89 / 75.51%	58.08 / 77.30%
MPNN-mean (Gilmer et al., 2017)	0.021 / 98.57%	23.73 / 89.29%	91.58 / 86.81%
MPNN-sum (Gilmer et al., 2017)	0.156 / 98.09%	4.745 / 88.11%	$+\infty$ / 87.71%
MPNN-max (Gilmer et al., 2017)	**0.005** / 98.89%	**0.013 / 98.58%**	**0.238 / 97.82%**
MPNN-max (*curriculum*)	0.021 / **98.99%**	0.351 / 96.34%	3.650 / 92.34%
MPNN-max (*no-reach*)	0.452 / 80.18%	2.512 / 91.77%	2.628 / 85.22%

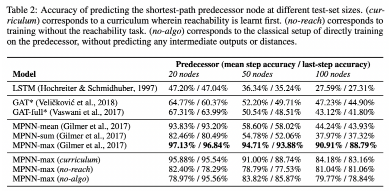


Table 2: Accuracy of predicting the shortest-path predecessor node at different test-set sizes. (*curriculum*) corresponds to a curriculum wherein reachability is learnt first. (*no-reach*) corresponds to training without the reachability task. (*no-algo*) corresponds to the classical setup of directly training on the predecessor, without predicting any intermediate outputs or distances.

	Predecessor (mean step accuracy / last-step accuracy)		
Model	*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 (*curriculum*)	95.88% / 95.54%	91.00% / 88.74%	84.18% / 83.16%
MPNN-max (*no-reach*)	82.40% / 78.29%	78.79% / 77.53%	81.04% / 81.06%
MPNN-max (*no-algo*)	78.97% / 95.56%	83.82% / 85.87%	79.77% / 78.84%

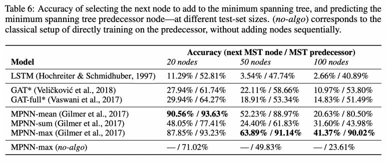


Table 6: Accuracy of selecting the next node to add to the minimum spanning tree, and predicting the minimum spanning tree predecessor node—at different test-set sizes. (*no-algo*) corresponds to the classical setup of directly training on the predecessor, without adding nodes sequentially.

	Accuracy (next MST node / MST predecessor)		
Model	*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 (*no-algo*)	— / 71.02%	— / 49.83%	— / 23.61%

Conclusion

The tasks in this paper only focus on node-level representation (due to the requirement of the experiments).

In theory, this model could also easily include:

- edge-level outputs;
- graph-level inputs / outputs.

Not considering corner-case inputs (e.g. negative weight cycles).

Pointer Graph Networks

Pointer Graph Networks (PGNs)

The previous work make GNNs learn graph algorithms, and transfer between them (MTL), using a single neural core (Process Network P) capable of: sorting, path-finding, binary addition.

PGNs is a framework that further **expands** the space of general-purpose algorithms that can be neurally executed.

Compare to Neural Execution of Graph Algorithms

Similar yet different. Different data structure:

- Previous: sequence of graphs $G = (V, E)$
- PGNs: sequence of pointer-based structures, pointer adjacency matrix $\mathbf{\Pi}^{(t)} \in \mathbb{R}^{n\times n}$ is dynamic (like (V, Π))

Problem setup is different. PGN:

- A sequence of operation inputs (of n entities at each step):

$$\mathcal{E}^{(t)} = \{\mathbf{e}_1^{(t)}, \mathbf{e}_2^{(t)}, \ldots \mathbf{e}_n^{(t)}\},$$

  $\mathbf{e}_i^{(t)}$ represents feature of entity i at time t, denoting some operation (add / remove edge etc.).
- Problem: predicting target outputs $\mathbf{y}_i^{(t)}$ from $\mathcal{E}^{(1)}, \ldots \mathcal{E}^{(t)}$

Task: Motivation

Tasks on *Dynamic Graph Connectivity* are used to illustrate the benefits of PGNs in the paper.

- DSU: disjoint-set unions, incremental graph connectivity
- LCT: link/cut trees, fully dynamic tree connectivity

Recap: Neural Execution of Graph Algorithms

Following the encoder-process-decoder paradigm on a sequence $(t = 1, \dots T)$ graph-structured inputs $G = (V, E)$:

- an *encoder* network f_A for **each** A: $\mathbf{X}^{(t)}, \mathbf{H}^{(t-1)} \to \mathbf{Z}^{(t)}$
    - $\mathbf{z}_i^{(t)} = f_A(\mathbf{x}_i^{(t)}, \mathbf{h}_i^{(t-1)}), \qquad \mathbf{h}_i^{(0)} = 0, i \in V$
    - implemented as linear projections
- a *processor* network P (**shared**): $\mathbf{Z}^{(t)}, \mathbf{E}^{(t)} \to \mathbf{H}^{(t)}$
    - $\mathbf{H}^{(t)} = P(\mathbf{Z}^{(t)}, \mathbf{E}^{(t)})$
    - implemented as MPNNs
- a *decoder* network g_A for **each** A: $\mathbf{Z}^{(t)}, \mathbf{H}^{(t)} \to \mathbf{Y}^{(t)}$
    - $\mathbf{y}_i^{(t)} = g_A(\mathbf{z}_i^{(t)}, \mathbf{h}_i^{(t)})$
    - implemented as linear projections

Pointer Graph Networks

Also encoder-process-decoder paradigm, on sequence of pointer-based inputs: $\mathcal{E}^{(t)} = \{\mathbf{e}_i^{(t)}\}_{i=1}^n$, pointer adjacency matrix $\mathbf{\Pi}^{(t)} \in \mathbb{R}^{n\times n}$:

- an *encoder* network f: $\mathcal{E}^{(t)}, \mathbf{H}^{(t-1)} \rightarrow \mathbf{Z}^{(t)}$
  - $\mathbf{z}_i^{(t)} = f(\mathbf{e}_i^{(t)}, \mathbf{h}_i^{(t-1)}), \qquad \mathbf{h}_i^{(0)} = 0, i \in \{1, \dots n\}$
  - implemented as linear projections
- a *processor* network P: $\mathbf{Z}^{(t)}, \mathbf{\Pi}^{(t-1)} \rightarrow \mathbf{H}^{(t)}$
  - $\mathbf{H}^{(t)} = P(\mathbf{Z}^{(t)}, \mathbf{\Pi}^{(t-1)})$
  - implemented as MPNNs
- a *decoder* network g: $\mathbf{Z}^{(t)}, \mathbf{H}^{(t)} \rightarrow \mathbf{Y}^{(t)}$
  - $\mathbf{y}^{(t)} = g(\bigoplus_i \mathbf{z}_i^{(t)}, \bigoplus_i \mathbf{h}_i^{(t)})$
  - $\bigoplus$: permutation-invariant aggregator (e.g. sum / max)
  - implemented as linear projections

PGNs: Masking for Sparsity

Inductive Bias: Many efficient algorithms only modify a small subset of the entities at once.

To incorporate it: Introducing masking $\mu_i^{(t)} \in \{0, 1\}$ for each node at each step,

$$\mu_i^{(t)} = \mathbb{I}_{\psi(\mathbf{z}_i^{(t)}, \mathbf{h}_i^{(t)}) > 0.5},$$

where ψ is the *masking network*, implemented as *linear* layers of appropriate dimensionality, with output activation being logistic sigmoid (enforcing probabilistic interpretation).

Updating $\Pi^{(t)}$

$$\mathbf{\Pi}_{ij}^{(t)} = \tilde{\mathbf{\Pi}}_{ij}^{(t)} \vee \tilde{\mathbf{\Pi}}_{ji}^{(t)} \,,$$

where it is found that symmetrise the matrix is beneficial, and $\tilde{\mathbf{\Pi}}^{(t)}$ denotes the pointers before symmetrisation.

$$\tilde{\mathbf{\Pi}}_{ij}^{(t)} = \mu_i^{(t)} \tilde{\mathbf{\Pi}}_{ij}^{(t-1)} + (1 - \mu_i^{(t)}) \mathbb{I}_{j=\arg\max_k(\alpha_{ik}^{(t)})} \,,$$

where μ_i are the sparsity mask we've mentioned before, $(1 - \mu_i^{(t)})$ is negating the mask. α is self-attention coefficient of $\mathbf{h}_i^{(t)}$:

$$\alpha_{ik}^{(t)} = \text{softmax}_k \left(\left\langle \mathbf{W}_{\text{query}} \mathbf{h}_i^{(t)}, \mathbf{W}_{\text{key}} \mathbf{h}_i^{(t)} \right\rangle \right)$$

where $\mathbf{W}_{\text{query}}$ and $\mathbf{W}_{\text{key}}$ are learnable linear transformations.
i.e. Nodes i, j are linked together ($\mathbf{\Pi}_{ij}^{(t)} = 1$) if they are (1) selected by the sparse mask (2) the most relevant to each other.

PGNs: P

In the previous work, P using MPNNs with U, M being linear layers with ReLU activation functions:

$$\mathbf{h}_i^{(t)} = U\left(\mathbf{z}_i^{(t)}, \bigoplus_{(j,i)\in E} M\left(\mathbf{z}_i^{(t)}, \mathbf{z}_j^{(t)}, \mathbf{e}_{ij}^{(t)}\right)\right).$$

In PGNs, P is also using MPNN with linear U, M with ReLU.

$$\mathbf{h}_i^{(t)} = U\left(\mathbf{z}_i^{(t)}, \bigoplus_{\mathbf{\Pi}_{ji}^{(t-1)}=1} M\left(\mathbf{z}_i^{(t)}, \mathbf{z}_j^{(t)}\right)\right),$$

where among all possible choices of aggregator $\bigoplus$, once again, (element-wise) max outperforms the rest.

Process Visualization

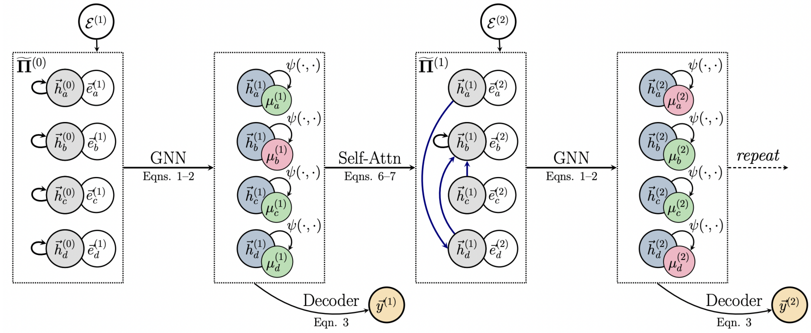


Figure: Visualization of pointer graph network (PGN) dataflow. (Figure 1 in the paper.)

Training Objectives

PGNs consider loss of three components at the same time:

- The downstream query loss in $\mathbf{y}^{(t)}$ prediction
- Difference between $\alpha^{(t)}$ and ground-truth pointers $\hat{\mathbf{\Pi}}^{(t)}$ (cross-entropy)
- Output from masking network ψ compared to ground-truth modification at time step t (binary cross-entropy)

Thereby, domain knowledge is introduced while training.

Task: Explanation

DSU: disjoint-set unions

QUERY-UNION(u, v) is called each step t, specified by

$$\mathbf{e}_i^{(t)} = r_i || \mathbb{I}_{i=u \vee i=v} \,,$$

- r_i: priority of node i
- $\mathbb{I}_{i=u \vee i=v}$: is node i being operated on?
- $\hat{\mathbf{y}}^{(t)}$: u, v in the same set?
- $\hat{\mu}_i^{(t)}$: node i visible by FIND(u) or FIND(v)?
- $\hat{\mathbf{\Pi}}_{ij}^{(t)}$: $\hat{\pi}_i = j$ after executing?

LCT: link/cut trees

QUERY-TOGGLE(u, v) is called each step t, specified by

$$\mathbf{e}_i^{(t)} = r_i || \mathbb{I}_{i=u \vee i=v} \,,$$

- r_i: priority of node i
- $\mathbb{I}_{i=u \vee i=v}$: is node i being operated on?
- $\hat{\mathbf{y}}^{(t)}$: u, v connected?
- $\hat{\mu}_i^{(t)}$: node i visible while executing?
- $\hat{\mathbf{\Pi}}_{ij}^{(t)}$: $\hat{\pi}_i = j$ after executing?

More Related Works

In Addition

More keywords: program synthesis, learning to execute, message-passing neural network, neural execution engines, etc.

Important previous works:

- Neural Programmer-Interpreters (ICLR'16)
- Deep Sets (NeurIPS'17)

Application to reinforcement learning:

- XLVIN: eXecuted Latent Value Iteration Nets (NeurIPS'20 Workshop)

Thank You! ☺