Algorithmic Reasoning with GNNs

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

Non-Markovian Inputs

GNNs typically overwrite their internal states in every step
- Previous applications: only latest version of the data relevant
- Here: queries require knowledge of previous versions of the data
- This places significant “pressure” on internal states

Current GNNs cannot explicitly memorize their past states

Persistent Message Passing

Idea: endow GNNs with an explicit, persistent memory
- Instead of overwriting nodes -> persisting nodes
- Paired with an efficient relevance / query mechanism
- Effectively an episodic memory of past computation

Strong performance on non-Markovian tasks

Task: Dynamic Range Minimum Queries

Compute (historic) minimum across ranges in continuously updated array

Solved by Segment Trees
- $O(\log n)$ query time
- Leaf nodes store array
- Intermediate nodes store minimum of children

Input Encoding

Initial connectivity

$$\Pi^{(0)} = \Pi$$
$$A^{(0)} = I$$

Node representations

$$u^{(t)} = \text{function}(\text{timestamp}(t), n^{(t-1)})$$
$$z^{(t)} = \text{function}(\text{expand}(z^{(t)}), n^{(t-1)})$$

Messages

Next-step candidates

$$\hat{z}^{(t)} = U \left( z^{(t)}, \max_{u^{(t-1)}} M \left( z^{(t)}, u^{(t-1)} \right) \right)$$

Relevance latents

$$\rho^{(t)} = U \left( u^{(t)}, \max_{v^{(t-1)}} M \left( v^{(t)}, u^{(t-1)} \right) \right)$$

Masking

$$\nu^{(t)} = \psi_{\text{random}}(\hat{z}^{(t)}), \in [0, 1]$$
$$\phi^{(t)} = \psi_{\text{random}}(\nu^{(t)}), \in [0, 1]$$

Persistency

- “Persist” selected nodes
- Original nodes untouched
- Track connectivity

Results

- PMP generalizes out-of-distribution to 2x larger test inputs
- Significantly outperforms GNNs which overwrite states
- Supervised on response (binary encoding), ground-truth masks, and node-values

https://arxiv.org/abs/2103.01043