Improving algorithmic alignment with autoregressive memory

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Introduction

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Algorithmic alignment

Definition 1

$\varepsilon > 0$ – error parameter, $\delta \in (0, 1)$ – error probability. $\{x_i, y_i\}_{i=1}^M$ – i.i.d from $\mathcal{D}$ and $y_i = g(x_i)$ for some function g. Let $f = \mathcal{A}(\{x_i, y_i\}_{i=1}^M)$ be the function generated by a learning algorithm $\mathcal{A}$. Then g is (M, ε, δ)-*learnable* with $\mathcal{A}$ if

$$\mathbb{P}_{x \sim \mathcal{D}} \left[\|f(x) - g(x)\| \leq \varepsilon \right] \geq 1 - \delta$$

Definition 2

Sample complexity $\mathcal{C}_{\mathcal{A}}(g, \varepsilon, \delta)$ is the minimum M so that g is (M, ε, δ)-learnable with $\mathcal{A}$.

Definition 3

Let g be a reasoning function, $\mathcal{N}$ – neural network with n modules $\mathcal{N}_i$. Module functions $f_1, \ldots, f_n$ generate g for $\mathcal{N}$ if, by replacing $\mathcal{N}_i$ with f_i, the network $\mathcal{N}$ simulates g. Then $\mathcal{N}$ (M, ε, δ)-*algorithmically aligns* with g if $f_1, \ldots, f_n$ generate g and there are learning algorithms $\mathcal{A}_i$ for the $\mathcal{N}_i$ such that $n \cdot \max_i C_{\mathcal{A}_i}(f_i, \varepsilon, \delta) \leq M$.

Algorithmic alignment impoves sample complexity

Theorem 1 (Keyulu Xu, et. al. 2020)

$\mathcal{A}$ – an overparameterized and randomly initialized 2-layer MLP trained with GD for a sufficient number of iterations. Suppose $g: \mathbb{R}^d \to \mathbb{R}^m$ with components $g(x)^{(i)} = \sum_j \alpha_j^{(i)} \left(\beta_j^{(i)\top} x\right)^{p_j^{(i)}}$, where $\beta_j^{(i)} \in \mathbb{R}^d,\ \alpha \in \mathbb{R}$ and $p_j^{(i)} = 1$ or $p_j^{(i)} = 2l,\ (l \in \mathbb{N})$. Then the sample complexity $\mathcal{C}(g, \varepsilon, \delta)$ is

$$\mathcal{C}_{\mathcal{A}}(g, \varepsilon, \delta) = O\left(\frac{\max_i \sum_{j=1}^{K} p_j^{(i)} |\alpha_j^{(i)}| \cdot \|\beta_j^{(i)}\|_2^{p_j^{(i)}} + \log(m/\delta)}{(\varepsilon/m)^2}\right)$$

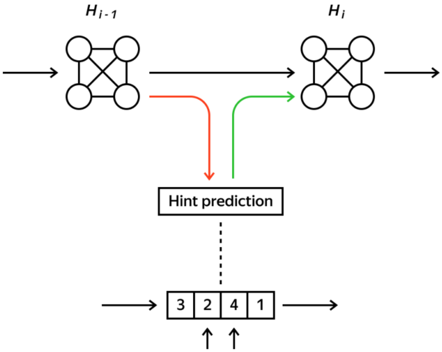
Theorem 2 (Keyulu Xu, et. al. 2020)

For some ε, δ suppose $\{S_i, y_i\}_{i=1}^{M} \sim \mathcal{D},\ |S_i| < N,\ y_i = g(S_i)$ for some g. Suppose $\mathcal{N}_1 \ldots \mathcal{N}_n$ are sequential MLP modules of $\mathcal{N}$. Suppose $\mathcal{N}$ and g (M, ε, δ)-algorithmically align via $f_1 \ldots f_n$. Then g is $(M, O(\varepsilon), O(\delta))$-learnable by $\mathcal{N}$.

Corollary 1

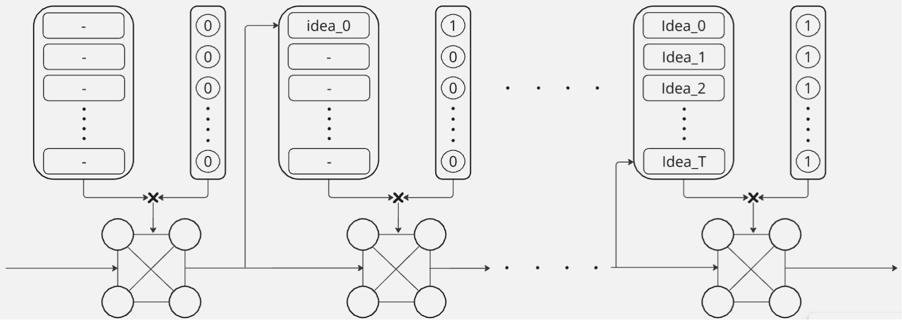
Suppose universe S has n objects $x_1 \ldots x_n$ and $g(S) = \sum_{i,j}(x_i - x_j)^2$. Then the sample complexity of MLP is $O(n^2)$ times larger than that of GNN.

Neural algorithmic reasoning, processor network



- Trained to follow trajectory of classical algorithm
- Aligns poorly with multiple algorithms at once
- Needs implicit hints on each step to enforce trajectory following

Processor network with autoregressive memory



$$L = -\sum_{X \in \mathcal{X}} \sum_{X_a \in \mathcal{X}_X} \log \frac{\exp\left(\sum_{t=1}^{T} \phi\left(M_t^X, M_t^{X_a}\right)\right)}{\exp\left(\sum_{t=1}^{T} \phi\left(M_t^X, M_t^{X_a}\right)\right) + \sum_{X_a \in \overline{\mathcal{X}_X}} \exp\left(\sum_{t=1}^{T} \phi\left(M_t^X, M_t^{\overline{X_a}}\right)\right)}$$

$\mathcal{X}$ – set of inputs, $M_t^X \in \mathbb{R}^k$ – the «idea» generated on step t for input X,
$\mathcal{X}_X$ – set of inputs similar to X, $\overline{\mathcal{X}_X}$ – set of inputs dissimilar to X

Processor network with autoregressive memory

- Mimics the step-by-step behaviour of classical algorithms not the exact trajectories
- Much less constraint compared to usual hint-prediction approach
- Does not require explicit hints
- Force processor to extract similar features («ideas») for similar algorithms at each step that might help with multi-algorithm learning