Some Mechanisms in Transformers and their Emergence

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Flatiron Institute, Simons Foundation

Foundation models for science workshop.
Flatiron Institute. April 30, 2025.

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w/ V. Cabannes, E. Dohmatob, D. Bouchacourt, H. Jégou, L. Bottou (Meta AI),
E. Nichani, Z. Wang, J. Lee (Princeton), L. Chen, D. Wu, J. Bruna (NYU), D. Hsu (Columbia)

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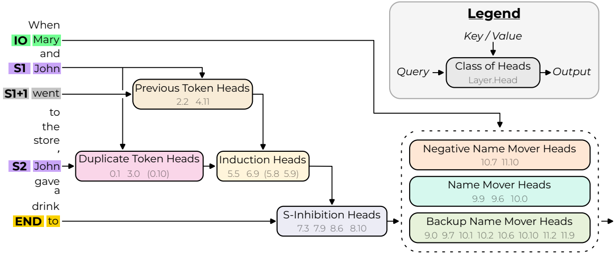
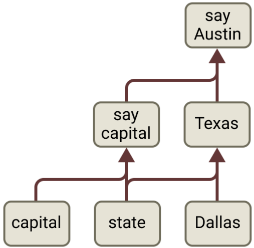
Mechanisms inside Transformer LLMs

Reasoning over context

- Circuits of attention heads (Elhage et al., 2021; Olsson et al., 2022; Wang et al., 2022)
- A "biology" of circuits found by mechanistic interpretability (*e.g.*, Anthropic, 2025)





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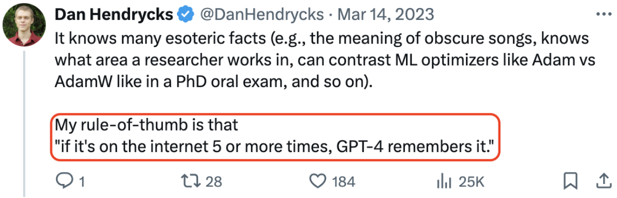
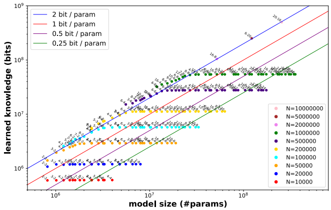
Knowledge storage

- Memorization, factual recall, parameter scaling
  - (Geva et al., 2020; Meng et al., 2022; Allen-Zhu and Li, 2024)
- Learn rules that help higher-level reasoning





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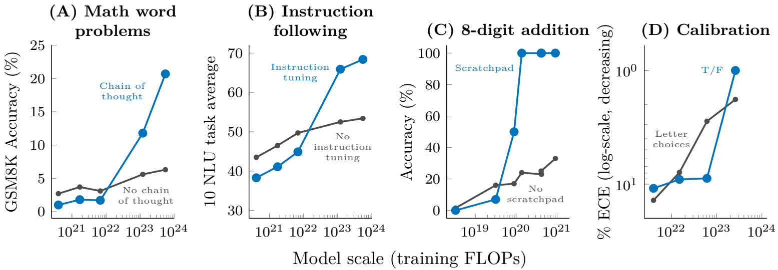
Q: How do these arise during training?

Emergence and training dynamics

Emergent capabilities and sequential learning (Wei et al. 2022; Power et al., 2022; Saxe et al. 2013)



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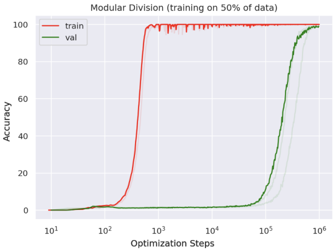

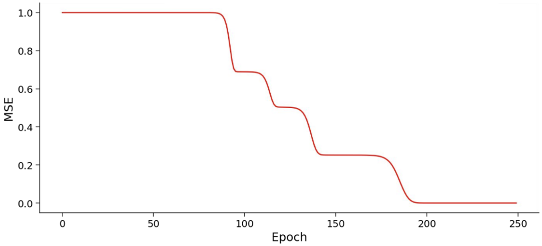

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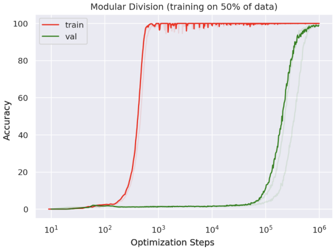

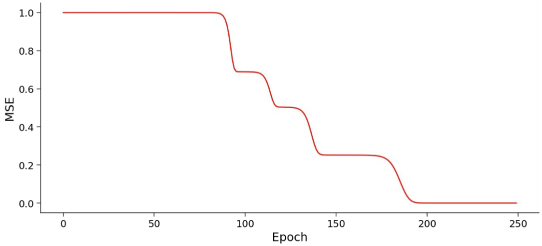

Why do we care about understanding?

- Highlight role of **data**, training **algorithm**, **architecture**
- $\Longrightarrow$ improve training methodology

Transformer setup

Input: sequence of discrete tokens $(z_1, \dots, z_T) \in [N]^T$

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Residual streams (Elhage et al., 2021)

- embed each token $z_t \in [N]$ as $x_t := e_{z_t} + p_t$
- (causal) self-attention $x_t := x_t + \mathrm{MHSA}(x_t, x_{1:t})$

$$\mathrm{MHSA}(x_t, x_{1:t}) = \sum_{h=1}^{H} \sum_{s=1}^{t} \beta_s^h W_O^{h\top} W_V^h x_s, \quad \text{with } \beta_s^h = \frac{\exp(x_s^\top W_K^{h\top} W_Q^h x_t)}{\sum_{s=1}^t \exp(x_s^\top W_K^{h\top} W_Q^h x_t)}$$

where $W_K, W_Q, W_V, W_O \in \mathbb{R}^{d_h \times d}$ (key/query/value/output matrices)

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- feed-forward $x_t := x_t + \mathrm{MLP}(x_t)$

$$\mathrm{MLP}(x_t) = V^\top \sigma(U x_t)$$

where $U, V \in \mathbb{R}^{m \times d}$, often $m = 4d$

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Next-token prediction

- cross-entropy loss

$$\sum_{t<T} \ell(z_{t+1}; ({u_j}^\top x_t)_j)$$

Outline

1. Memorization and factual recall

2. In-context reasoning

Weights as associative memories

- Consider sets of **nearly orthonormal embeddings** $\{e_z\}_{z \in \mathcal{Z}}$ and $\{u_y\}_{y \in \mathcal{Y}}$:

$$\|e_z\| \approx 1 \quad \text{and} \quad {e_z}^\top e_{z'} \approx 0$$
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$$W = \sum_{(z,y) \in \mathcal{M}} \alpha_{zy} u_y {e_z}^\top$$

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  - Logits in attention heads: $x_k^\top W_{KQ} x_q$
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- Related to Hopfield (1982); Kohonen (1972); Willshaw et al. (1969); Iscen et al. (2017)

Gradients lead to associative memories

Lemma (Gradients as memories, B. et al., 2023)

Let p be a data distribution over $(z, y) \in [N]^2$, and consider the loss

$$L(W) = \mathbb{E}_{(z,y)\sim p}[\ell(y, F_W(z))], \quad F_W(z)_k = {u_k}^\top W e_z,$$

with ℓ the ***cross-entropy loss*** *and e_z, u_k input/output embeddings.*

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Note: related to (Ba et al., 2022; Damian et al., 2022; Oymak et al., 2023; Yang and Hu, 2021)

Application to factual recall: toy model

$$z_1 \cdots z_{i-1} \; s \; z_{i+1} \cdots z_{j-1} \; r \; z_{j+1} \cdots z_{T-1} \; \text{EOS} \longrightarrow a^*$$

The capital of France is Paris

- $s \in \mathcal{S}$: subject token
- $r \in \mathcal{R}$: relation token
- $a^*(s, r) \in \mathcal{A}_r$: attribute/fact to be stored
- $z_i \in \mathcal{N}$: noise tokens

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Q: How do Transformers solve this?

Two mechanisms

- One-layer Transformer, with or without MLP, random embeddings
- Embedding dimension d, head dimension d_h, MLP width m, H heads

Theorem (Nichani et al., 2024, informal)

A one-layer Transformer with or without MLP can achieve perfect factual recall with $\tilde{O}(SR)$ parameters. (note: attention-only needs large enough d)

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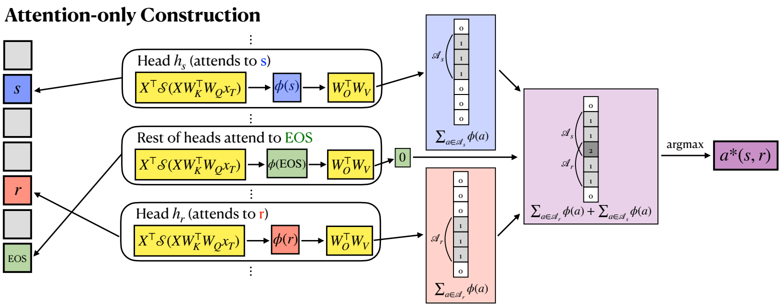

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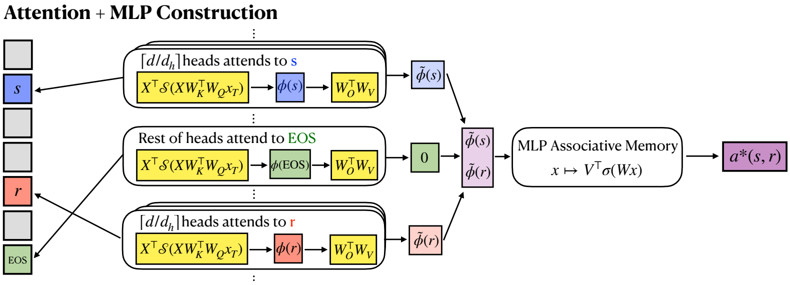

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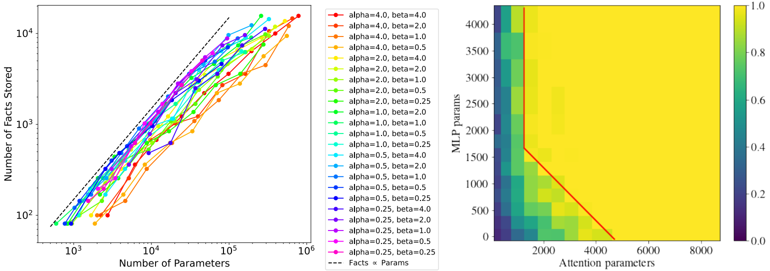

Training dynamics

- One-layer Transformer with **linear attention** and **one-hot** embeddings
- Gradient flow with initialization $W_{OV}(a, z), w_{KQ}(z) \approx \alpha > 0$

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- *There is global convergence to zero loss*
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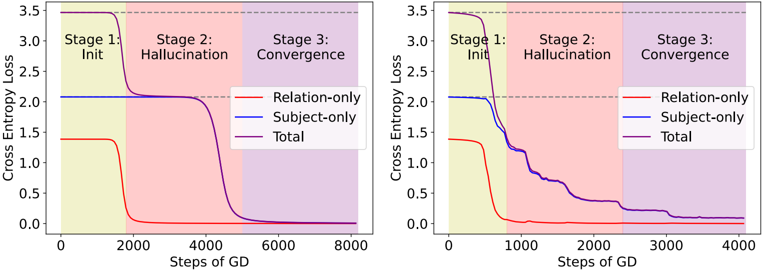
- *There is an intermediate phase where the model predicts using $p(a|r)$ instead of $p(a|s, r)$*

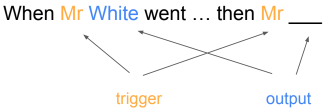
- Intermediate phase corresponds to **hallucination** (uniform over $\mathcal{A}_r$, ignoring s)



Outline

1. Memorization and factual recall
2. In-context reasoning

The bigram data model for in-context reasoning



When Mr White went to the mall, it started raining, then Mr White witnessed an odd occurrence. While walking around the mall with his family, Mr White heard the sound of a helicopter landing in the parking lot. Curious, he made his way over to see what was going on.

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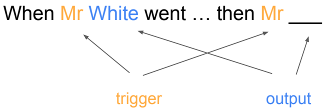

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Fix **trigger tokens**: $q_1, \dots, q_K$

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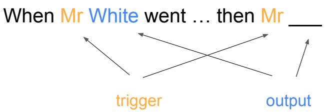

When Mr White went to the mall, it started raining, then Mr White witnessed an odd occurrence. While walking around the mall with his family, Mr White heard the sound of a helicopter landing in the parking lot. Curious, he made his way over to see what was going on.

Fix **trigger tokens**: $q_1, \ldots, q_K$

Sample each sequence $z_{1:T} \in [N]^T$ as follows

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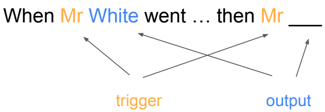

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$$p(j|i) = \begin{cases} \mathbb{1}\{j = o_k\}, & \text{if } i = q_k, \quad k = 1, \dots, K \\ \pi_b(j|i), & \text{o/w.} \end{cases}$$

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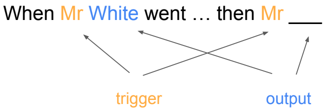

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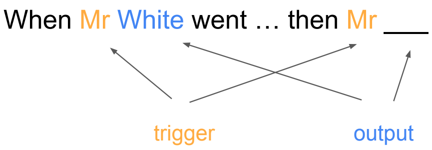
π_b: **global bigrams** model (estimated from Karpathy's character-level Shakespeare)

Transformers on the bigram task



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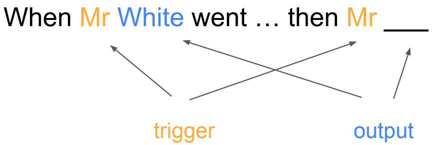

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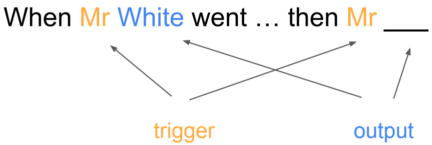

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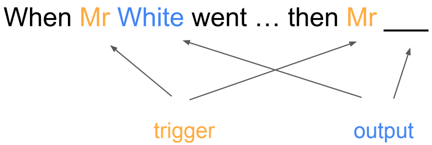

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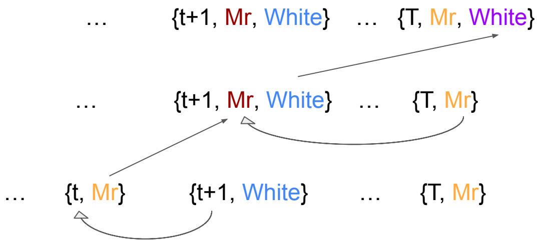
See (Sanford, Hsu, and Telgarsky, 2023, 2024b) for representational lower bounds

Induction head mechanism (Elhage et al., 2021; Olsson et al., 2022)



- 1st layer: **previous-token head**
  - attends to previous token and copies it to residual stream

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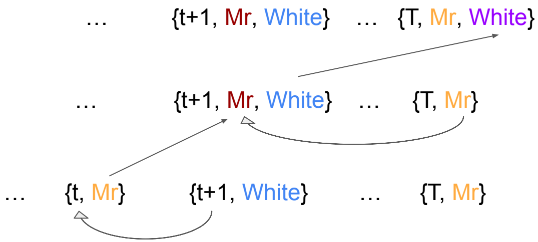

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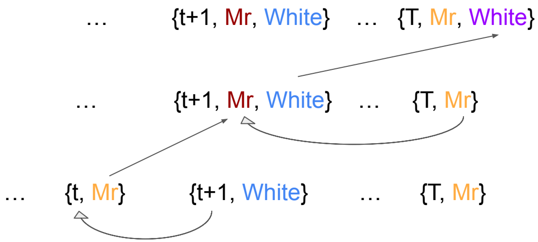

- 1st layer: **previous-token head**
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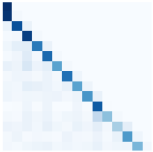
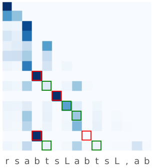
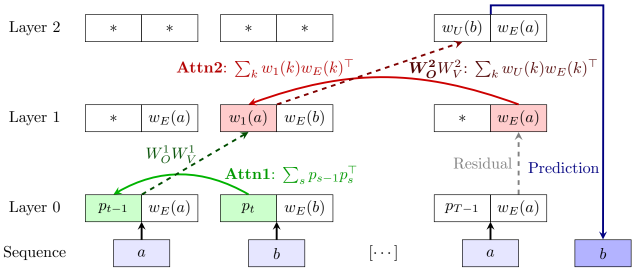
- Matches observed attention scores:





Induction head with associative memories



$$W_{KQ}^1 = \sum_{t=2}^{T} p_t p_{t-1}^\top, \quad W_{KQ}^2 = \sum_{k \in Q} e_k \tilde{e}_k^\top, \quad W_{OV}^2 = \sum_{k=1}^{N} u_k e_k^\top,$$

- Random embeddings e_k, u_k, random matrix W_{OV}^1 (frozen at init)
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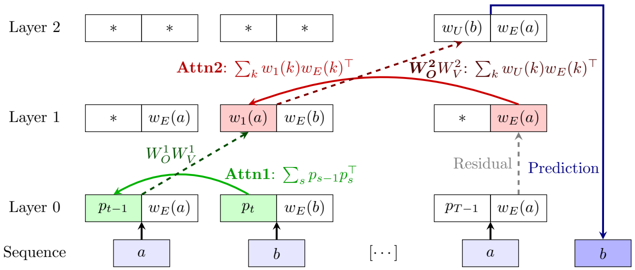

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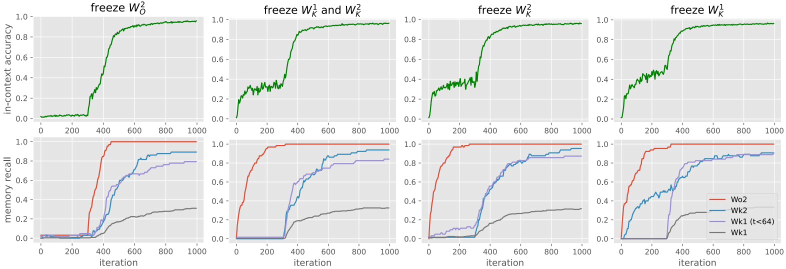
Q: Does this match practice?

Empirically probing the dynamics

Train only W_{KQ}^1, W_{KQ}^2, W_{OV}^2, loss on predictable tokens after trigger



- "Memory recall **probes**": for target memory $W_* = \sum_{i=1}^M u_i e_i^\top$, compute

$$R(\hat{W}, W_*) = \frac{1}{M} \sum_{i=1}^{M} \mathbb{1}\{i = \arg\max_j u_j^\top \hat{W} e_i\}$$

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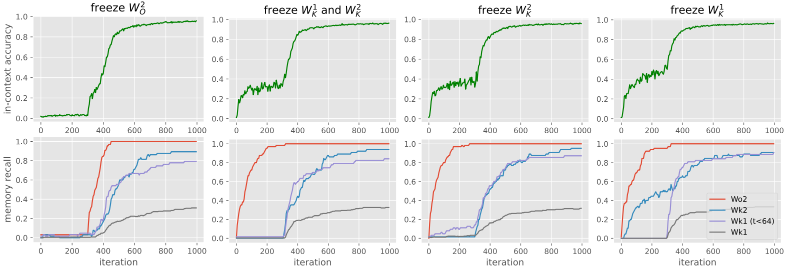

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- Natural learning “**order**”: W_{OV}^2 first, W_{KQ}^2 next, W_{KQ}^1 last
- Joint learning is faster

Gradient steps for the bigram task

Theorem (B. et al., 2023, informal)

In a simplified setup, we can recover the desired associative memories with ***3 sequential gradient steps*** *on the population loss: first on* W_{OV}^2, *then* W_{KQ}^2, *then* W_{KQ}^1.

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Key ideas

- Attention is uniform at initialization $\implies$ inputs are sums of embeddings
- W_{OV}^2: correct output appears w.p. 1, while other tokens are noisy and cond. indep. of z_T
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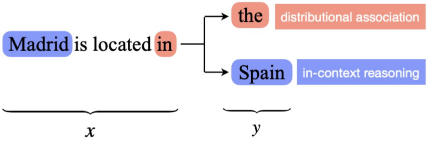
see also (Snell et al., 2021; Oymak et al., 2023)

Distributional vs in-context associations



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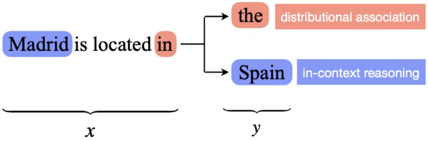

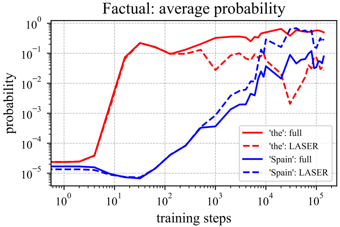

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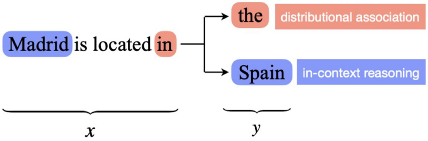

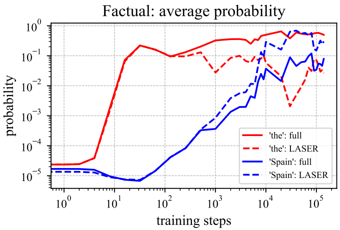

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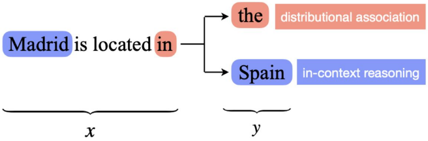

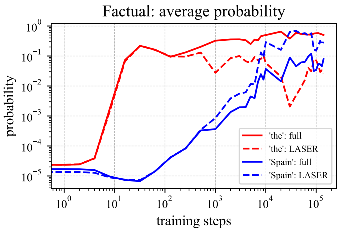

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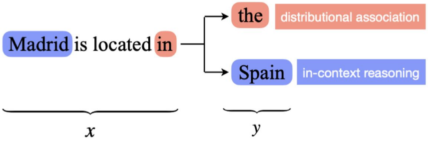

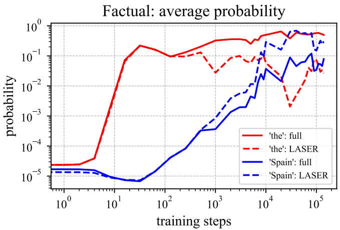

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Theorem (Chen, Bruna, and B., 2024, informal)

In toy model above, feed-forward layer learns global bigram after $O(1)$ samples, attention after $O(N)$ samples due to noise.

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- Composition of multiple statements given in context. Example:

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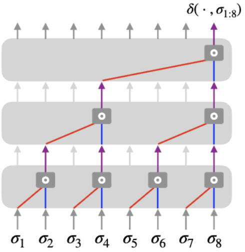

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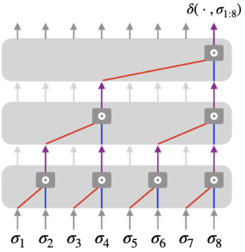

Q: what about training dynamics?

Training dynamics for k-hop reasoning

Failure of gradient descent (based on statistical query model)

Theorem (Wang, Nichani, et al., 2025+, informal)

Gradient descent requires either $\exp(k)$ *samples or* $\exp(k)$ *compute to solve the* k*-hop task.*

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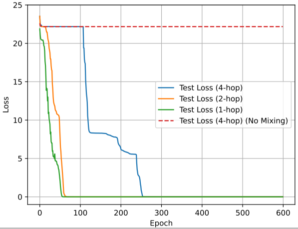

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Thank you!

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