Associative Memories as a Building Block in Transformers

Alberto Bietti

Flatiron Institute, Simons Foundation

AI + Physics Workshop, CUNY, September 2025

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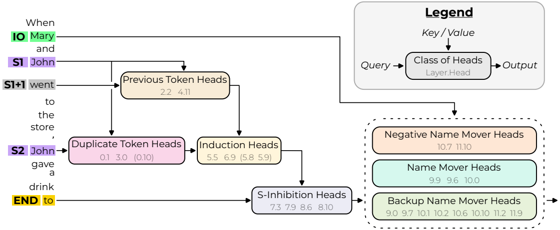
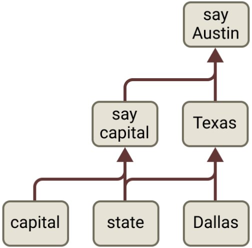
w/ V. Cabannes, E. Dohmatob, D. Bouchacourt, H. Jégou, L. Bottou (Meta),
E. Nichani, J. Lee (Princeton)

What are Transformer LLMs doing?

Reasoning over context

- A “biology” of circuits (Elhage et al., 2021; Wang et al., 2022), (Anthropic, 2025)
- Many results on expressivity (e.g., circuits, formal languages, graph algorithms)
  - e.g., (Merrill et al., 2022; Liu et al., 2023; Sanford et al., 2023)





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- Memorization, factual recall, parameter scaling
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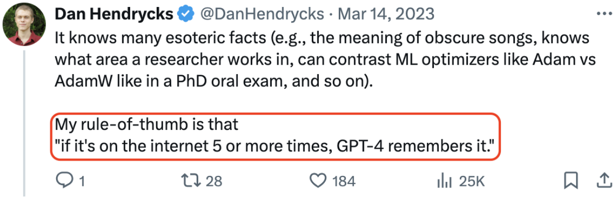
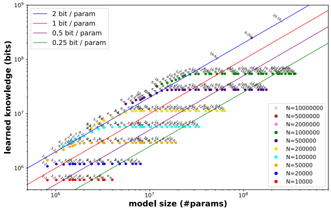
- Allows higher-level reasoning





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Goal: tractable model for both + training dynamics?

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

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- input e_z, positional p_t, output u_y, in $\mathbb{R}^d$
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- 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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$$\mathrm{MLP}(x_t) = V^\top \sigma(U x_t)$$

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. Associative memories
2. Application to Transformers I: in-context reasoning (B. et al., 2023)
3. Application to Transformers II: factual recall (Nichani et al., 2025)

Associative memories: background

Hopfield nets (Hopfield, 1982)

- Store N patterns $\xi_i \in \{\pm 1\}^d$ using Hebb's rule:

$$W = \sum_{i=1}^{N} \xi_i \xi_i^\top \in \mathbb{R}^{d \times d}$$

- Recover pattern from corrupted version by iterating: $x' = \text{sign}(Wx)$

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- Can store $N = \tilde{\Theta}(d)$ patterns (Amit et al., 1985; McEliece et al., 1988)

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Modern Hopfield nets (a.k.a dense associative memories)

- Improve capacity through higher-order energy function
  - (Krotov and Hopfield, 2016; Demircigil et al., 2017; Lucibello and Mézard, 2024)
- e.g., capacity d^{k-1} when using energy $E(x) = -\sum_{i=1}^{N} (\xi_i^\top x)^k$

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Attention as associative memory

- Softmax attention as one step retrieval in dense associative memory over **context**
  - Ramsauer et al. (2020); Hoover et al. (2023)
  - Smart, B., and Sengupta (2025): emerges from in-context denoising

Transformer 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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Examples in Transformers

- e_z, u_y are input/output/positional embeddings, or intermediate representations
- Logits in attention heads: $x_k^\top W_{KQ} x_q$
- Logits in next-token prediction: $u_y^\top U \sigma(V x_t)$ or $u_y^\top W_{OV} x_k$

Gradient 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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  - After **one gradient step** on the population loss, assuming near-orthonormal embeddings

$$W_1 = \frac{\eta}{N} \sum_{z,k} \left(\mathbb{1}\{f_*(z) = k\} - \frac{1}{N} \right) u_k e_z{}^\top \quad \Longrightarrow \quad u_k{}^\top W_1 e_z \approx \frac{\eta}{N} \left(\mathbb{1}\{f_*(z) = k\} - \frac{1}{N} \right)$$

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

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  - $f^*(z) \in \{0, 1\}$: can store up to $N \approx d$ associations
  - Scaling laws: store the most frequent tokens with under-parameterized model

Capacity $\approx$ number of parameters

Low-rank

- $W = W_1^\top W_2$, with $W_1, W_2 \in \mathbb{R}^{m \times d}$ (e.g., key-query or output-value matrices)
- can store $N \approx md$ associations when $m \leq d$
- construction: random W_1, one step on W_2

(Nichani, Lee, and B., 2025), related to Krotov and Hopfield (2016); Demircigil et al. (2017)

Capacity ≈ number of parameters

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Non-linear MLP

- $\hat{f}(z) = \arg\max_y u_y{}^\top W_1 \sigma(W_2^\top e_z)$, $W_1, W_2 \in \mathbb{R}^{d \times m}$
- can store $N \approx md$ associations for any width m
- construction: using Hermite polynomials of degree $\approx \log N / \log d$ in kernel regime

(Nichani, Lee, and B., 2025), related to Krotov and Hopfield (2016); Demircigil et al. (2017)

Capacity ≈ number of parameters

Low-rank

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Note: matches information-theoretic lower bounds

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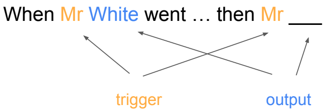
Outline

1. Associative memories
2. Application to Transformers I: in-context reasoning (B. et al., 2023)
3. Application to Transformers II: factual recall (Nichani et al., 2025)

The bigram data model for in-context reasoning

Goal: capture both in-context and global knowledge (*e.g.*, nouns vs syntax)



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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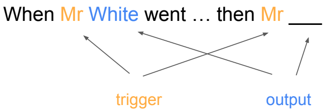

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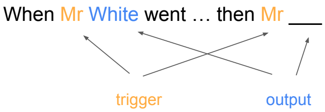

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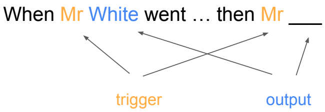

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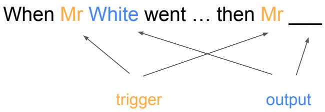

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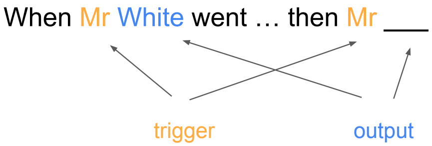
π_b: **global bigrams** model (estimated from Karpathy's character-level Shakespeare)

Transformers on the bigram task

When Mr White went … then Mr ___

trigger output

Transformers on the bigram task



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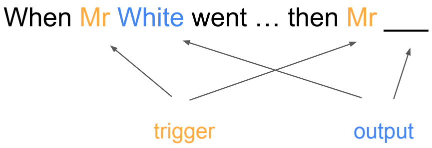

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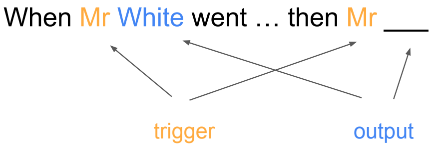

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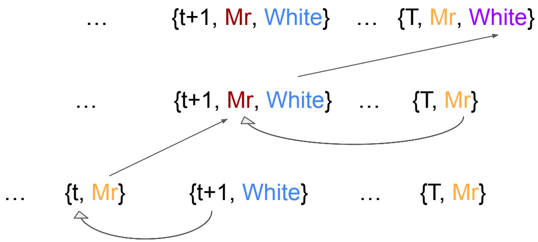
See (Sanford, Hsu, and Telgarsky, 2023, 2024) for representational lower bounds

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



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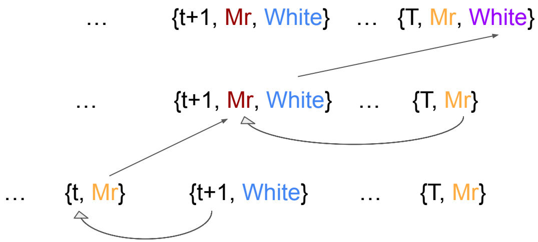

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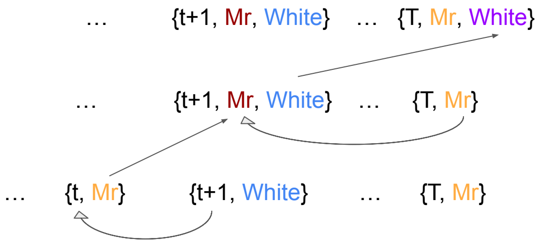

- 1st layer: **previous-token head**
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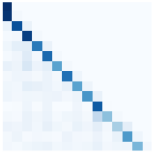
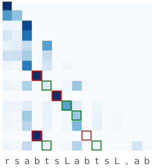
- Matches observed attention scores:





Random embeddings in high dimension

- We consider **random** embeddings u_i with i.i.d. $\mathcal{N}(0, 1/d)$ entries and d large

$$\|u_i\| \approx 1 \quad \text{and} \quad u_i^\top u_j = O(1/\sqrt{d})$$

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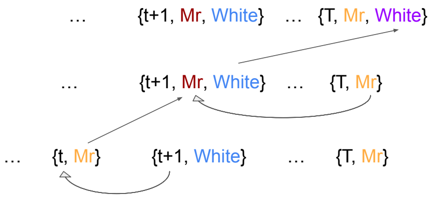
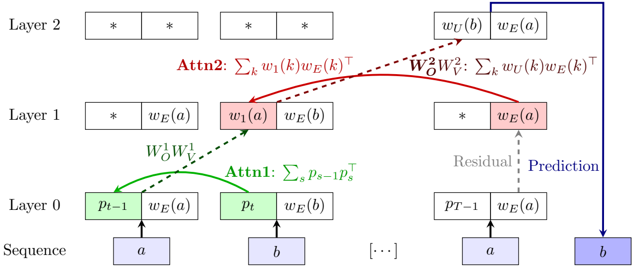
- Value/Output matrices help with token **remapping**: Mr $\mapsto$ Mr, White $\mapsto$ White



Induction head with associative memories



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

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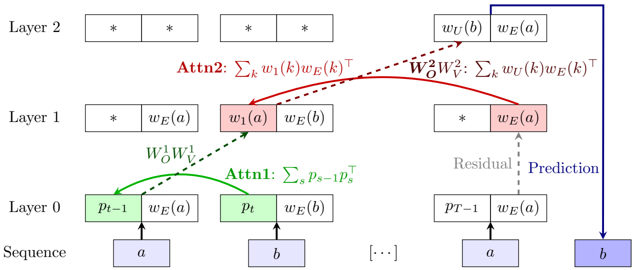

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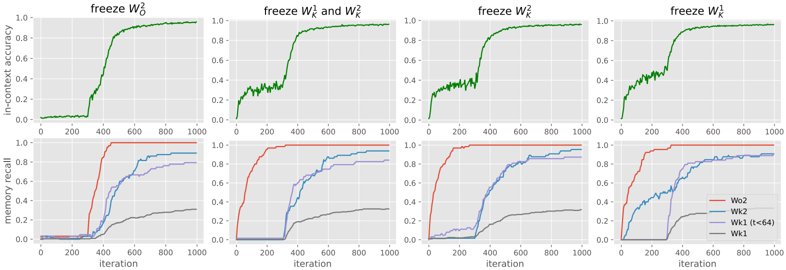
Q: Does this match practice?

Empirically probing the dynamics

Train only W_{KQ}^1, W_{KQ}^2, W_{OV}^2, loss on deterministic output tokens only



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

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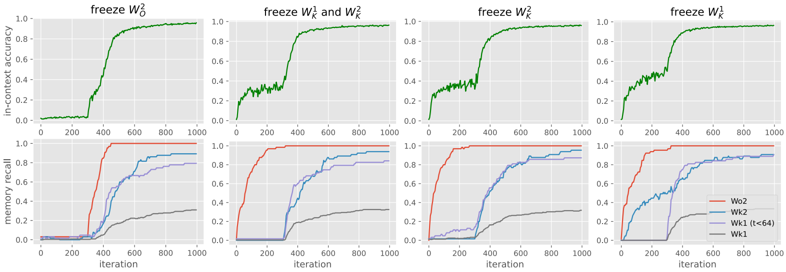

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- Natural learning "**order**": W^2_{OV} first, W^2_{KQ} next, W^1_{KQ} last
- Joint learning is faster

Gradient steps for the bigram task

Setting: transformer on the bigram task

- Focus on predicting second output token
- All distributions are uniform
- Some simplifications to architecture
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*In the setup above, we can recover the desired associative memories with **3 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
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- Extension to multi-hop with curriculum (Wang et al., 2025):

John holds the apple. John is in the kitchen. Where is the apple?

Key idea: gradient associative memories with noisy inputs

Insight: residual streams, attention output at init, are noisy sums of embeddings

Lemma (Gradients with noisy inputs, B. et al., 2023)

Let p be a data distribution over $(x, y) \in \mathbb{R}^d \times [N]$, and consider the loss

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

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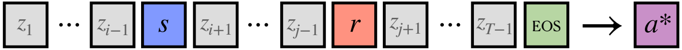
- Similar arguments for attention matrices

Outline

Toy model of factual recall



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
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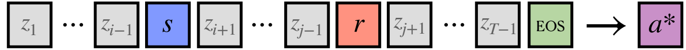

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Q: How many parameters do Transformers need to solve this?

How many parameters do we need?

- 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., 2025, informal)

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- Total parameters scale with number of facts SR (up to $A_{\max}$)
- Constructions are based on associative memories
- Attention-only needs large enough d
- Noise is negligible (log factors)

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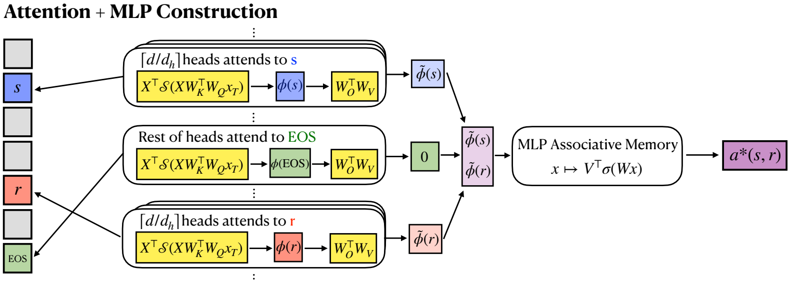

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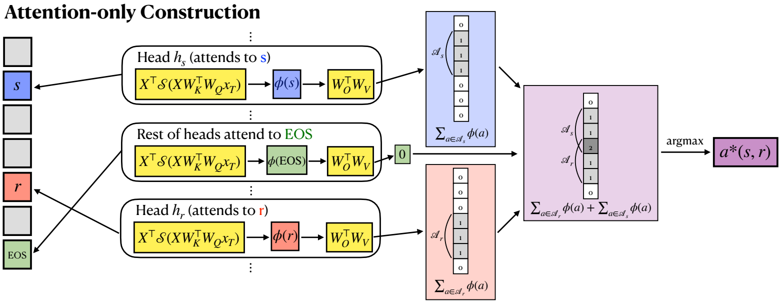
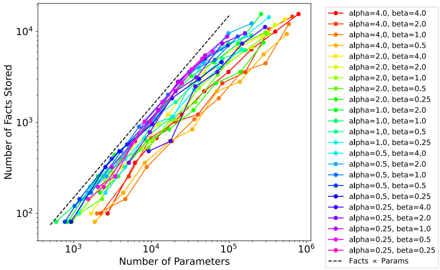


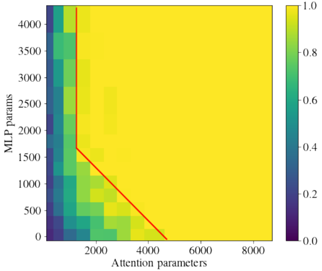
How many parameters do we need?

- 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., 2025, informal)

- *Attention + MLP:* $Hd_h \gtrsim S + R$ *and* $md \gtrsim SR$ *succeeds*
- *Attention-only:* $d \gtrsim R + A_{\max}$ *and* $Hd_h \gtrsim S + R$ *succeeds* ($A_{\max} := \max_r |\mathcal{A}_r|$)





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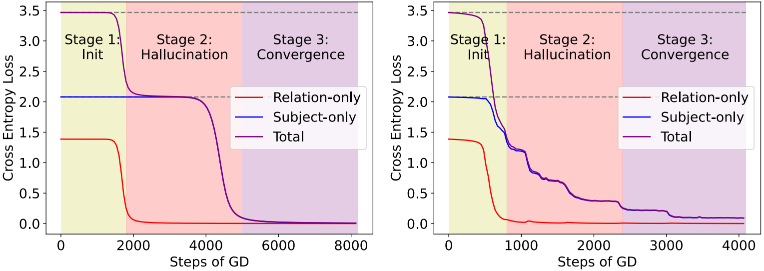
- Intermediate phase corresponds to **hallucination** (over $\mathcal{A}_r$, ignoring s)



Concluding remarks

Transformer weights as associative memories

- Storage capacity and gradient-based learning
- Toy models of reasoning and factual recall

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- Fine-grained optimization for multiple layers
- Analysis for more general tasks
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Thank you!

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Assume $d \gg \sqrt{N} \gg 1$ and $n \gg N$. The Transformer learns the desired mapping iff

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- If $T = \Theta(1)$, $d \gg \sqrt{N}$ is enough
- If $T \gg 1$, need $d \gg \sqrt{N}$ is **not** enough unless n is very large

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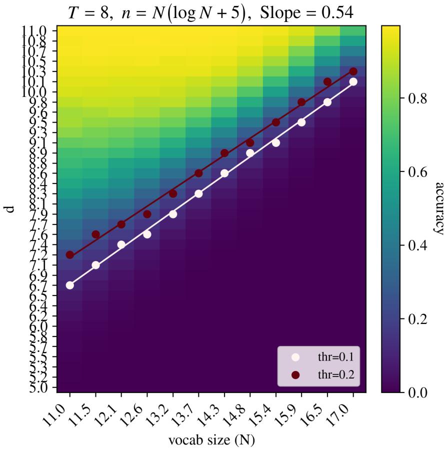

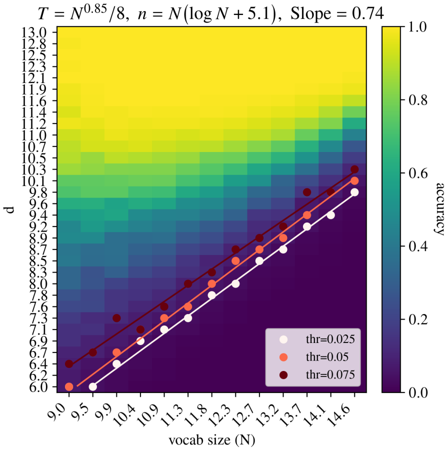

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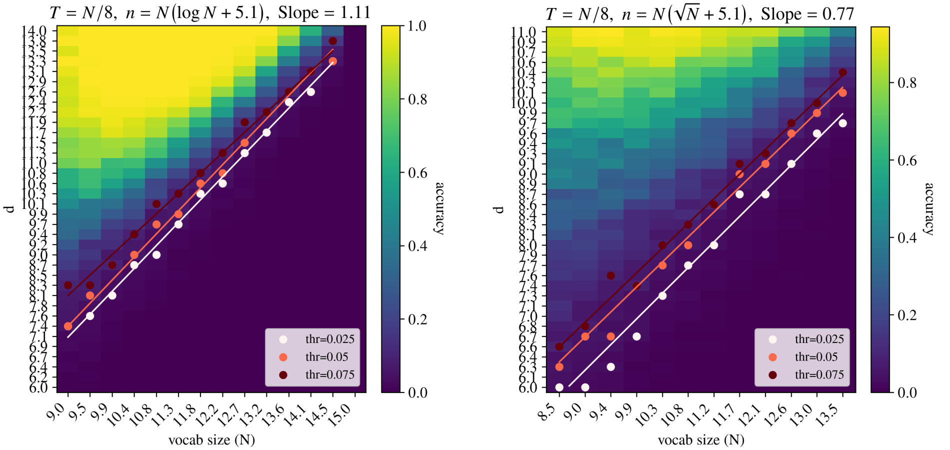

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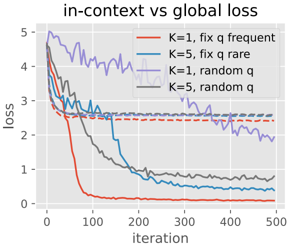

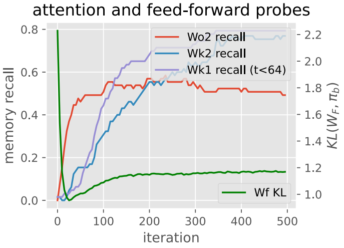

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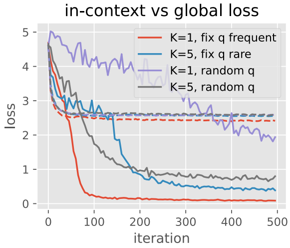

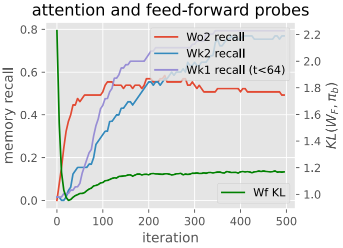

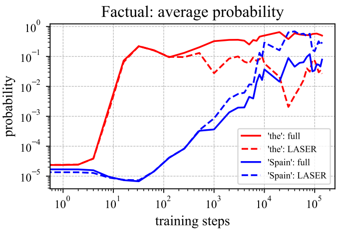

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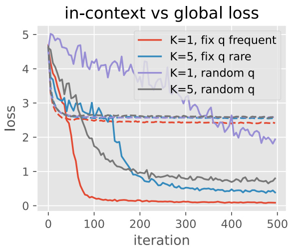

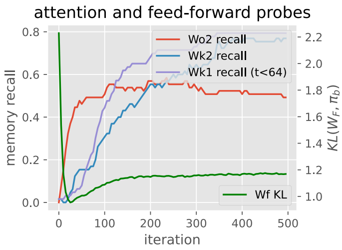

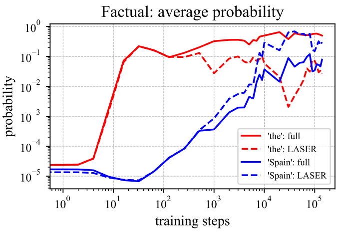

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Theorem (Chen et al., 2024, informal)

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

Setup with heavy-tailed data

Setting

- $z_i \sim p(z)$, $y_i = f^*(z_i)$, n samples: $S_n = \{z_1, \ldots, z_n\}$, 0/1 loss:

$$L(\hat{f}_n) = \mathbb{P}(y \neq \hat{f}_n(z))$$

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- **Q: What about finite capacity?**

Scaling laws with finite capacity

- Random embeddings $e_z, u_y \in \mathbb{R}^d$ with $\mathcal{N}(0, 1/d)$ entries
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- $n^{-\frac{\alpha-1}{\alpha}}$ is the same as (Hutter, 2021)
- $q = 1$ is best if we have enough capacity
- Can store at most d memories (approximation error: $d^{-\alpha+1}$)

Scaling laws with optimization algorithms

$$L(W) = \mathbb{E}_{z \sim p}[\ell(f^*(z), UWe_z)] \qquad \rightarrow \qquad W_{n,d} \approx \sum_{z=1}^{N} q(z) u_{f^*(z)} e_z{}^\top$$

Different algorithms lead to different memory schemes $q(z)$:

Scaling laws with optimization algorithms

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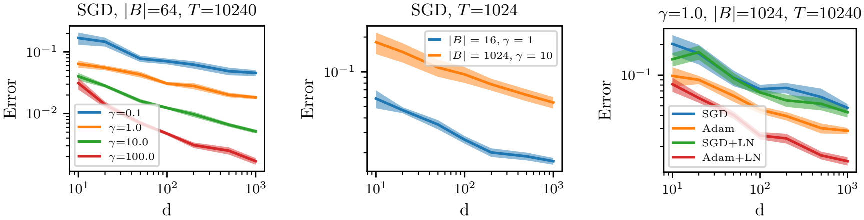

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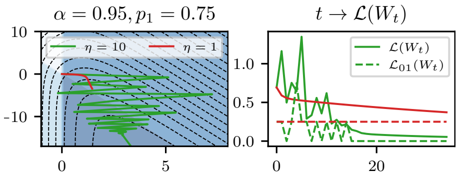

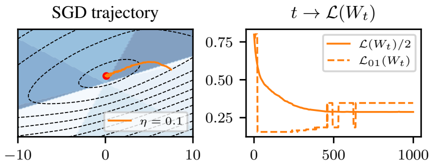

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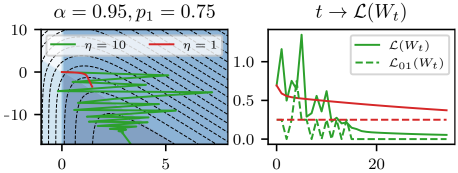

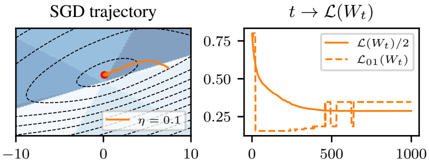

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