Associative Memories as a Building Block in Transformers

Alberto Bietti

Flatiron Institute, Simons Foundation

Cargèse, August 2025

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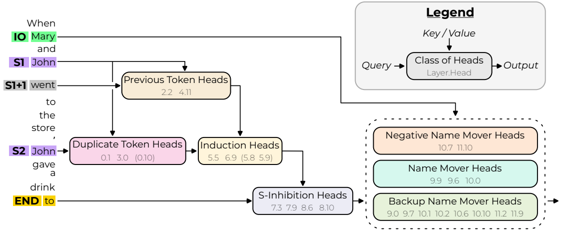
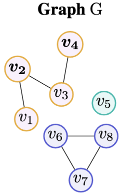
w/ V. Cabannes, E. Dohmatob, D. Bouchacourt, H. Jégou, L. Bottou (Meta), E. Nichani, J. Lee (Princeton), M. Vural (U Toronto), D. Wu (NYU/Flatiron)

What are Transformer LLMs doing?

Reasoning over context

- Circuits of attention heads (Elhage et al., 2021; Olsson et al., 2022; Wang et al., 2022)
- Many results on expressivity (e.g., circuits, formal languages, graph connectivity)
  - e.g., (Merrill et al., 2022; Liu et al., 2023; Sanford et al., 2023)





Task: Are v_2 and v_4 connected?

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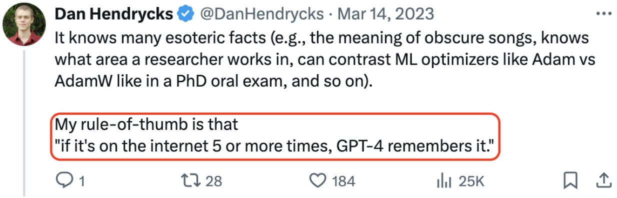
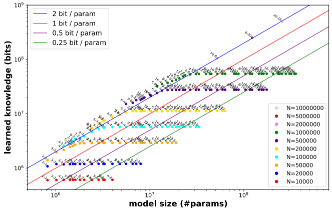
- Allows higher-level reasoning





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Goal: tractable model for both + training dynamics?

Transformer language models

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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- 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. Associative memories
2. Application to Transformers I: factual recall (Nichani et al., 2024)
3. Application to Transformers II: reasoning / retrieval (B. et al., 2023; Vural 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: $x' = \mathrm{sign}(Wx)$

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- Iterates descend on a quadratic energy landscape $E(x) = -x^\top W x$
- 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); 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: $u_y^\top U\sigma(Vx_t)$ 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

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

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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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- Random embeddings $e_z, u_y \sim \mathcal{N}(0, \frac{1}{d} I)$

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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., 2024), related to Krotov and Hopfield (2016); Demircigil et al. (2017)

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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., 2024), related to Krotov and Hopfield (2016); Demircigil et al. (2017)

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)
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Non-linear MLP

- $\hat{f}(z) = \arg\max_y u_y{}^\top W_1 \sigma(W_2^\top e_z)$, $W_1, W_2 \in \mathbb{R}^{d \times m}$
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Note: matches information-theoretic lower bounds

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Outline

Toy model of factual recall

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

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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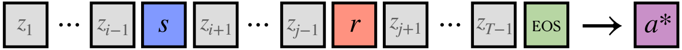

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Q: How many parameters do Transformers need to solve this?

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., 2024, informal)

- *Attention + MLP:* $Hd_h \gtrsim S + R$ *and* $md \gtrsim SR$ *succeeds*
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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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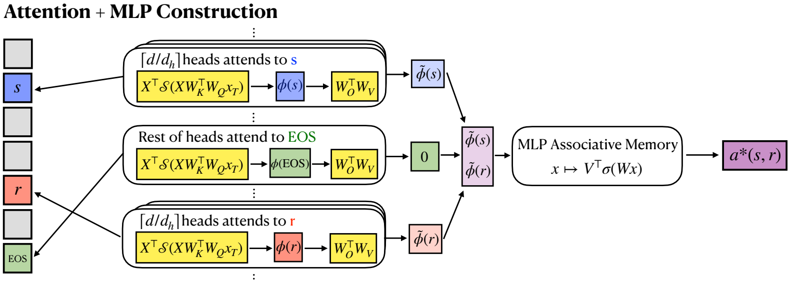

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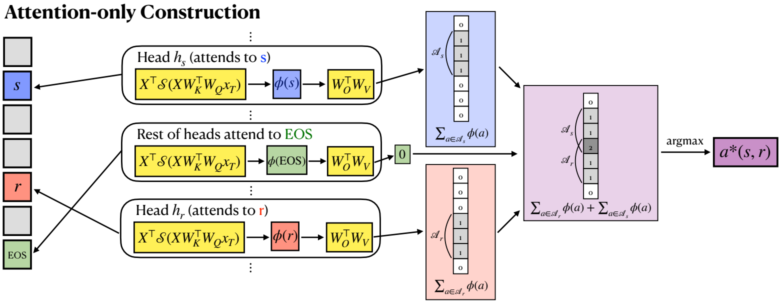

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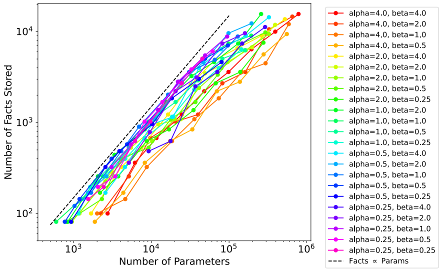

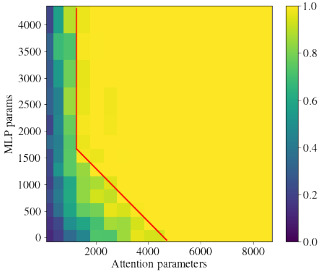

Training dynamics

- One-layer Transformer with **linear attention** and **one-hot** embeddings
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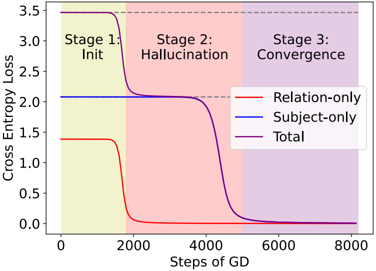
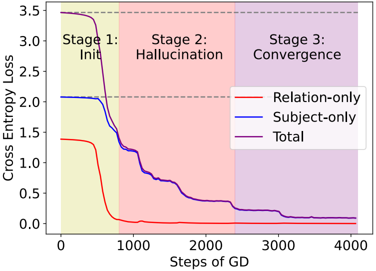
- Intermediate phase corresponds to **hallucination** (over $\mathcal{A}_r$, ignoring s)



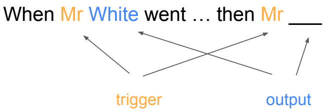


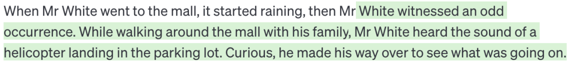
Outline

1. Associative memories
2. Application to Transformers I: factual recall (Nichani et al., 2024)
3. Application to Transformers II: reasoning / retrieval (B. et al., 2023; Vural et al., 2025+)

The bigram data model for in-context reasoning

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





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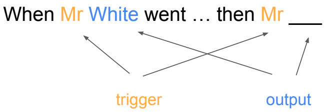

When Mr White went to the mall, it started raining, then Mr White witnessed an odd occurrence. While walking around the mall with his family, Mr White heard the sound of a helicopter landing in the parking lot. Curious, he made his way over to see what was going on.

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

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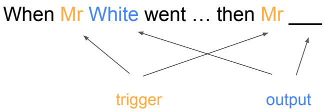

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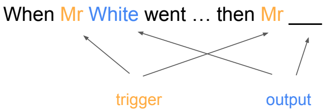

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$$p(j|i) = \begin{cases} \mathbb{1}\{j = o_k\}, & \text{if } i = q_k, \quad k = 1, \dots, K \\ \pi_b(j|i), & \text{o/w.} \end{cases}$$

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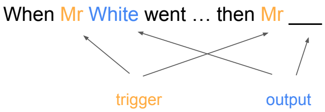

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π_b: **global bigrams** model (estimated from Karpathy's character-level Shakespeare)

Transformers on the bigram task

When Mr White went … then Mr ___

trigger output

Transformers on the bigram task

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- **1-layer transformer fails**: $\sim 55\%$ accuracy on in-context output predictions

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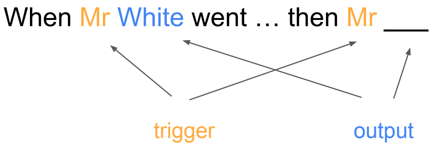

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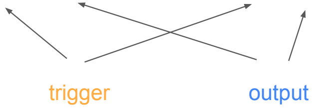

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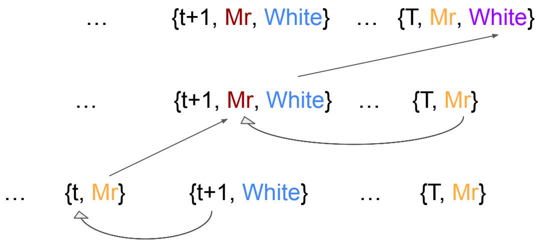
See (Sanford, Hsu, and Telgarsky, 2023, 2024) for representational lower bounds

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



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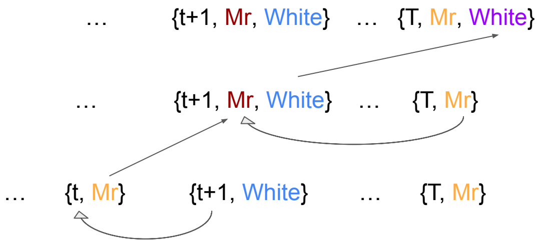

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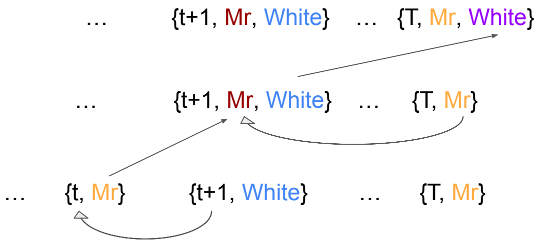

- 1st layer: **previous-token head**
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- 2nd layer: **induction head**
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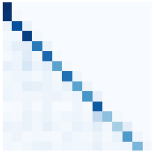
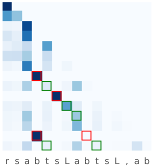
- Matches observed attention scores:





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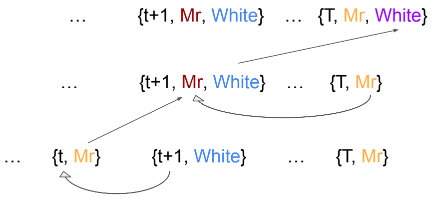
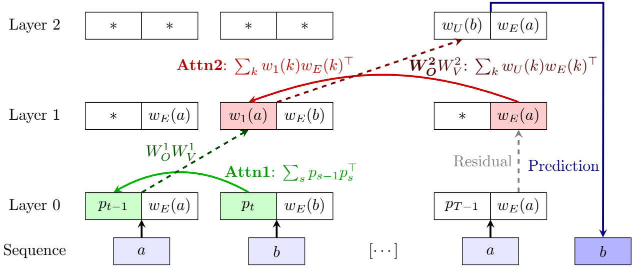
- Value/Output matrices help with token **remapping**: Mr $\mapsto$ Mr, White $\mapsto$ White



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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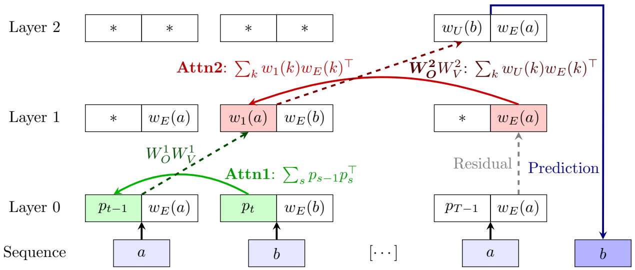

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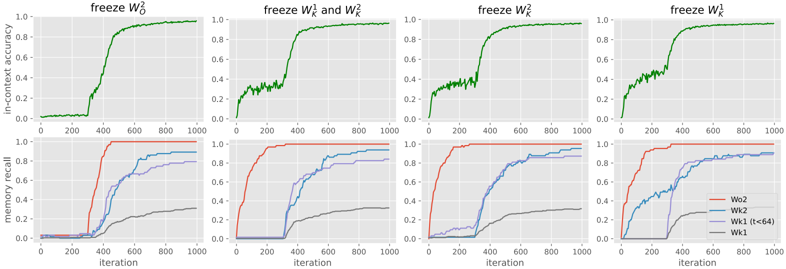
Q: Does this match practice?

Empirically probing the dynamics

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



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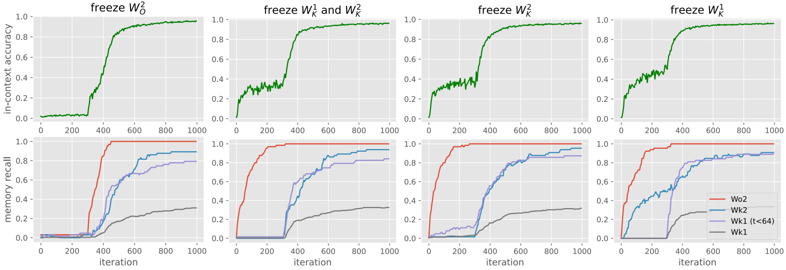

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- Natural learning "**order**": W_{OV}^2 first, W_{KQ}^2 next, W_{KQ}^1 last
- Joint learning is faster

Gradient steps for the bigram task

Setting: transformer on the bigram task

- Focus on predicting second output token
- All distributions are uniform
- Some simplifications to architecture
- Infinite width, infinite data, $N \gg T$

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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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- Attention is uniform at initialization $\implies$ inputs are sums of embeddings
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- $W_{KQ}^{1/2}$: correct associations lead to more focused attention

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- See also Eshaan's talk for k-hop with finite samples

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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Denoting $\mu_k := \mathbb{E}[x|y = k]$ *and* $\hat{\mu}_k := \mathbb{E}_x[\frac{\hat{p}_W(k|x)}{p(y=k)} x]$, *we have*

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

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- Similar arguments for attention matrices

Finite width and finite samples (Vural et al., 2025+)

- Data model: $y = f^*(z_{t^*})$, with **one planted relevant token** z_{t^*} in a context of length T

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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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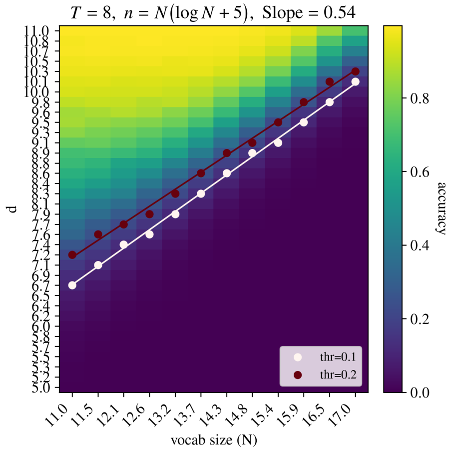

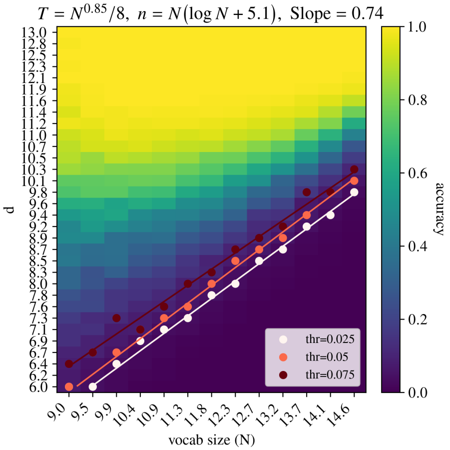

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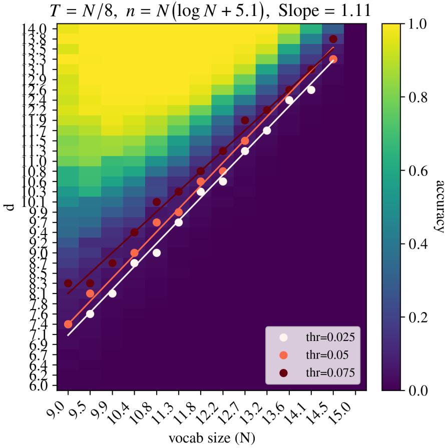

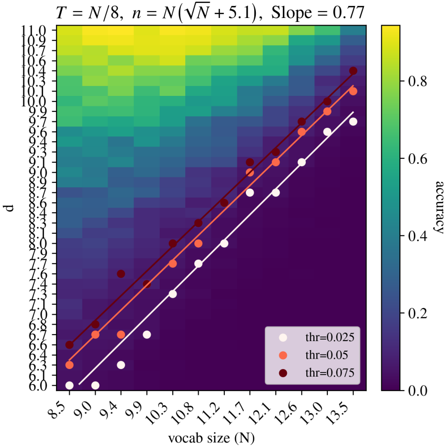

Concluding remarks

Transformer weights as associative memories

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

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Thank you!

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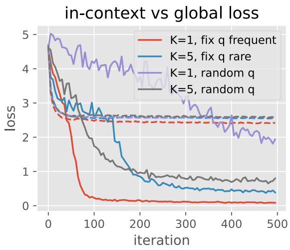
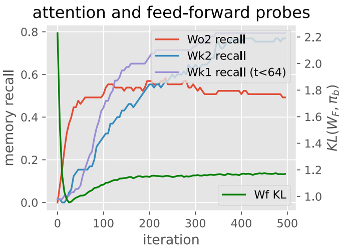
Global vs in-context associations





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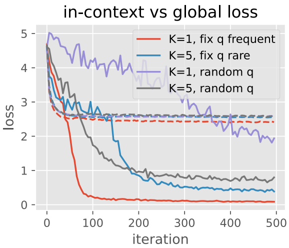

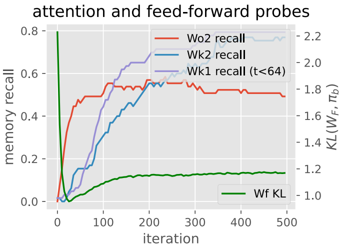

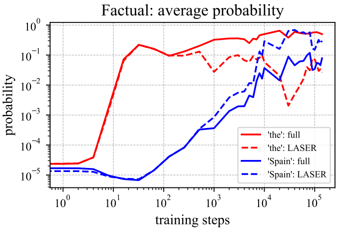

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  - "Madrid is located in" $\rightarrow$ {the, Spain} on Pythia-1B
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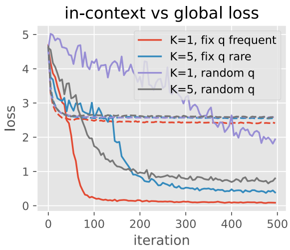

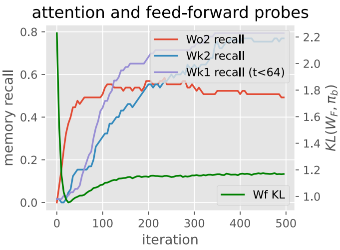

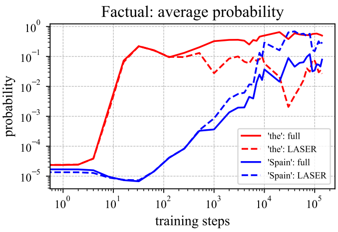

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Theorem (Chen et al., 2024, informal)

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:

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

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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: $d^{-\alpha+1}$)

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- Adam and layer-norm help with practical settings (large batch sizes + smaller step-size)

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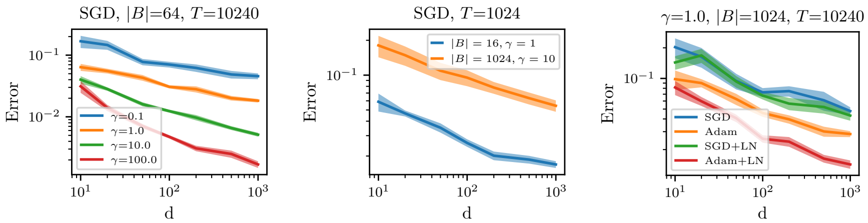
- For $d \leq N$, smaller step-sizes can help later in training
- Adam and layer-norm help with practical settings (large batch sizes + smaller step-size)



Optimization with imbalance and small capacity

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Benefits of large step-sizes + oscillations: (Cabannes, Simsek, and B., 2024b)

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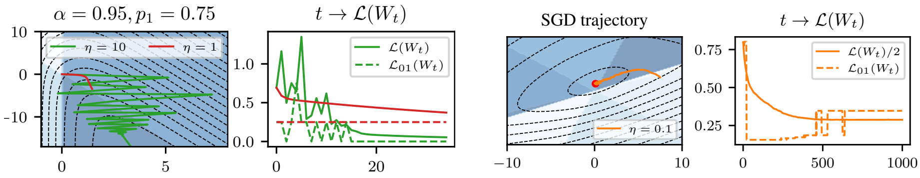

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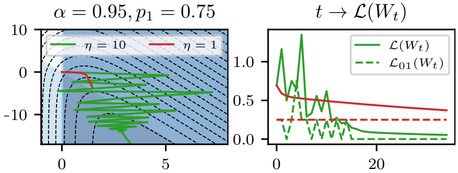

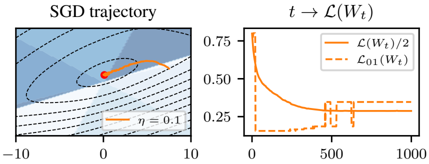

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- Correlated embeddings + imbalance $\implies$ oscillatory regimes
- Large step-sizes help reach perfect accuracy faster despite oscillations (empirically)
- Over-optimization can hurt in under-parameterized settings (empirically)