Associative Memories as a Building Block in Transformers

Alberto Bietti

Flatiron Institute, Simons Foundation

Inria Sierra, January 2025

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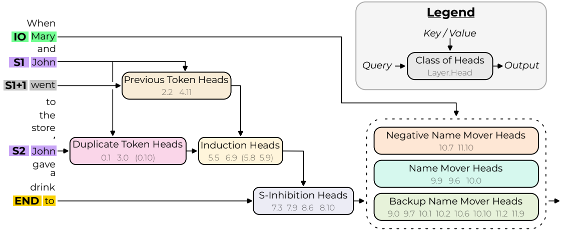
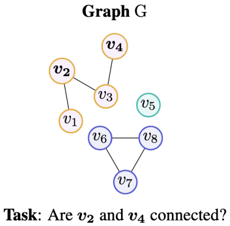
w/ V. Cabannes, E. Dohmatob, D. Bouchacourt, H. Jégou, L. Bottou (Meta AI),
E. Nichani, J. Lee (Princeton), B. Simsek, L. Chen, J. Bruna (NYU)

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)





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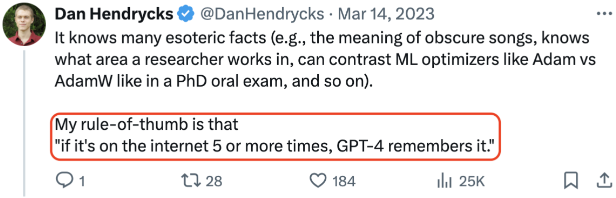
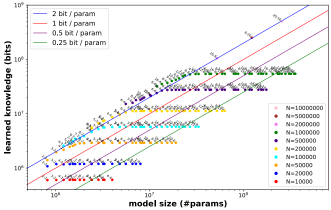
- Allows higher-level reasoning





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

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

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

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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- Consider **pairwise associations** $(z, y) \in \mathcal{M}$ with **weights** α_{zy} and define:

$$W = \sum_{(z,y) \in \mathcal{M}} \alpha_{zy} u_y {e_z}^\top$$

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- Examples in Transformers:
  - Logits in attention heads: $x_k^\top W_{KQ} x_q$
  - Logits in next-token prediction: $u_y^\top U\sigma(Vx_t)$ or $u_y^\top W_{OV} x_k$

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- Note: attention itself is also related to AM (Ramsauer et al., 2020; Schlag et al., 2021)

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; Oymak et al., 2023; Yang and Hu, 2021)

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  - 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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Multi-input

- $\hat{f}(z_1, z_2) = \arg\max_y u_y{}^\top W_1 \sigma(W_2^\top (e_{z_1} + \tilde{e}_{z_2}))$
- also $N \approx md$ capacity

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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

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

Multi-input

- $\hat{f}(z_1, z_2) = \arg\max_y u_y{}^\top W_1 \sigma(W_2^\top (e_{z_1} + \tilde{e}_{z_2}))$
- also $N \approx md$ capacity

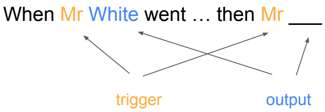
Note: matches information-theoretic lower bounds

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

Outline

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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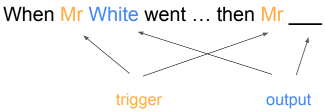

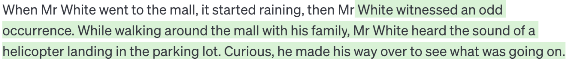

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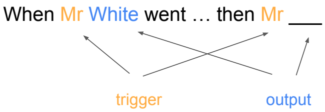

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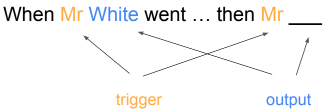

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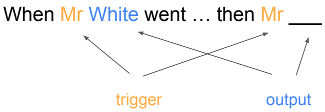

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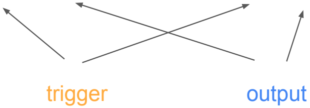
π_b: **global bigrams** model (estimated from Karpathy's character-level Shakespeare)

Transformers on the bigram task

When Mr White went … then Mr ___



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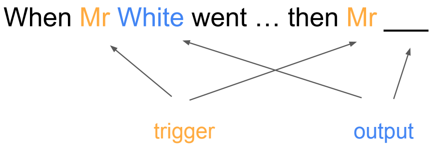

- **1-layer transformer fails**: $\sim 55\%$ accuracy on in-context output predictions

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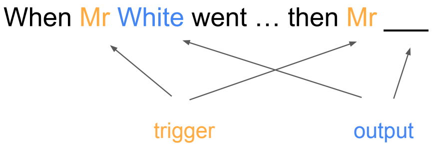

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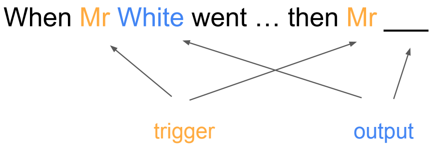

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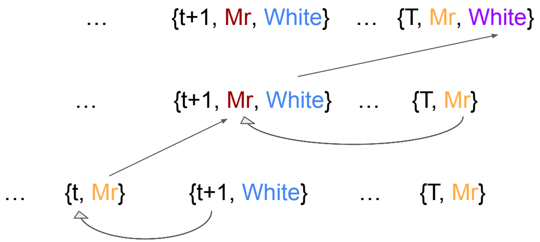
See (Sanford, Hsu, and Telgarsky, 2023, 2024) for representational lower bounds

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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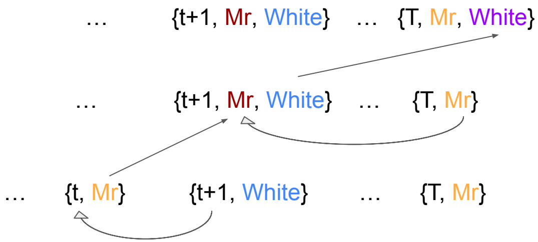

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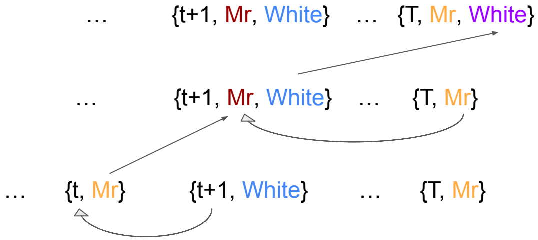
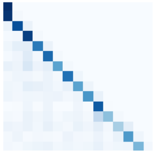
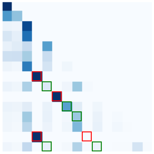


- 1st layer: **previous-token head**
  - attends to previous token and copies it to residual stream
- 2nd layer: **induction head**
  - attends to output of previous token head, copies attended token
- Matches observed attention scores:





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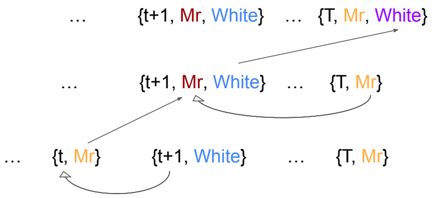
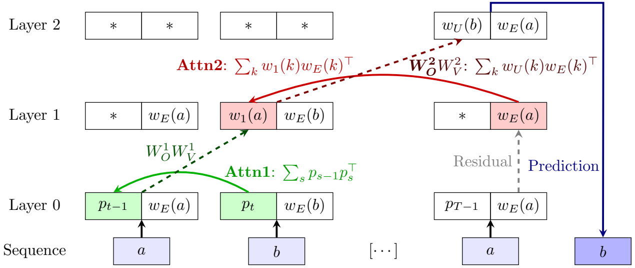
- Value/Output matrices help with token **remapping**: Mr $\mapsto$ Mr, White $\mapsto$ White



Induction head with associative memories



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

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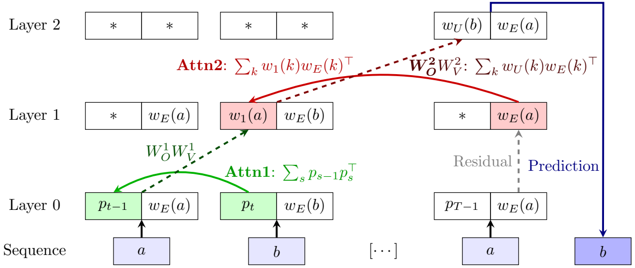

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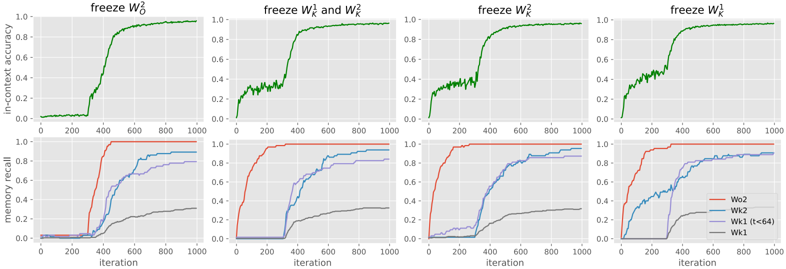
Q: Does this match practice?

Empirically probing the dynamics

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



- "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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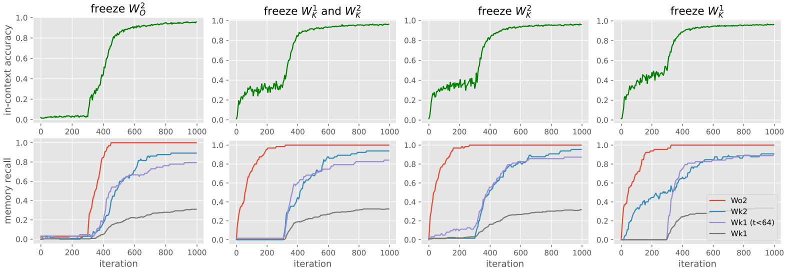

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- Natural learning "**order**": W^2_{OV} first, W^2_{KQ} next, W^1_{KQ} last
- Joint learning is faster

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
- Infinite width, infinite data, $N \gg T$

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

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
- W_{OV}^2: correct output appears w.p. 1, while other tokens are noisy and cond. indep. of z_T
- $W_{KQ}^{1/2}$: correct associations lead to more focused attention

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see also (Snell et al., 2021; Oymak et al., 2023)

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)

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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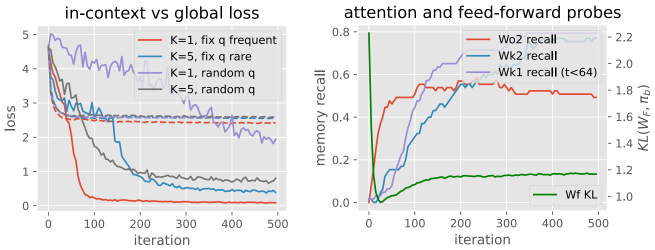
- Similar arguments for attention matrices

Global vs in-context associations



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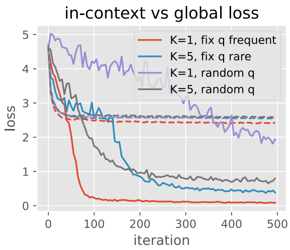

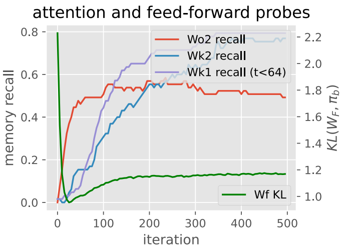

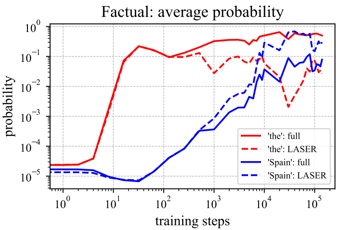

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Trade-offs between global and in-context predictions (Chen, Bruna, and B., 2024)

- Trade-offs also appear in LLMs
  - "Madrid is located in" $\rightarrow$ {the, Spain} on Pythia-1B
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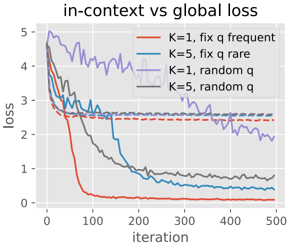

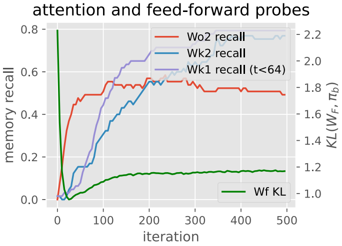

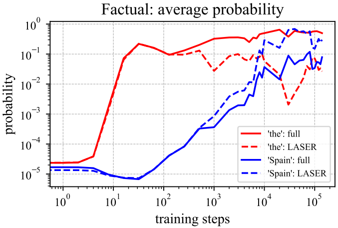

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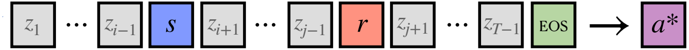
Theorem (Chen et al., 2024, informal)

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

Outline

Toy model of factual recall



The capital of France is Paris

- $s \in \mathcal{S}$: subject token
- $r \in \mathcal{R}$: relation token
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- $z_i \in \mathcal{N}$: noise tokens

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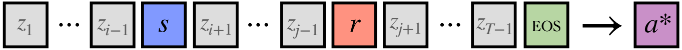

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Q: How many parameters do Transformers need to solve this?

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

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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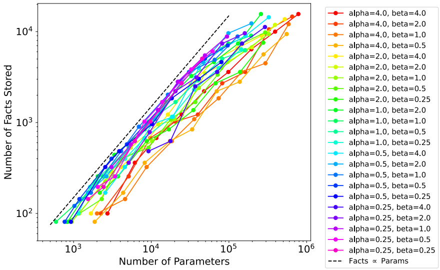

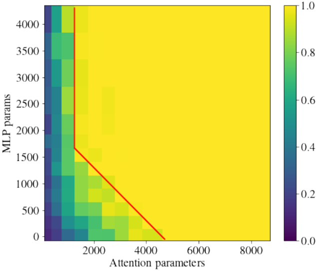

Training dynamics

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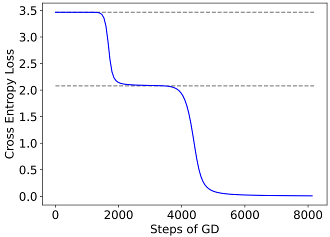
- Intermediate phase corresponds to **hallucination** (over $\mathcal{A}_r$, ignoring s)



Outline

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?**

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

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

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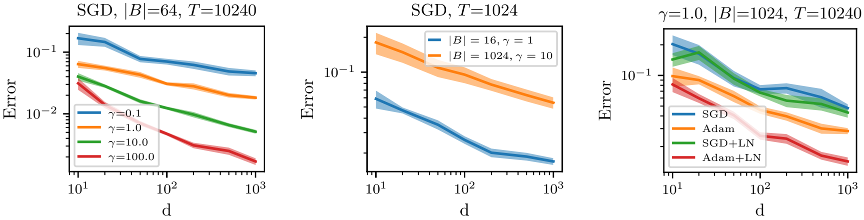

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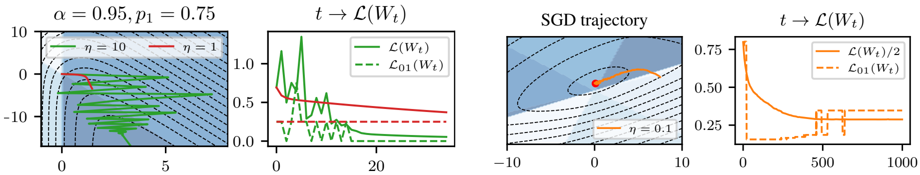

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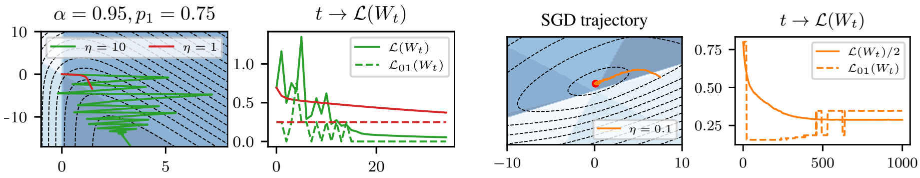

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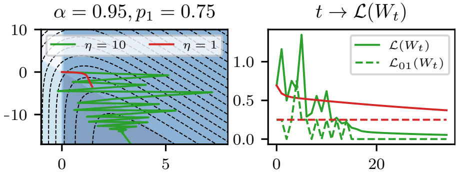

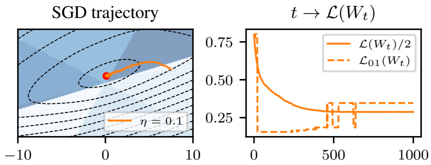

Concluding remarks

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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