Associative Memories as a Tractable Building Block in Transformers

Alberto Bietti

Flatiron Institute, Simons Foundation

FLAIR Seminar, EPFL, December 2024.

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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)

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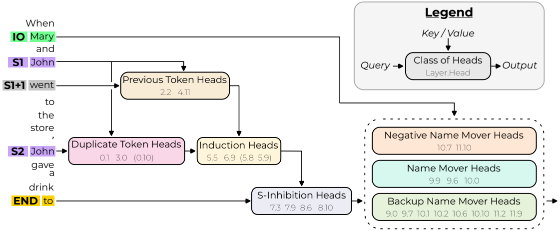
What are Transformer LLMs doing?

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/logic/MPC)



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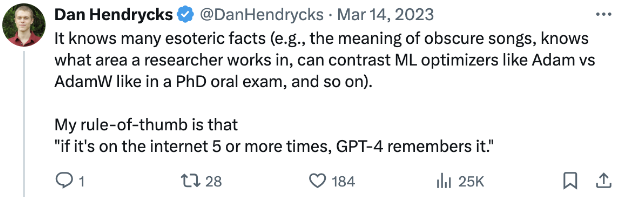
- Factual recall, memorization, scaling parameters
  - (Geva et al., 2020; Meng et al., 2022; Allen-Zhu and Li, 2024)
- Allows higher-level reasoning



Congress shall make no law respecting an establishment of religion, or prohibiting the free exercise thereof; or abridging the freedom of speech, or of the press; or the right of the people peaceably to assemble, and to petition the Government for a redress of grievances.

This is known as the First Amendment to the United States Constitution and it is designed to protect the fundamental rights of citizens of the United States. It guarantees citizens the right to practice any religion of their choosing, the freedom of speech and of the press, and the right to peacefully assemble and to petition the government.

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Q: What is a good model for these + training dynamics?

Transformer setup

Embeddings

- input e_z, positional p_t, output u_y, in $\mathbb{R}^d$
- this talk: **fixed** to **random** init $\mathcal{N}(0, 1/d)$

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

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

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** $\{u_i\}_{i \in \mathcal{I}}$ and $\{v_j\}_{j \in \mathcal{J}}$:

$$\|u_i\| \approx 1 \quad \text{and} \quad {u_i}^\top u_j \approx 0$$
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$$W = \sum_{(i,j) \in \mathcal{M}} \alpha_{ij} v_j {u_i}^\top$$

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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

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

with ℓ the cross-entropy loss and u_z, v_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)

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  - $f^*(z) = z \mod 2$: can store up to $N \approx d$ associations

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 $m \leq d$
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(Nichani, Lee, and Bietti, 2024), related to Krotov and Hopfield (2016); Demircigil et al. (2017)

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Note: matches information-theoretic lower bounds

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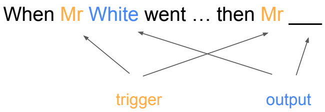
Outline

1. Associative memories
2. Application to Transformers I: induction heads (B. et al., 2023)
3. Application to Transformers II: factual recall (Nichani et al., 2024)
4. Scaling laws and optimization (Cabannes et al., 2024a,b)

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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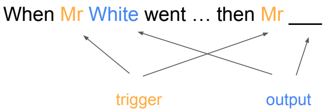

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Fix **trigger tokens**: $q_1, \ldots, q_K$

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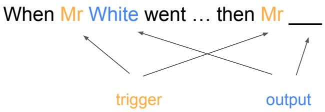

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Sample each sequence $z_{1:T} \in [N]^T$ as follows

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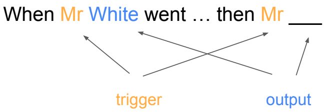

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$$p(j|i) = \begin{cases} \mathbb{1}\{j = o_k\}, & \text{if } i = q_k, \quad k = 1, \dots, K \\ \pi_b(j|i), & \text{o/w.} \end{cases}$$

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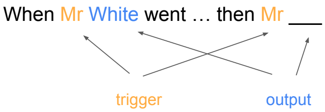

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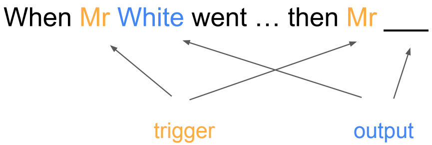
π_b: **global bigrams** model (estimated from Karpathy's character-level Shakespeare)

Transformers on the bigram task



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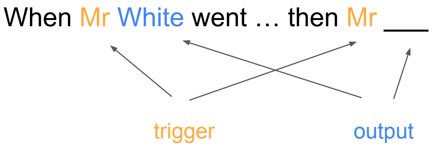

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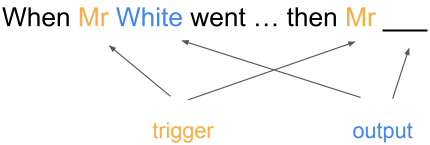

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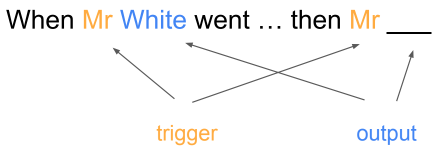
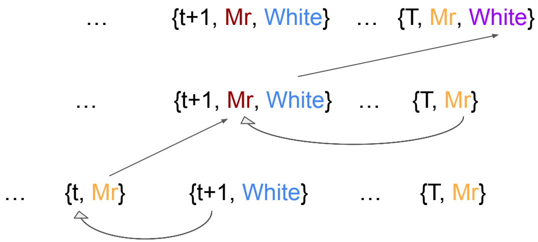


- **1-layer transformer fails**: $\sim$ 55% accuracy on in-context output predictions
- **2-layer transformer succeeds**: $\sim$ 99% accuracy

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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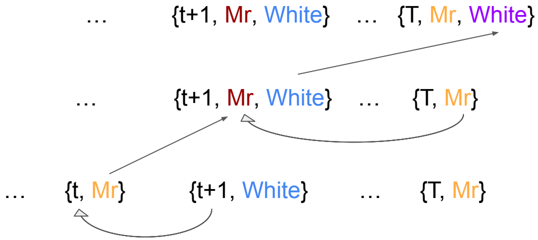

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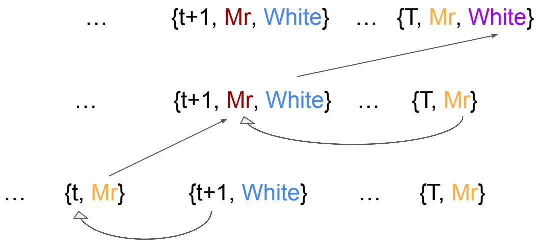

- 1st layer: **previous-token head**
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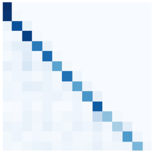
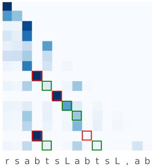
- 2nd layer: **induction head**
  - attends to output of previous token head, copies attended token
- Matches observed attention scores:





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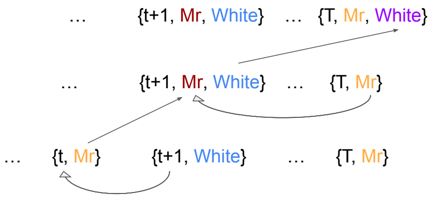
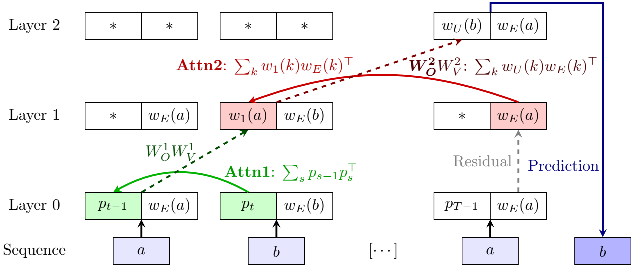
- Value/Output matrices help with token **remapping**: Mr $\mapsto$ Mr, White $\mapsto$ White



Induction head with associative memories



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

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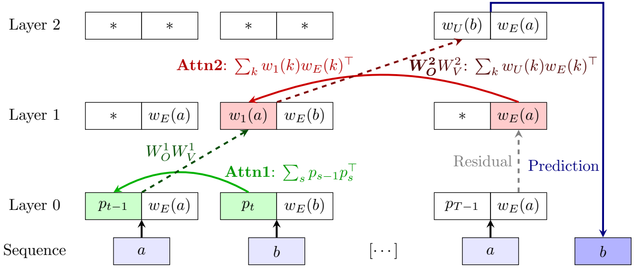

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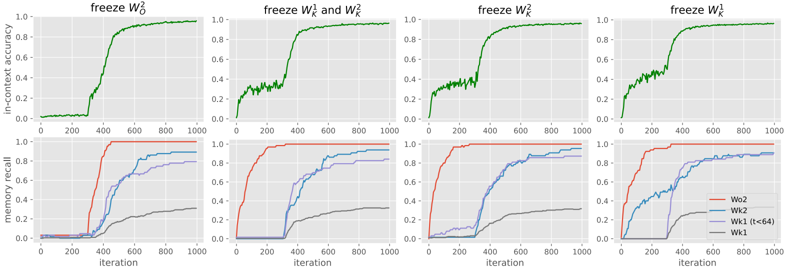
Q: Does this match practice?

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 $W_* = \sum_{i=1}^M v_i u_i^\top$, compute

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

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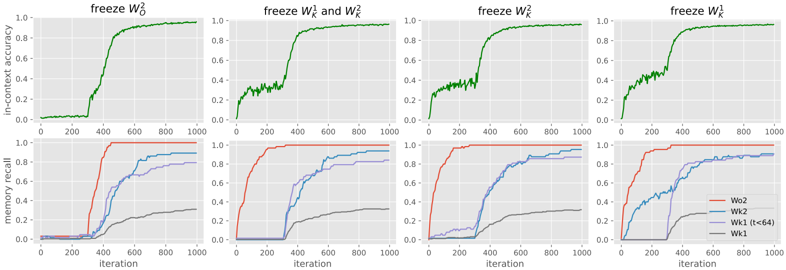

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- Natural learning "**order**": W_{OV}^2 first, W_{KQ}^2 next, W_{KQ}^1 last
- Joint learning is faster

Gradient steps for the bigram task

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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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

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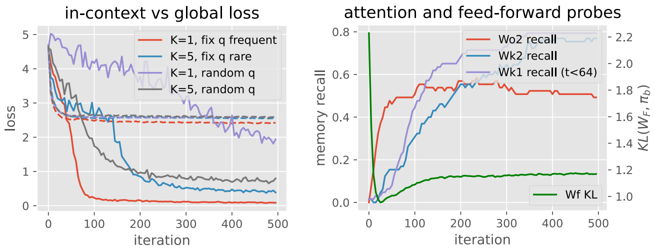
- Similar arguments for attention matrices

Global vs in-context associations



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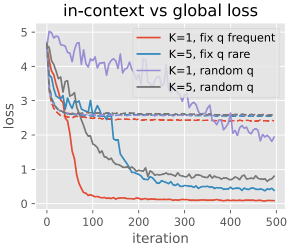

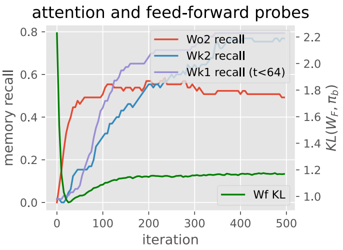

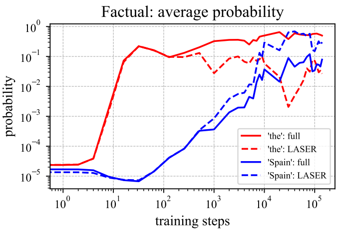

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- Trade-offs also appear in LLMs
  - "Madrid is located in" $\rightarrow$ {the, Spain} on Pythia-1B
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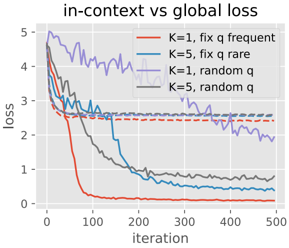

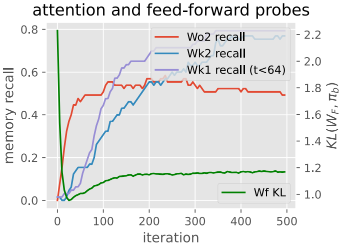

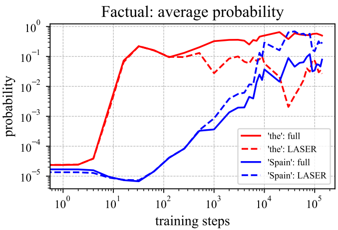

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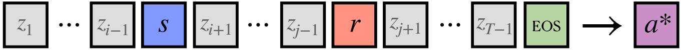
Theorem (Chen et al., 2024, informal)

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

Outline

1. Associative memories
2. Application to Transformers I: induction heads (B. et al., 2023)
3. Application to Transformers II: factual recall (Nichani et al., 2024)
4. Scaling laws and optimization (Cabannes et al., 2024a,b)

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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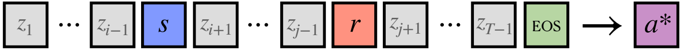

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Q: How many parameters do Transformers need to solve this?

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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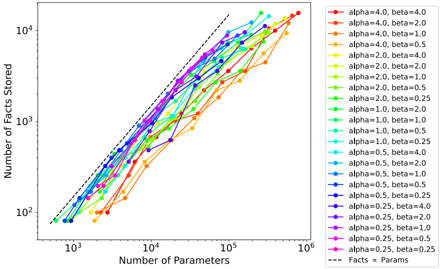

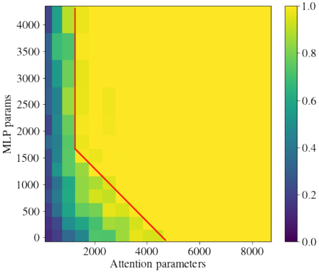

Training dynamics

- One-layer Transformer with **linear attention**, one-hot embeddings
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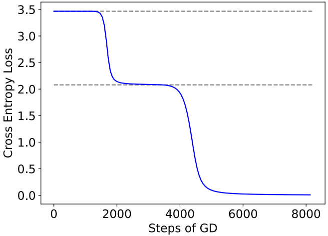
- *There is an intermediate phase where the model predicts with $p(a|r)$ instead of $p(a|s, r)$*

- 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:

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

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

Scaling laws with finite capacity

- Random embeddings $u_z, v_y \in \mathbb{R}^d$ with $\mathcal{N}(0, 1/d)$ entries
- Estimator: $\hat{f}_{n,d}(x) = \arg\max_y v_y^\top W_{n,d} u_z$, with

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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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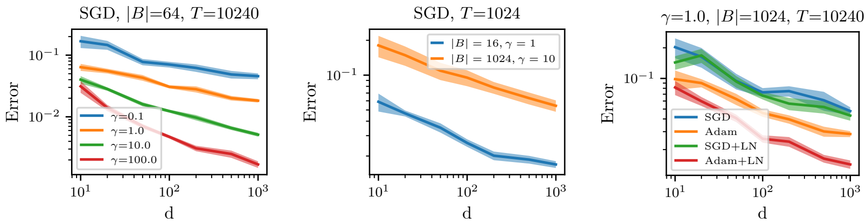

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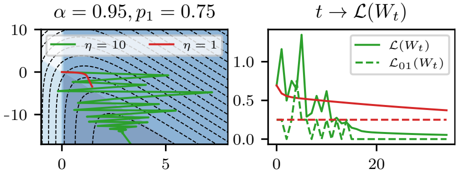
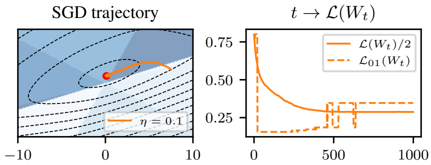
Benefits of large step-sizes + oscillations: (Cabannes, Simsek, and B., 2024b)

- Orthogonal embeddings $\implies$ logarithmic growth of margins for any step-size
- 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)





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Transformer weights as associative memories

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Thank you!

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Matrices as associative memories

- Consider sets of **nearly orthonormal embeddings** $\{u_i\}_{i \in \mathcal{I}}$ and $\{v_j\}_{j \in \mathcal{J}}$:

$$\|u_i\| \approx 1 \quad \text{and} \quad {u_i}^\top u_j \approx 0$$
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note: closely related to Hopfield (1982); Kohonen (1972); Willshaw et al. (1969)

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- Simple **differentiable model** to learn such associative memories:

$$z \in [N] \to u_z \in \mathbb{R}^d \to W u_z \in \mathbb{R}^d \to ({v_k}^\top W u_z)_k \in \mathbb{R}^M$$

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$$\nabla L(W) = \sum_{k=1}^{M} \mathbb{E}_z[(\hat{p}_W(y = k|z) - p(y = k|z)) v_k u_z{}^\top],$$

with $\hat{p}_W(y = k|z) = \exp(\xi_W(z)_k) / \sum_j \exp(\xi_W(z)_j)$.

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- After **one gradient step** on the population loss from $W_0 = 0$ with step η, we have

$$W_1 = W_0 - \eta \sum_{k=1}^{N} \mathbb{E}_z[(\hat{p}_W(y = k|z) - p(y = k|z)) v_k u_z{}^\top]$$

$$= \eta \sum_{z,k} p(z)(p(y = k|z) - \hat{p}_W(y = k|z)) v_k u_z{}^\top$$

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

Gradient associative memories with noisy inputs

- In practice, inputs are often a collection of tokens / sum of embeddings

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Maximal updates:

- First gradient update from standard initialization ($[W_0]_{ij} \sim \mathcal{N}(0, 1/d)$) take the form

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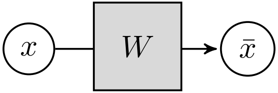
Large gradient steps on shallow networks:

- Useful for feature learning in **single-index** and **multi-index** models

$$y = f^*(x) + \text{noise}, \quad f^*(x) = g^*(Wx), \quad W \in \mathbb{R}^{r \times d}$$

- Sufficient to break the curse of dimensionality when $r \ll d$
- (Ba et al., 2022; Damian et al., 2022; Dandi et al., 2023; Nichani et al., 2023)

Associative memories inside deep models



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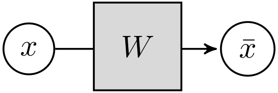

- Consider W that connects two nodes $x, \bar{x}$ in a feedforward computational graph
- The loss gradient takes the form

$$\nabla_W L = \mathbb{E}[\nabla_{\bar{x}} \ell \cdot x^\top]$$

  where $\nabla_{\bar{x}} \ell$ is the **backward** vector (loss gradient w.r.t. $\bar{x}$)
- Often, this expectation may lead to associative memories as before
- A similar form can arise in attention matrices (see later!)

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$\Longrightarrow$ **study through scaling laws** (a.k.a. generalization bounds/statistical rates)

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 $u_z, v_y \in \mathbb{R}^d$ 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: $d^{-\alpha+1}$)

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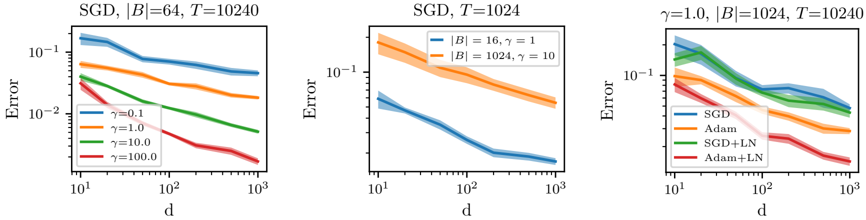

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But: higher computational cost, more sensitive to noise, harder to learn