Transformers and Associative Memories

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Oberwolfach. September 19, 2023.

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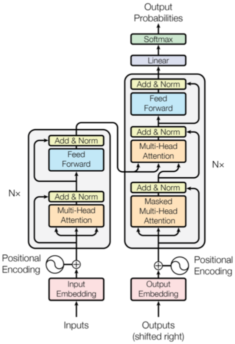
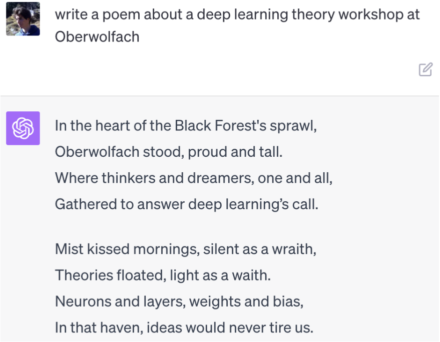
Transformers and language models

- **Transformers**: self-attention + MLPs + residual connections





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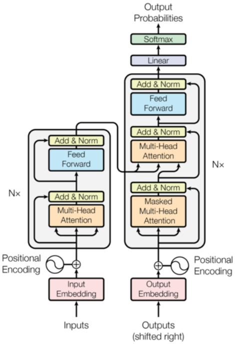

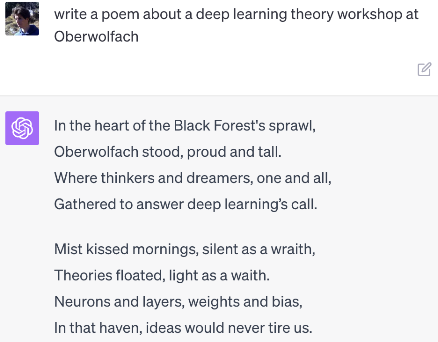

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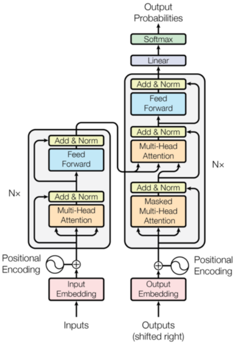
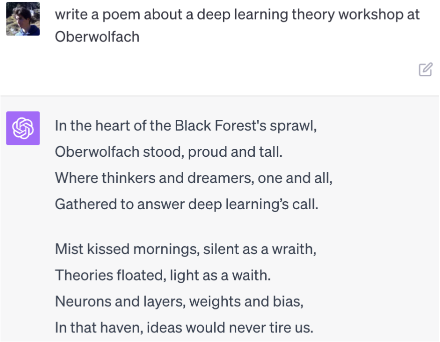
- **Large language models**: train to predict next token on all the web (+ fine-tune)
- **In-context "reasoning" vs memorization**: transformers seem to use a mix of "reasoning" from context and "knowledge" from training set





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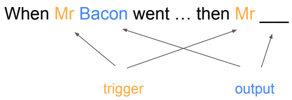
- **Training dynamics**: how is this learned during training?
- **Role of depth**: can we go beyond shallow models?
- **Experimental/theory setup**: what is a simple setup for studying this?

The bigram data model

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



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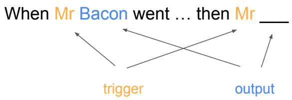

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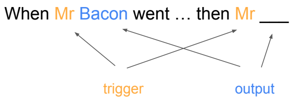

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- **Sequence-specific Markov model**: $z_1 \sim \pi_1 \quad z_t|z_{t-1} \sim p(\cdot|z_{t-1})$

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

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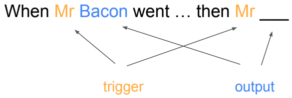

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π_b: **global bigrams** model (estimated from Karpathy's character-level Shakespeare)

Transformers I: embeddings and residual stream

- **Input sequence**: $[z_1, \ldots, z_T] \in [N]^T$
- **Embedding layer**:

$$x_t := w_E(z_t) + p_t \in \mathbb{R}^d$$

  - $w_E(z)$: token embedding of $z \in [N]$
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- **Loss** for next-token prediction (cross-entropy)

$$\sum_{t=1}^{T-1} \ell(z_{t+1}, \xi_t)$$

Transformers II: self-attention

Causal self-attention layer:

$$x'_t = \sum_{s=1}^{t} \beta_t W_O W_V x_s, \quad \text{with } \beta_s = \frac{\exp(x_s^\top W_K^\top W_Q x_t)}{\sum_{s=1}^{t} \exp(x_s^\top W_K^\top W_Q x_t)}$$

- $W_K, W_Q \in \mathbb{R}^{d \times d}$: **key** and **query** matrices
- $W_V, W_O \in \mathbb{R}^{d \times d}$: **value** and **output** matrices
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- **Single-head** attention (in practice, multi-head with multiple such matrices, $d_h \times d$)
- Each x'_t is then added to the corresponding residual stream

$$x_t := x_t + x'_t$$

Transformers III: feed-forward

Feed-forward layer: apply simple transformation to each token representation

- MLP (practice):

$$x_t' = W_2 \sigma(W_1 x_t), \qquad W_2 \in \mathbb{R}^{d \times D}, W_1 \in \mathbb{R}^{D \times d}$$

- Linear (in this work):

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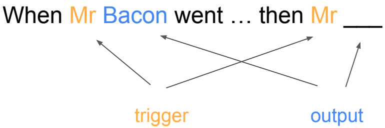
- Some evidence that feed-forward layers store "global knowledge" (Geva et al., 2020; Meng et al., 2022)

Transformers on the bigram task



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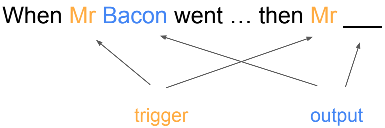

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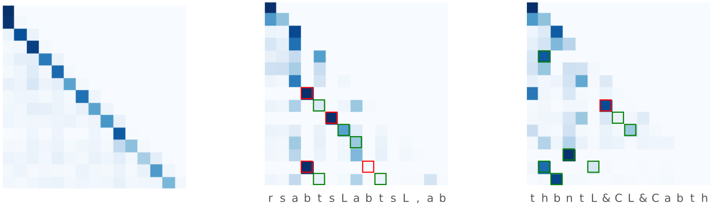
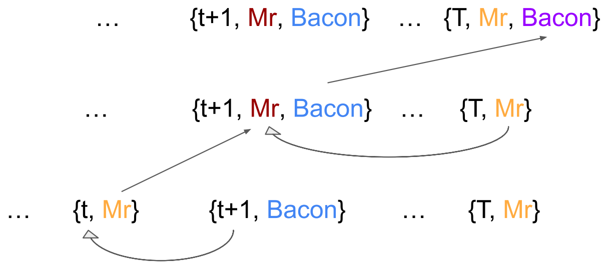
- Attention maps reveal a structured 2-layer “induction” mechanism (Elhage et al., 2021)



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



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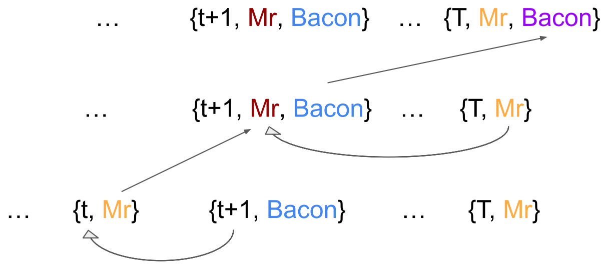

- 1st layer: **previous-token head**
  - attends to previous token and copies it to residual stream
- 2nd layer: **induction head**
  - attends to output of previous token head, copies attended token

Matrices as associative memories

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

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- Consider **pairwise associations** $(i, j) \in \mathcal{M}$ with **weights** α_{ij} and define:

$$W = \sum_{(i,j) \in \mathcal{M}} \alpha_{ij} v_j u_i^\top$$

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note: closely related to Hopfield and Willshaw networks (Hopfield, 1982; Willshaw et al., 1969)

Random embeddings in high dimension

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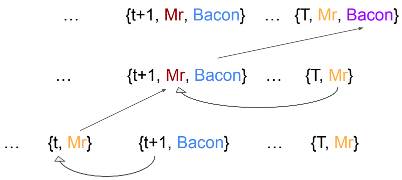
- Value/Output matrices help with token remapping: Mr $\mapsto$ Mr, Bacon $\mapsto$ Bacon



Gradient associative memories

Lemma (Gradients as memories)

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

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

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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

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

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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

$$\nabla_W L(W) = \sum_{k=1}^{N} p(y = k) v_k (\hat{\mu}_k - \mu_k)^\top.$$

Gradient associative memories with noisy inputs

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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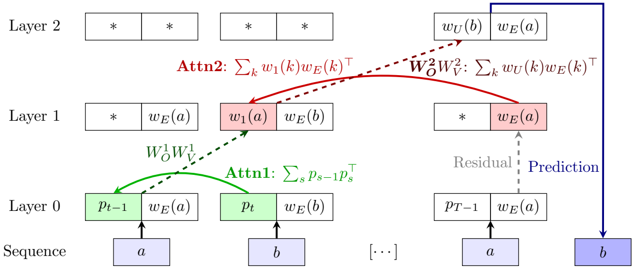
$$v_k^\top W_1(u_y + p_t) \approx \frac{\eta}{N} \mathbb{1}\{y = k\} + O\left(\frac{1}{N^2}\right)$$

Induction head with associative memories



$$W_K^1 = \sum_{t=2}^{T} p_t p_{t-1}^\top, \quad W_K^2 = \sum_{k \in Q} w_E(k) w_1(k)^\top, \quad W_O^2 = \sum_{k=1}^{N} w_U(k)(W_V^2 w_E(k))^\top,$$

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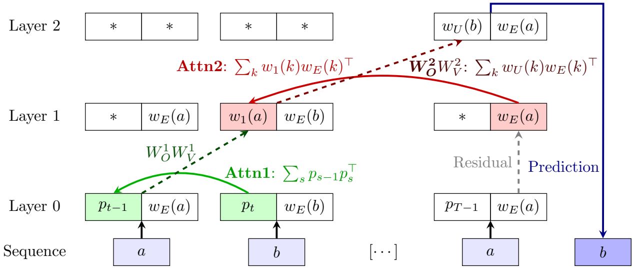

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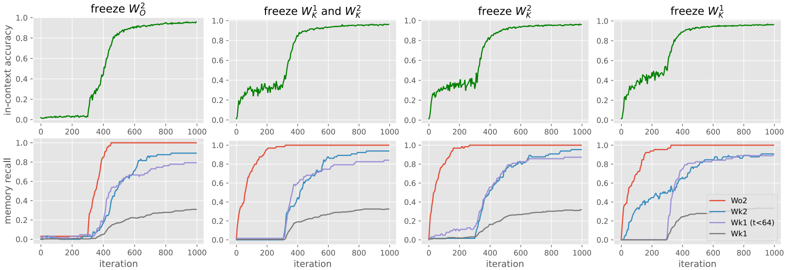
Q: Does this match practice?

Empirically probing the dynamics

Train only W_K^1, W_K^2, W_O^2, loss on deterministic output tokens only



- "Memory recall **probes**": for target memory $W_* = \sum_{(i,j)\in\mathcal{M}} v_j u_i^\top$, compute

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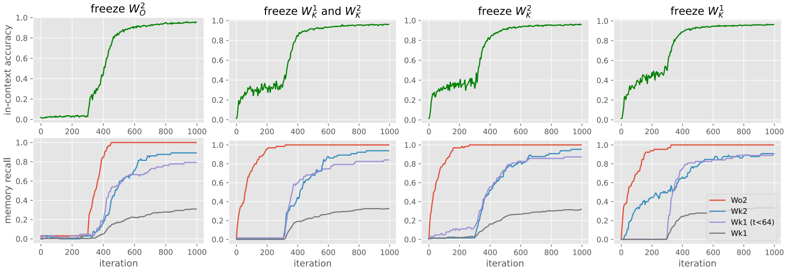

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- Natural learning "**order**": W_O^2 first, W_K^2 next, W_K^1 last
- Joint learning is faster

Theoretical analysis with single gradient steps

Setting

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In the setup above, we can recover the desired associative memories with ***3 gradient steps*** *on the population loss, assuming near-orthonormal embeddings: first on W_O^2, then W_K^2, then W_K^1.*

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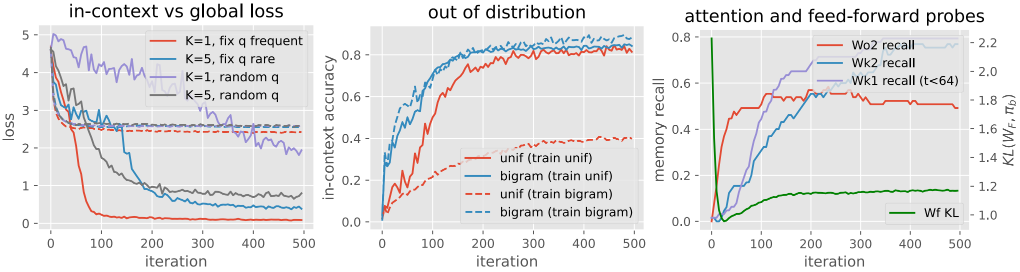
Key ideas

- Attention is uniform at initialization $\implies$ inputs are sums of embeddings
- W_O^2: correct output appears w.p. 1, while other tokens are noisy and cond. indep. of z_T
- $W_K^{1/2}$: correct associations lead to more focused attention

Global vs in-context learning and role of data

Train on all tokens, with added W_F after second attention layer



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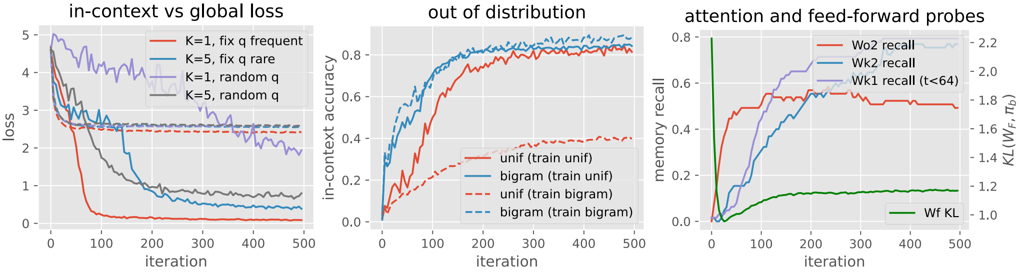

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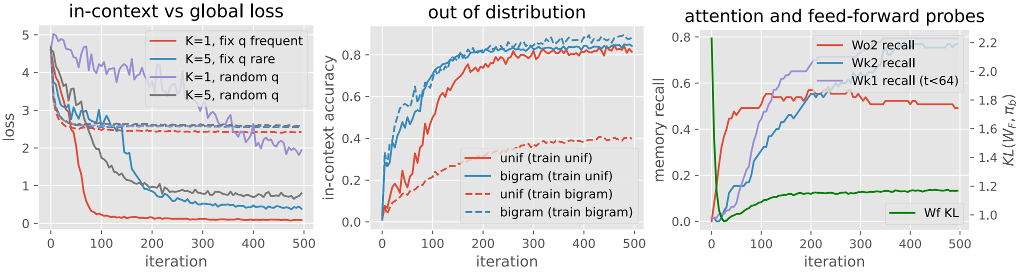

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- More frequent *triggers* $\implies$ faster learning of induction head
- More uniform *output* tokens helps OOD performance

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- **Factorizations** (*e.g.*, $W_K^\top W_Q$): $y^\top UVx$
  - Low rank factorization can save parameters/compute
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- **But**: adding heads and layers loses identifiability

What about finite samples/width? “scaling laws”/rates

Setting

- $z_i \sim p(z)$, $y_i = f^*(z_i)$, $i = 1, \dots, n$, $S_n = \{z_i\}_i$

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- Finite-memory version of (Hutter, 2021)
- 2 and 3 are related to Adam and layer-norm

Discussion and next steps

Summary

- Bigram model: simple but rich toy model for discrete data
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Thank you!

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