Session: **Deep Learning Theory**

4th Italian Meeting on Probability and Mathematical Statistics. Rome, June 2024

Understanding Transformers through Associative Memories

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Flatiron Institute, Simons Foundation

4th Italian Meeting on Probability and Mathematical Statistics. Rome, June 2024

w/ Vivien Cabannes, Elvis Dohmatob, Diane Bouchacourt, Hervé Jegou, Léon Bottou (Meta)

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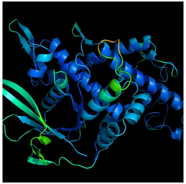
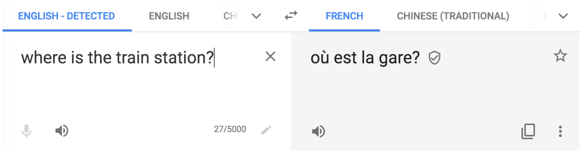
Success of deep learning

State-of-the-art models in various domains (images, language, speech, biology, ...)





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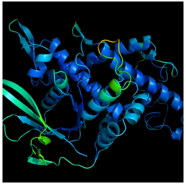

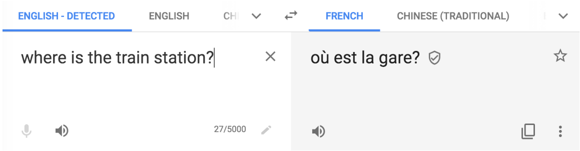

$$f(x) = W_L \sigma(W_{L-1} \cdots \sigma(W_1 x) \cdots)$$

Recipe: **huge models** + **lots of data** + **compute** + **simple algorithms**

Breaking the curse of dimensionality I: feature learning

Curse of dimensionality:

- Image/text/genomics/etc. data are **high-dimensional**: $x \in \mathbb{R}^d$, d large
- Curse of dimensionality $\implies$ need additional **structure** for learning

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Feature learning:

- **Single-index/multi-index** models:

$$\mathbb{E}[y|x] = f^*(w_1^\top x, \dots, w_r^\top x), \qquad r \ll d$$

- Example: CNNs learn Gabor-like filters

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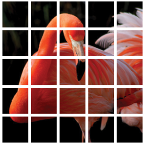
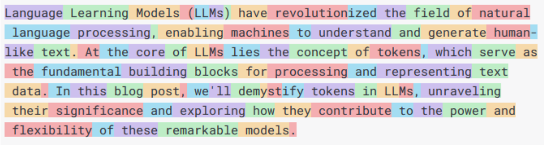
- Example: CNNs learn Gabor-like filters
- **Goal**: $O(n^{-1/r})$ instead of $O(n^{-1/d})$ rates (Bach, 2017)
- Gradient descent can achieve this (e.g., Ba et al., 2022; B. et al., 2022; Damian et al., 2022)

Breaking the curse of dimensionality II: locality + architecture

- **Local structure**: split input into small local patches / “tokens”: $x = (x_1, \ldots, x_T)$





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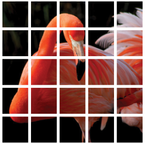

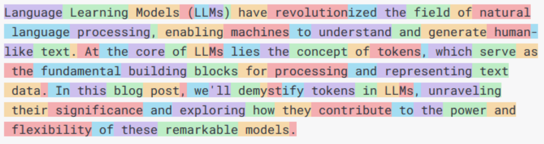

- Target may involve **interactions** between tokens, e.g. (Wahba, 1990)

$$\mathbb{E}[y|x] = \sum_i f_i^*(x_i) + \sum_{i,j} f_{ij}^*(x_i, x_j)$$

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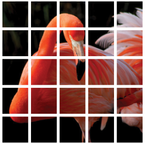

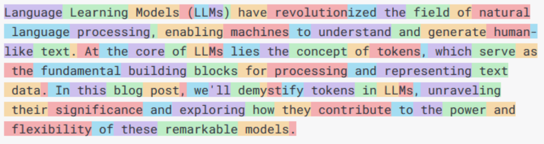

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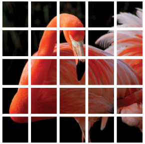

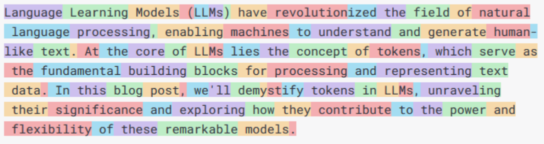

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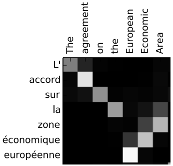
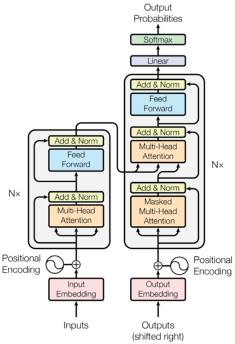
Role of architectures:

- **Convolution**: local interactions at different scales
- **Attention**: non-local interactions



Transformers and language models

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



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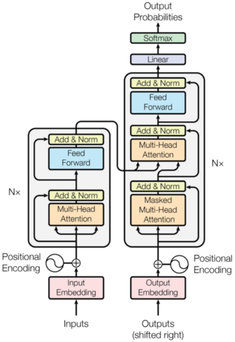
- **Large language models**: train to predict next token on all the web (+ fine-tune)



write a poem about probability near the Colosseum

In Rome where ancient stones convene,
The Colosseum stands serene.
A relic of time, of fights once grand,
Now whispers secrets through the land.

Beneath its arches, shadows play,
As if to speak of yesterday.
Where gladiators fought their fate,
Each clash a turn, a random state.

Probability dances here,
In every arch, in every tear.
For who could know which soul would stand,
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Transformers and language models

- **Transformers**: attention + MLPs + residual connections
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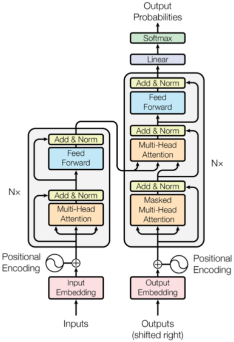
- **In-context "reasoning" vs memorization**: transformers seem to use a mix of "reasoning" from context and "knowledge" from training set



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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.

How Transformer language models use context

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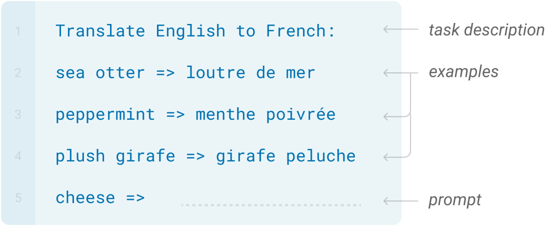
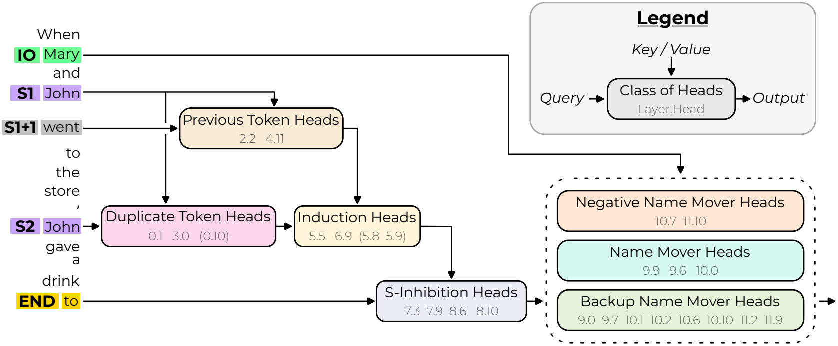


(Brown et al., 2020)

How Transformer language models use context

- Few-shot learning, basic "reasoning", math, linguistic capabilities
- Transformers may achieve this using "circuits" of attention heads



(Wang et al., 2022)

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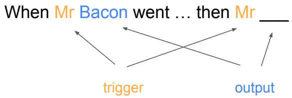
This work: (B. et al., 2023, see also **Vivien Cabannes**' talk)

- Empirical+theoretical study by viewing parameters as **associative memories**

The bigram data model

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



When Mr Bacon went to the mall, it started raining, then Mr Bacon decided to buy a raincoat and umbrella. He went to the store and bought a red raincoat and yellow polka dot umbrella.

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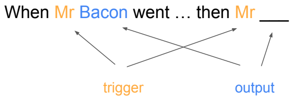

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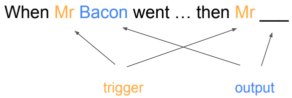

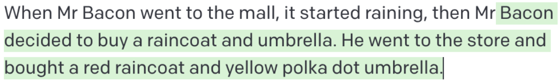

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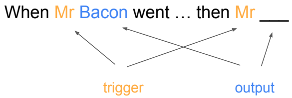

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$$p(j|i) = \begin{cases} \mathbb{1}\{j = o_k\}, & \text{if } i = q_k, \quad k = 1, \dots, K \\ \pi_b(j|i), & \text{o/w.} \end{cases}$$

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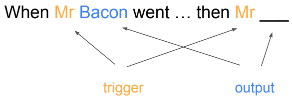

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π_b: **global bigrams** model (estimated from Karpathy's character-level Shakespeare)

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

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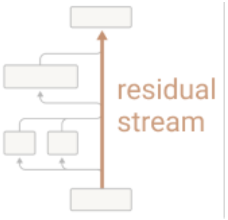

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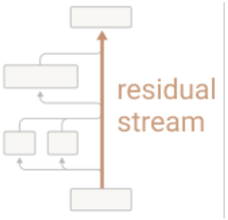
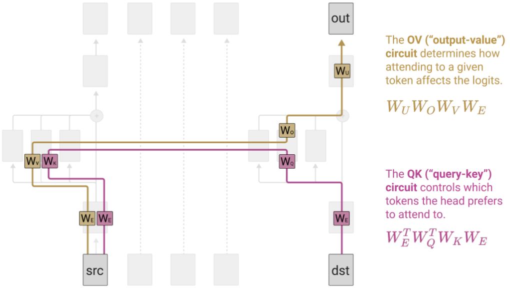
- **Loss** for next-token prediction (ℓ: cross-entropy)

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



Transformers II: self-attention



Causal self-attention layer (single head):

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

- $W_K, W_Q \in \mathbb{R}^{d \times d}$: **key** and **query** matrices, $W_V, W_O \in \mathbb{R}^{d \times d}$: **value** and **output** matrices
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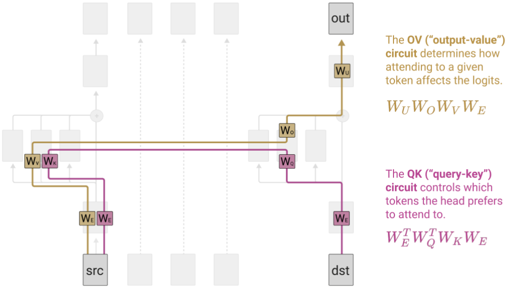

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- Each x'_t is then added to the corresponding residual stream

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

Transformers III: feed-forward

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

- MLP:
$$x'_t = W_2 \sigma(W_1 x_t), \qquad W_2 \in \mathbb{R}^{d \times D}, W_1 \in \mathbb{R}^{D \times d}$$
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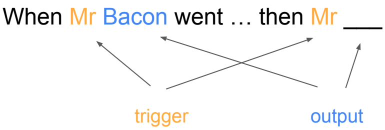
- Added to the residual stream: $x_t := x_t + x'_t$
- Some evidence that feed-forward layers store "global knowledge", *e.g.*, for factual recall (Geva et al., 2020; Meng et al., 2022; Chen et al., 2024)

Transformers on the bigram task



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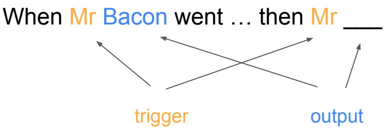

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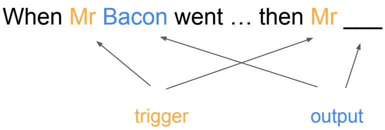

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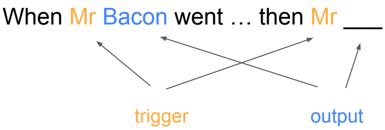

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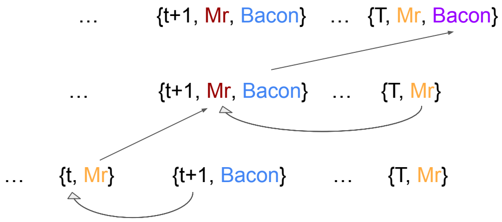
See also representation lower bounds (Sanford, Hsu, and Telgarsky, 2023)

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



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  - attends to previous token and copies it to residual stream

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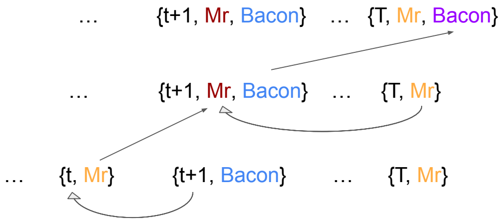
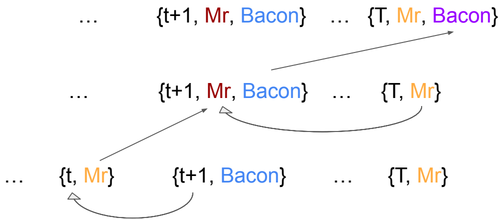
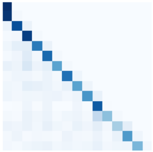


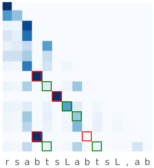
- 1st layer: **previous-token head**
  - attends to previous token and copies it to residual stream
- 2nd layer: **induction head**
  - attends to output of previous token head, copies attended token

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





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)

Random embeddings in high dimension

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

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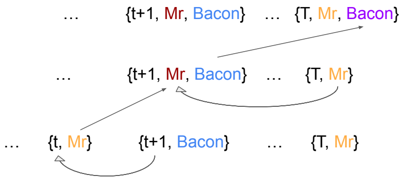
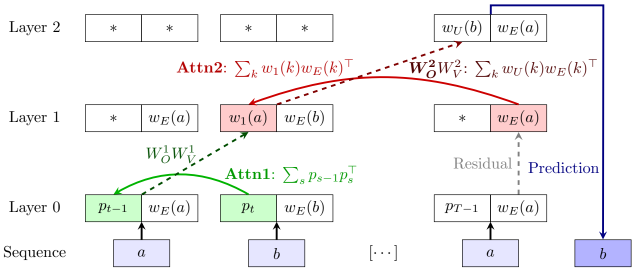
- Value/Output matrices help with token remapping: Mr $\mapsto$ Mr, Bacon $\mapsto$ Bacon



Induction head with associative memories



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

- Random embeddings $w_E(k)$, $w_U(k)$, random matrices W_V^1, W_O^1, W_V^2, fix $W_Q = I$
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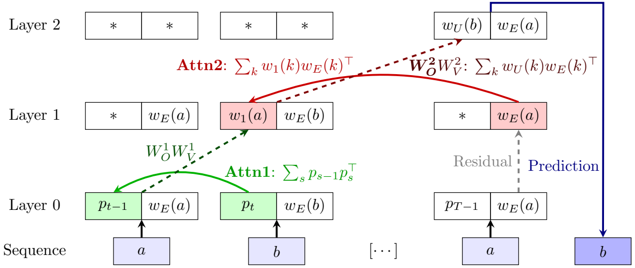

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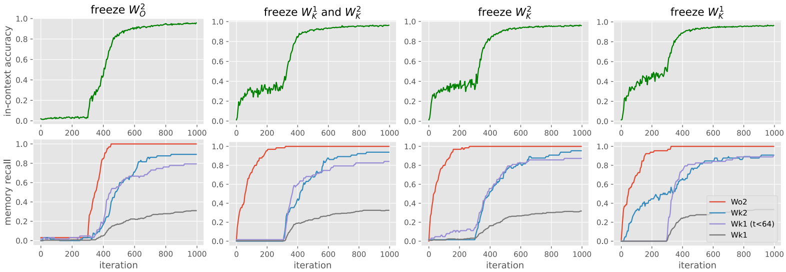
Q: Does this match practice?

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

$$R(\hat{W}, W_*) = \frac{1}{|\mathcal{M}|} \sum_{(i,j)\in\mathcal{M}} \mathbb{1}\{j = \arg\max_{j'} v_{j'}^\top \hat{W} u_i\}$$

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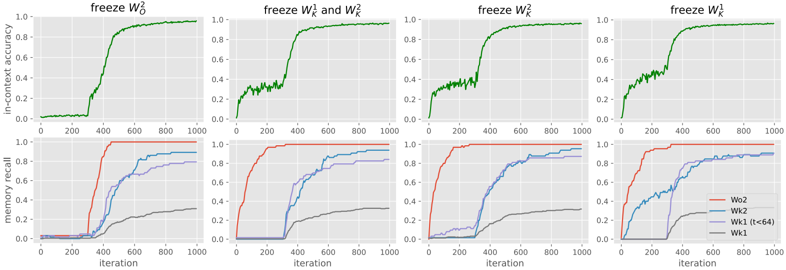

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- Natural learning "**order**": W_O^2 first, W_K^2 next, W_K^1 last
- Joint learning is faster

Gradients as associative memories

- **Simple model** to learn 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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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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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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Setting: transformer on the bigram task

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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

Discussion and next steps

Summary

- Bigram model: simple but rich toy model for discrete data
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Future directions

- More complex "reasoning" mechanisms, links with "emergence"
- Learning dynamics: multiple gradient steps? joint training? embeddings?

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- Typically $\hat{f}(z) = \arg\max_y f_y(z)$ with $f_y : [N] \to \mathbb{R}$ for each $y \in [M]$

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

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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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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

$$\mathbf{z} = \{z_1, \ldots, z_s\} \subset [N], \quad x = \sum_{j=1}^{s} u_{z_s} \in \mathbb{R}^d$$

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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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Link with feature learning

Maximal updates:

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

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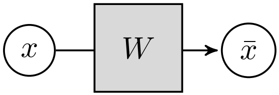
Large gradient steps on shallow networks:

- 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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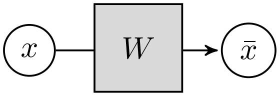

- Consider W that connects two nodes $x, \bar{x}$ in a feedforward computational graph
- The loss gradient takes the form

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

  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

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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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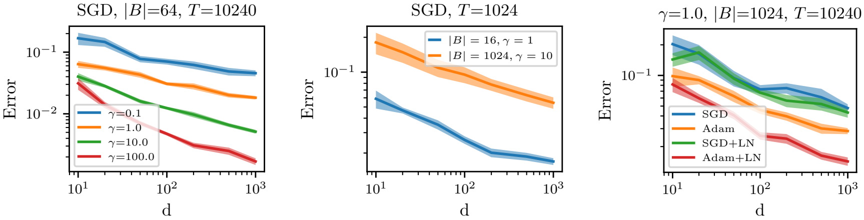

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Main idea: there are $\exp(d)$ near-orthogonal directions on the sphere

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