Understanding Transformers through Associative Memories

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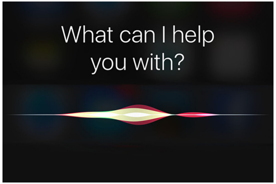
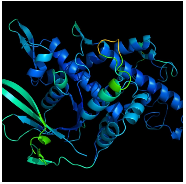
NTU CSIE, April 12, 2024.

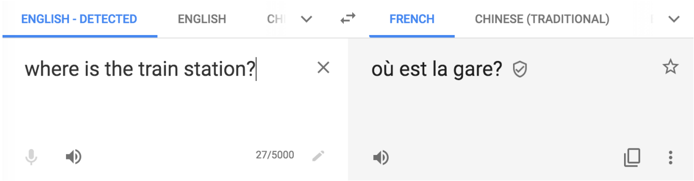
w/ V. Cabannes, E. Dohmatob, D. Bouchacourt, H. Jegou, L. Bottou (Meta AI)

Success of deep learning

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







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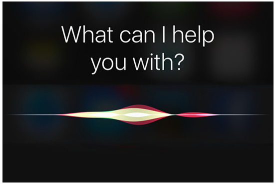

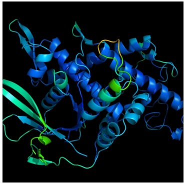

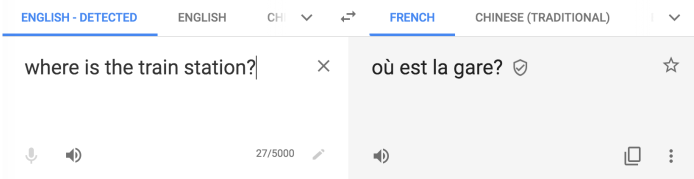

Recipe: **huge models** + **lots of data** + **compute** + **simple algorithms**

Deep learning basics

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- Train by (stochastic) **gradient descent** on loss function ℓ (e.g., cross-entropy)

$$\sum_{i=1}^{n} \ell(y^{(i)}, x_L^{(i)})$$

- Gradients are computed using **back-propagation** (chain rule)

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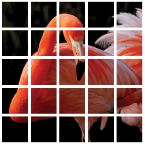

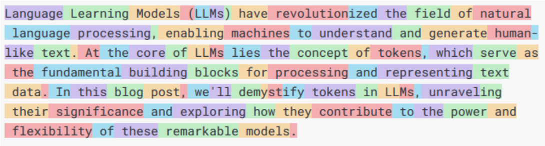

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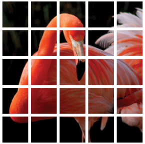

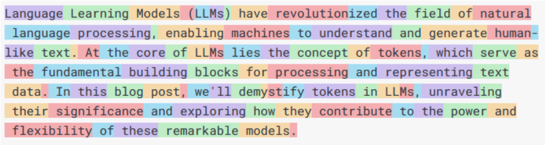

Language Learning Models (LLMs) have revolutionized the field of natural language processing, enabling machines to understand and generate human-like text. At the core of LLMs lies the concept of tokens, which serve as the fundamental building blocks for processing and representing text data. In this blog post, we'll demystify tokens in LLMs, unraveling their significance and exploring how they contribute to the power and flexibility of these remarkable models.

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- Exploit **symmetries/invariances** among tokens

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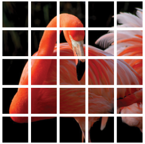
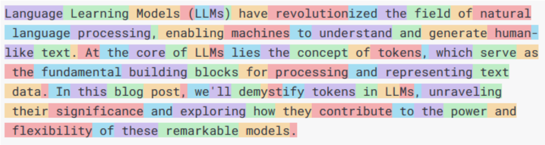
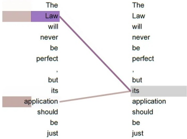


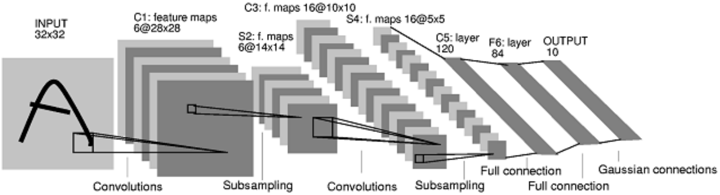


Architectures:

- Exploit **symmetries/invariances** among tokens
- Model **interactions/correlations** across tokens



Convolutional networks (CNNs)



(LeCun et al, 1998)

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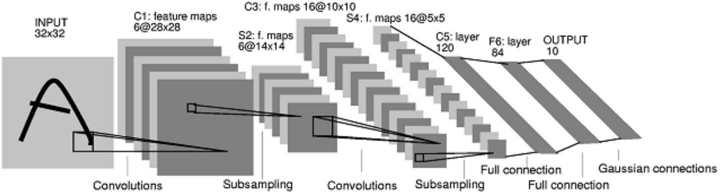

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- Model **local interactions** at different scales
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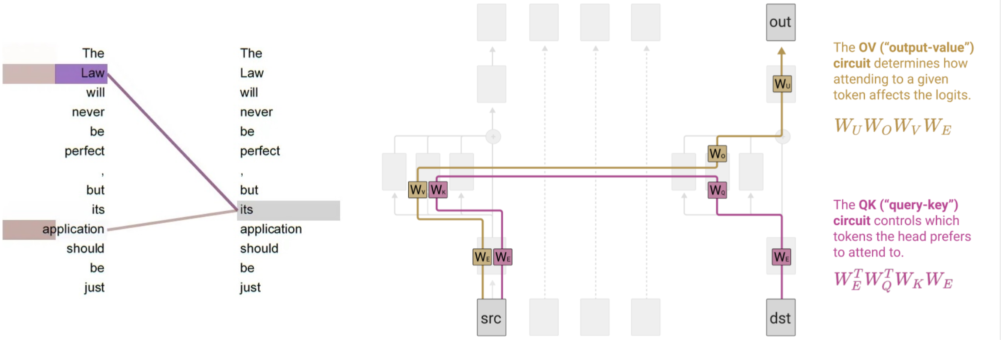
- Some theoretical benefits: (B. and Mairal, 2019; B. et al., 2021; B., 2022)

Attention heads in Transformers

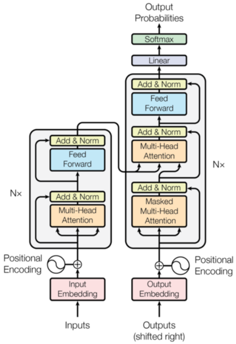


(Vaswani et al., 2017; Elhage et al., 2021)

- Model **non-local interactions** using **key-query attention**
  - "Learn" interactions instead of fixing them as in CNNs?

Transformers and language models

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



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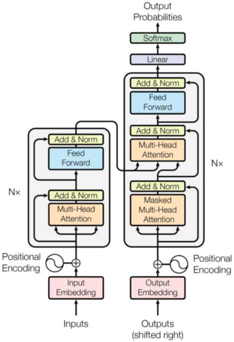


You

write a short poem about machine learning in Taipei

ChatGPT

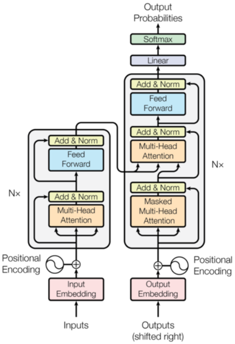
In Taipei's embrace, where modern meets tradition,
Among the lanterns' glow and temples' sedition,
There lies a silent thread, unseen yet bold,
A tale of machine learning, patiently told.

Beneath the towering Taipei 101's might,
Where day gives way to neon-lit night,
Algorithms dance in intricate flair,
Patterns emerge from data, layer by layer.

In night markets bustling, rich with life's tapestry,
Machine learning whispers secrets of the city's mystery.
Predicting, learning, in an endless strive,
To make sense of the chaos, to help us thrive.

Transformers and language models

- **Transformers**: attention + MLPs + residual connections
- **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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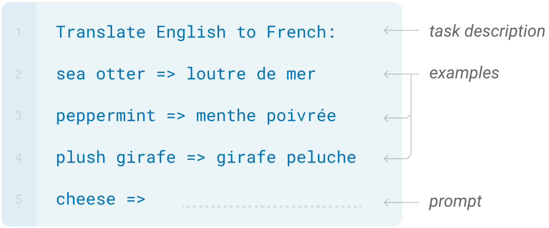
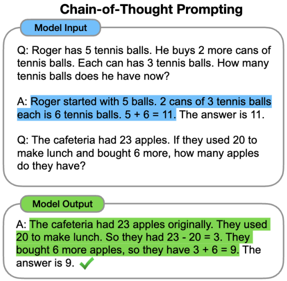
Congress shall make no law respecting an establishment of religion, or prohibiting the free exercise thereof; or abridging the freedom of speech, or of the press; or the right of the people peaceably to assemble, and to petition the Government for a redress of grievances.

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

- Few-shot learning, chain-of-thought “reasoning”, math, linguistic capabilities





(Brown et al., 2020; Wei et al., 2022)

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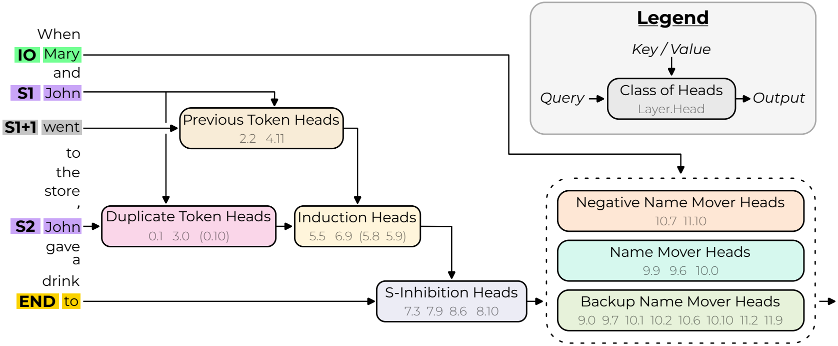
- Few-shot learning, chain-of-thought “reasoning”, math, linguistic capabilities
- Transformers may achieve this using “circuits” of attention heads



(Wang et al., 2022)

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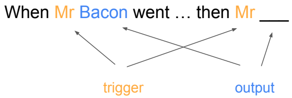
This work: (B. et al., 2023; Cabannes et al., 2024)

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

Outline

The bigram data model

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



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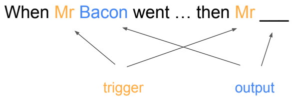

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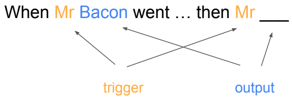

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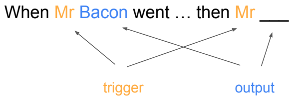

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$$p(j|i) = \begin{cases} \mathbb{1}\{j = o_k\}, & \text{if } i = q_k, \quad k = 1, \ldots, K \\ \pi_b(j|i), & \text{o/w.} \end{cases}$$

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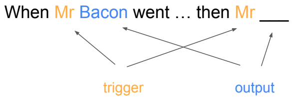

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π_b: **global bigrams** model (estimated from Karpathy's character-level Shakespeare)

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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  - Attention and feed-forward layers

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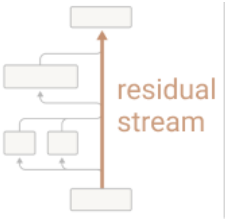
- **Loss** for next-token prediction (ℓ: cross-entropy)

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



Transformers II: self-attention

Causal self-attention layer:

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

- $W_K, W_Q \in \mathbb{R}^{d \times d}$: **key** and **query** matrices
- $W_V, W_O \in \mathbb{R}^{d \times d}$: **value** and **output** matrices
- β_s: attention weights, $\sum_{s=1}^{t} \beta_s = 1$

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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 (practice):

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

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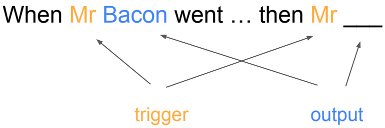
- Added to the residual stream: $x_t := x_t + x_t'$
- Some evidence that feed-forward layers store "global knowledge", *e.g.*, for factual recall (Geva et al., 2020; Meng et al., 2022)

Transformers on the bigram task



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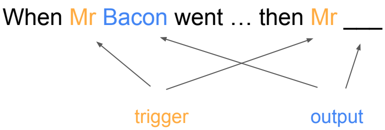

- **1-layer transformer fails**: $\sim 55\%$ accuracy on in-context output predictions

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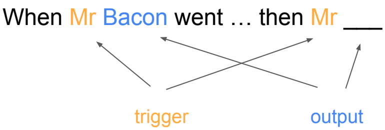

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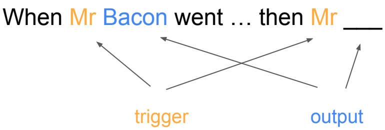

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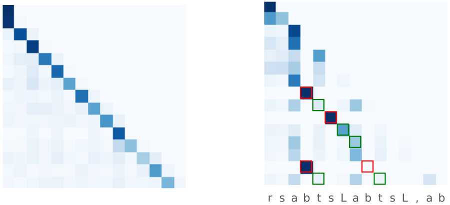

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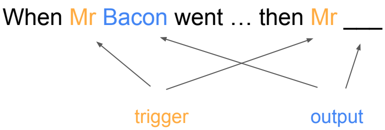

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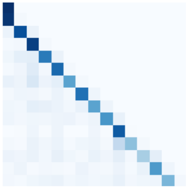
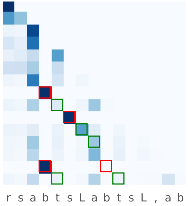
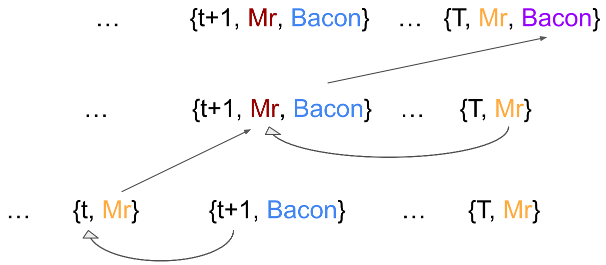




See also representation lower bounds (Sanford, Hsu, and Telgarsky, 2023)

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



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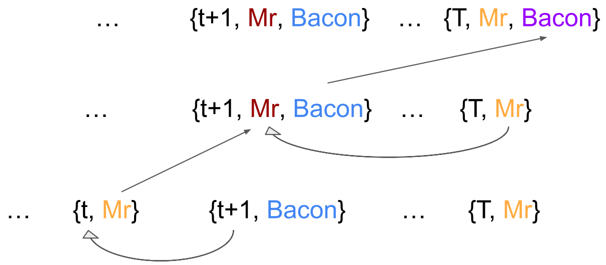

- 1st layer: **previous-token head**
  - attends to previous token and copies it to residual stream
- 2nd layer: **induction head**
  - attends to output of previous token head, copies attended token

Matrices as associative memories

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

$$\|u_i\| \approx 1 \quad \text{and} \quad {u_i}^\top u_j \approx 0$$
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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 (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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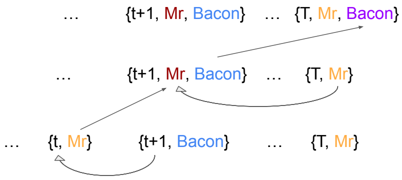
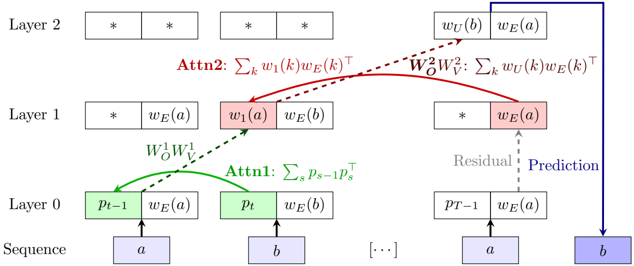
- Value/Output matrices help with token remapping: Mr $\mapsto$ Mr, Bacon $\mapsto$ Bacon



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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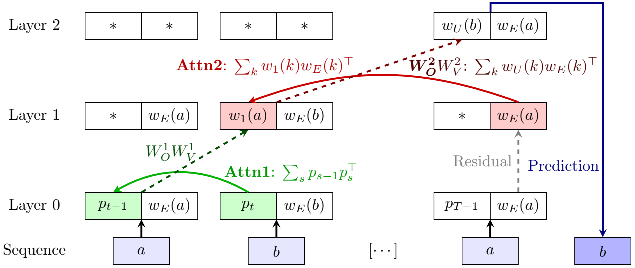

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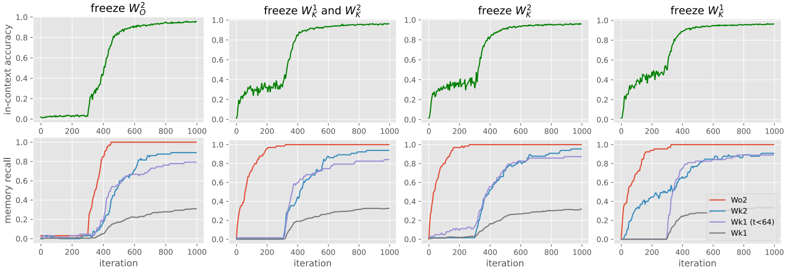
Q: Does this match practice?

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

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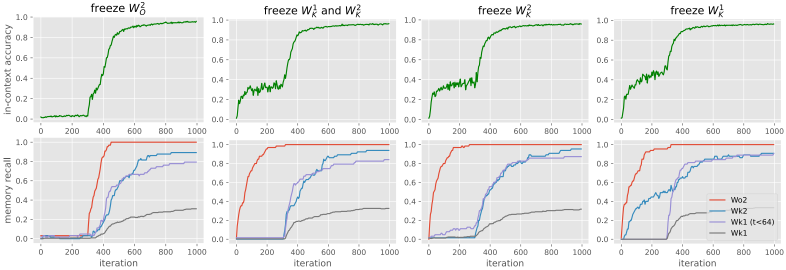

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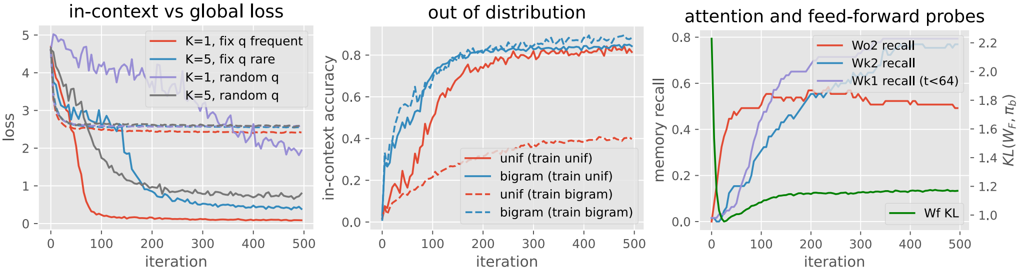
- Natural learning "**order**": W_O^2 first, W_K^2 next, W_K^1 last
- Joint learning is faster

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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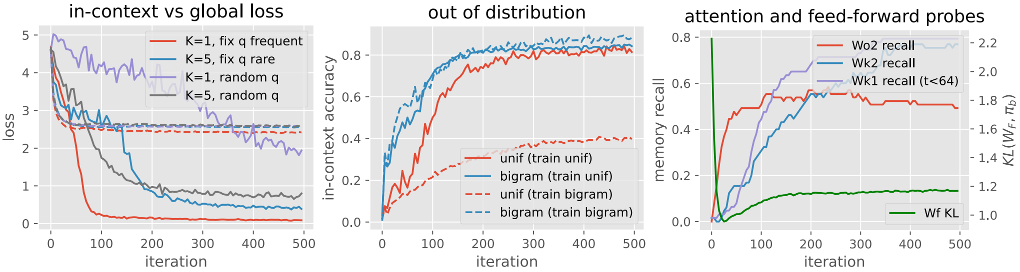

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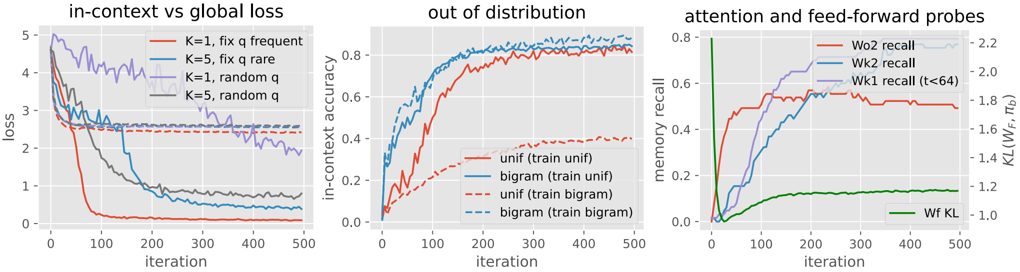

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- More uniform *output* tokens helps OOD performance

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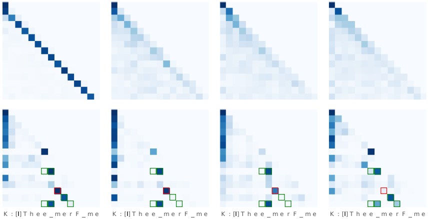
- **But**: adding heads and layers loses identifiability



Outline

1. Transformers on the bigram task

2. Learning with gradient steps

Learning associative memories with gradients

- **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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Let p be a data distribution over $(z, y) \in [N] \times [M]$, and consider the loss

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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

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

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v_k{}^\top W_1 x \approx \frac{\eta}{N} \mathbb{1}\{k = y\} + O\left(\frac{\eta}{N^2}\right)
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- **Corollary**: $\hat{f}(x) = \arg\max_k v_k^\top W_1 x$ has near-perfect accuracy

Gradient steps for the bigram task

Setting: transformer on the bigram task

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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

Finite data and finite capacity?

Questions:

- **Finite capacity?** how much can we “store” with finite d?

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Scaling laws analysis: (Cabannes, Dohmatob, and B., 2024)

- Heavy-tailed distribution of input tokens (Zipf law)
- Linear associative memory can only store d tokens
- $\implies$ Storing d most frequent tokens is best!
- Multiple gradient steps + Adam help achieve that
- Non-linear memory (e.g., MLP layers) can store more

Discussion and next steps

Summary

- Bigram model: simple but rich toy model for discrete data
- Transformer weights as associative memories
- Learning via few top-down gradient steps
- Better algorithms help for better scaling laws on heavy-tailed data

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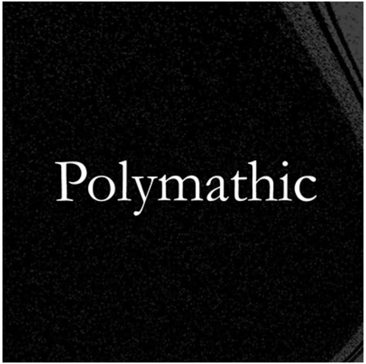
Future directions

- More complex “reasoning” mechanisms, links with “emergence”
- Learning dynamics: multiple gradient steps? joint training? embeddings?
- Applications: interpretability, model editing, factual recall, efficient fine-tuning
- Beyond text data: images and scientific data?

Thank you!



Internships and postdocs at Flatiron Institute and Polymathic AI in New York

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Learning associations

Motivation:

- DL theory often focuses on learning/approximation of **continuous** target functions
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- Data distribution $p(z, y)$ over pairs of **discrete tokens** $(z, y) \in [N] \times [M]$

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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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- 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 (1982); Kohonen (1972); Willshaw et al. (1969)

Learning associative memories with gradients

- 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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with ℓ the cross-entropy loss and u_z, v_k input/output embeddings.

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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

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

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

Example: filter out exogenous noise

- **Data model**: $y \sim \text{Unif}([N]), \quad t \sim \text{Unif}([T]), \quad x = u_y + n_t \in \mathbb{R}^d$
  - where $\{n_t\}_{t=1}^T$ are another collection of embeddings, *e.g.*, positional embeddings
- After **one gradient step** on the population loss from $W_0 = 0$ with step η, we have

$$
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- **Corollary**: $\hat{f}(x) = \arg\max_k v_k^\top W_1 x$ has near-perfect accuracy

Link with feature learning

Maximal updates:

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

$$W_1 = W_0 + \Delta W \in \mathbb{R}^{d \times d}, \quad \Delta W := \sum_j \alpha_j v_j u_j^\top, \quad \alpha_j = \Theta_d(1)$$

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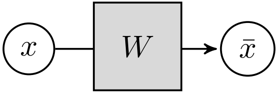
Large gradient steps on shallow networks:

- 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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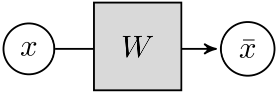

- Consider W that connects two nodes $x, \bar{x}$ in a feedforward computational graph
- The loss gradient takes the form

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

  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
- 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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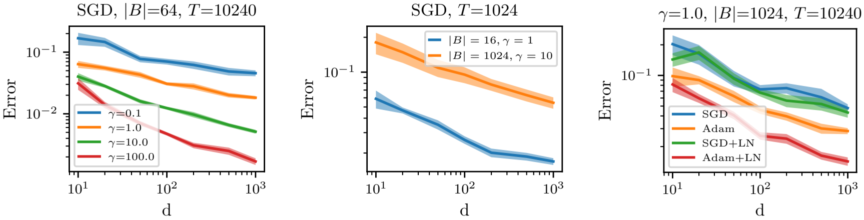

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Main idea: there are $\exp(d)$ near-orthogonal directions on the sphere

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