How do transformers work? (Part II)

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Simons Bootcamp, September 4th

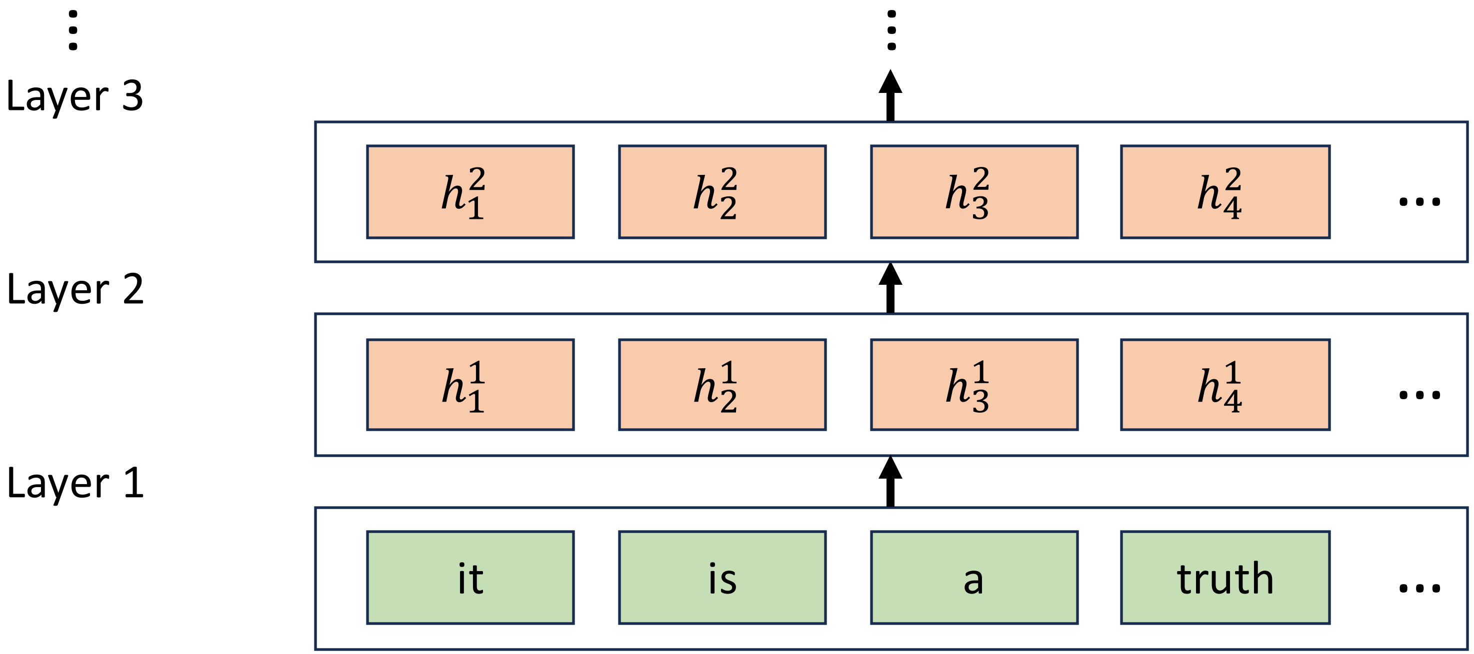
Plan for Part II

1. What can transformers do?
2. Overview of some theoretical perspectives

1. What can transformers do?

TRANSFORMERS

Transforms sequence of N tokens to sequence of N vectors by composing several sequence-to-sequence maps



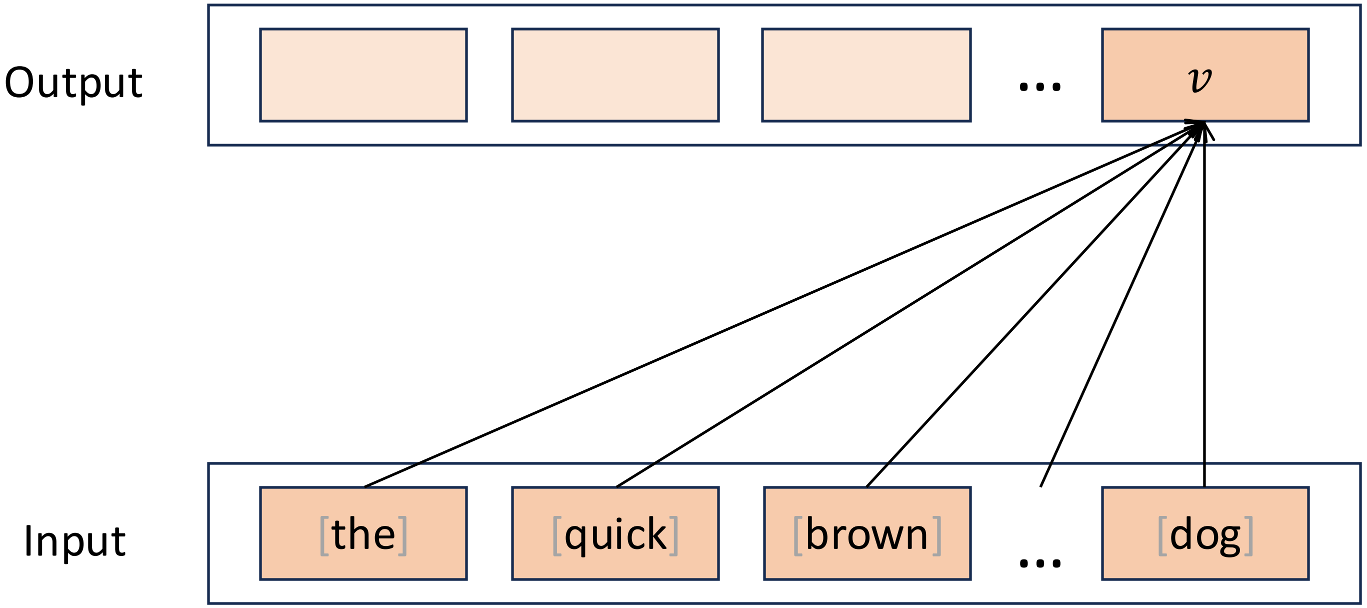
SINGLE QUERY ATTENTION

Given a query q, and keys and values for previous words compute

$$v = \sum_t \alpha_t v_t \quad \text{where} \quad \alpha_t = \frac{\exp(q^T k_t/\sqrt{d})}{\sum_u \exp(q^T k_u/\sqrt{d})}$$

weighted average of other values

weights are given by softmax



ATTENTION PATTERNS

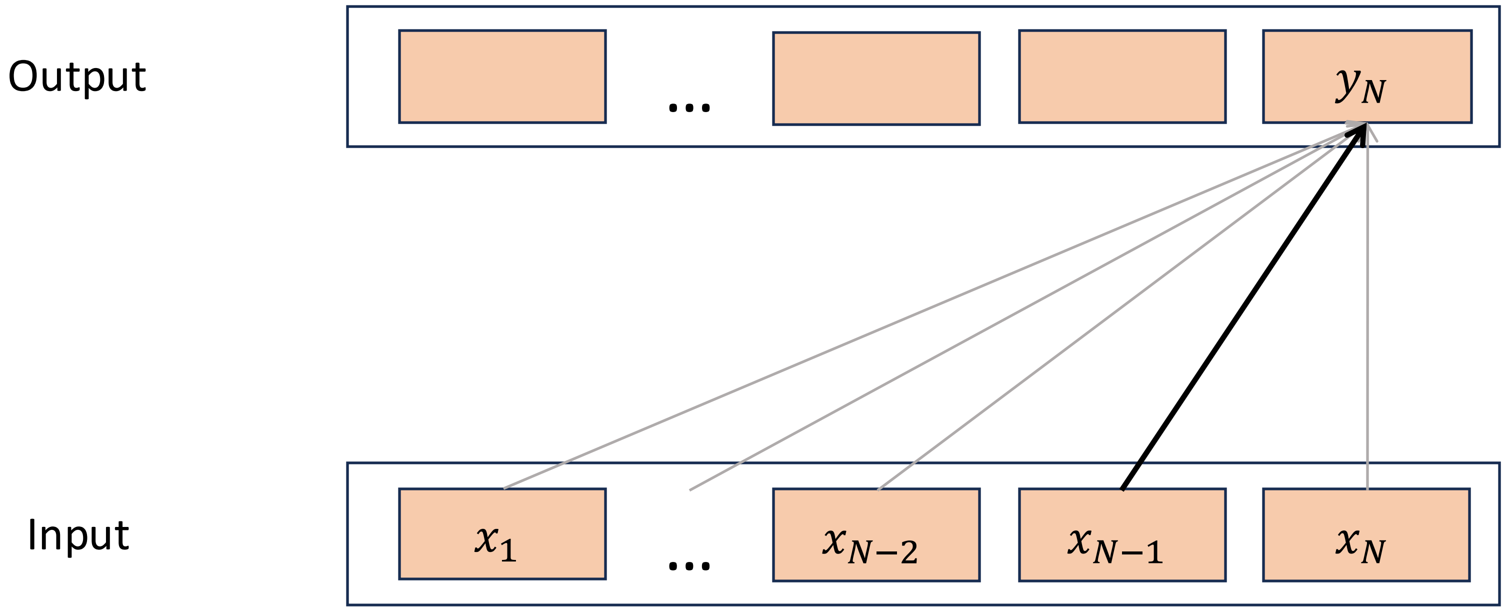
1. Query aligns with only a few keys
   → sparse weighted average of values

2. Query equally (mis)aligned with all previous keys
   → uniform average all previous values

How might these patterns arise?

EXAMPLE: POSITIONAL PATTERN

Query aligns only with previous token's key

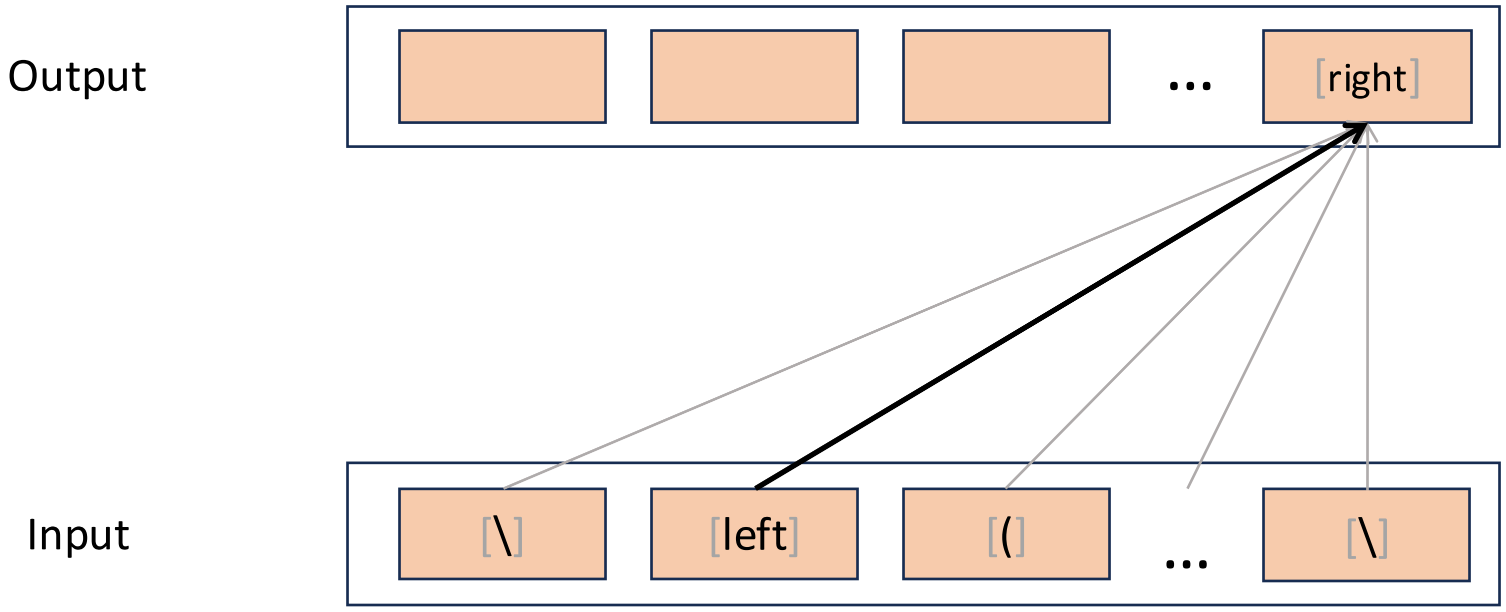


(Recall: input vectors = word embeddings + positional embeddings)

EXAMPLE: SKIP-GRAM PATTERN

[Elhage et al, 2021]

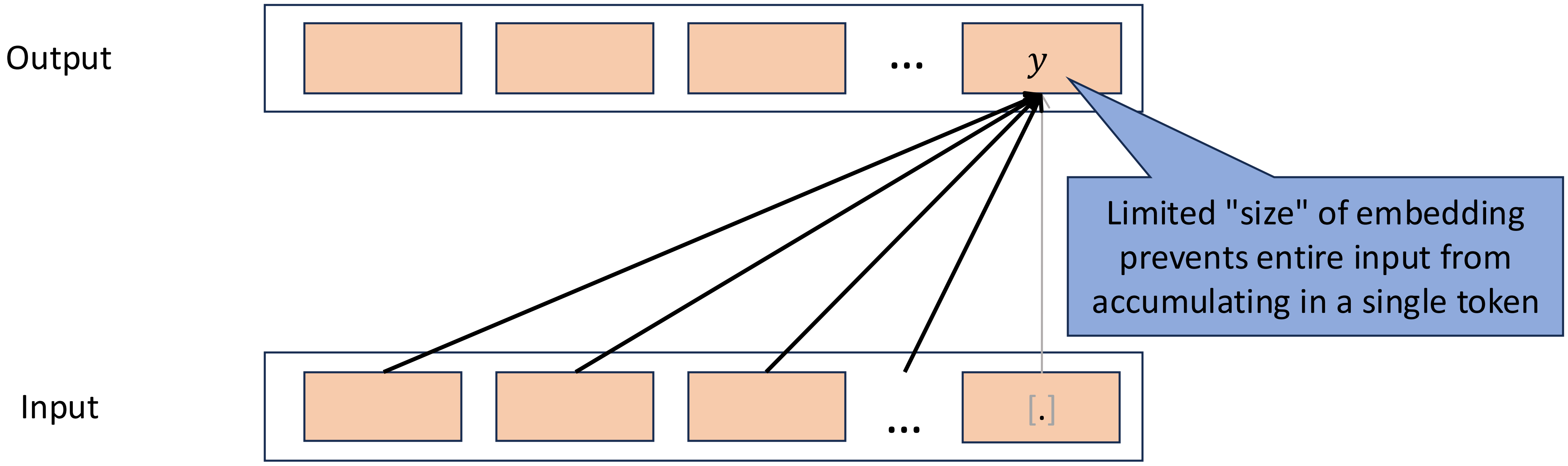
Query for "\" token aligns with key of "left"



Training identifies "skip-grams"---e.g., ("left", "\")---that help predict next token

EXAMPLE: AGGREGATION PATTERN

Query for "." (period) token aligns with keys of all previous tokens



What information gets passed up the layers?

EXAMPLE: INDUCTION HEADS

[Elhage et al, 2021; Olsson et al, 2022]

Prompt (after tokenization):

[Mr] [and] [Mrs] [Durs] [ley] [,] [of] [number] [four] [,] [Pri] [vet] [Drive] [,] [were] [proud] [to] [say] [that] [they] [were] [perfectly] [normal] [,] [thank] [you] [very] [much] [.] [They] [were] [the] [last] [people] [you] ['d] [expect] [to] [be] [involved] [in] [anything] [strange] [or] [mysterious] [,] [because] [they] [just] [didn] ['t] [hold] [with] [such] [nonsense] [.] [Mr] [Durs]

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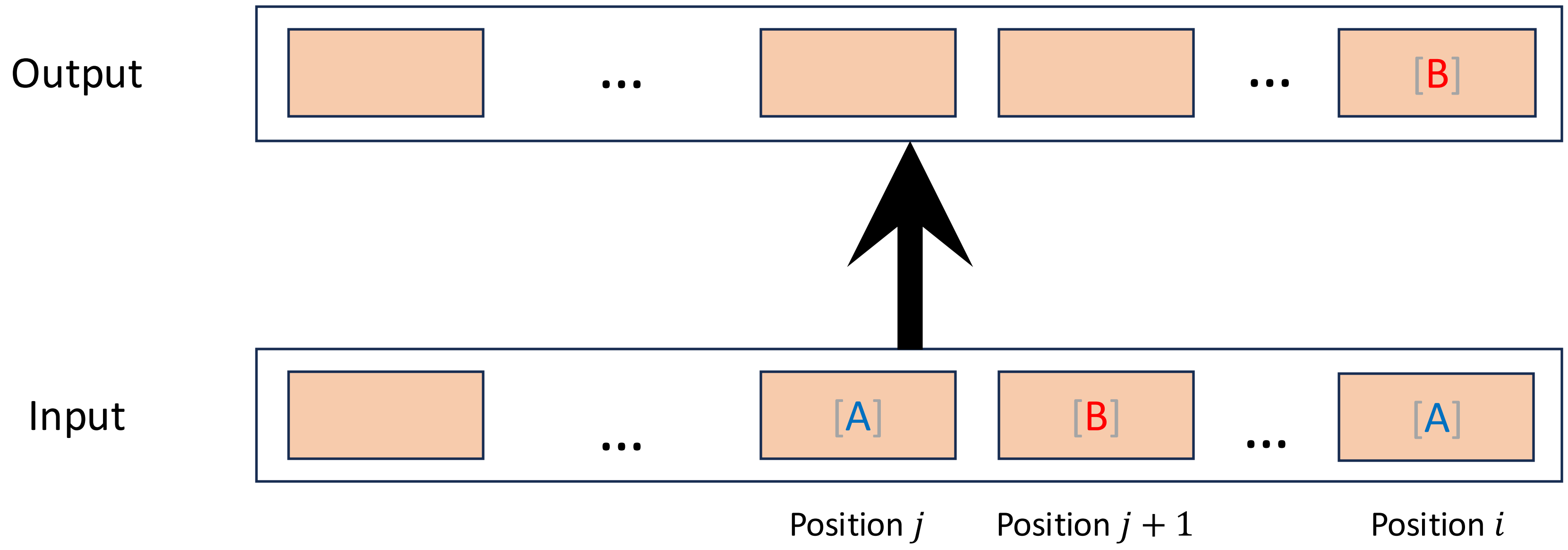
INDUCTION HEADS ABSTRACTION

[Elhage et al, 2021; Olsson et al, 2022]

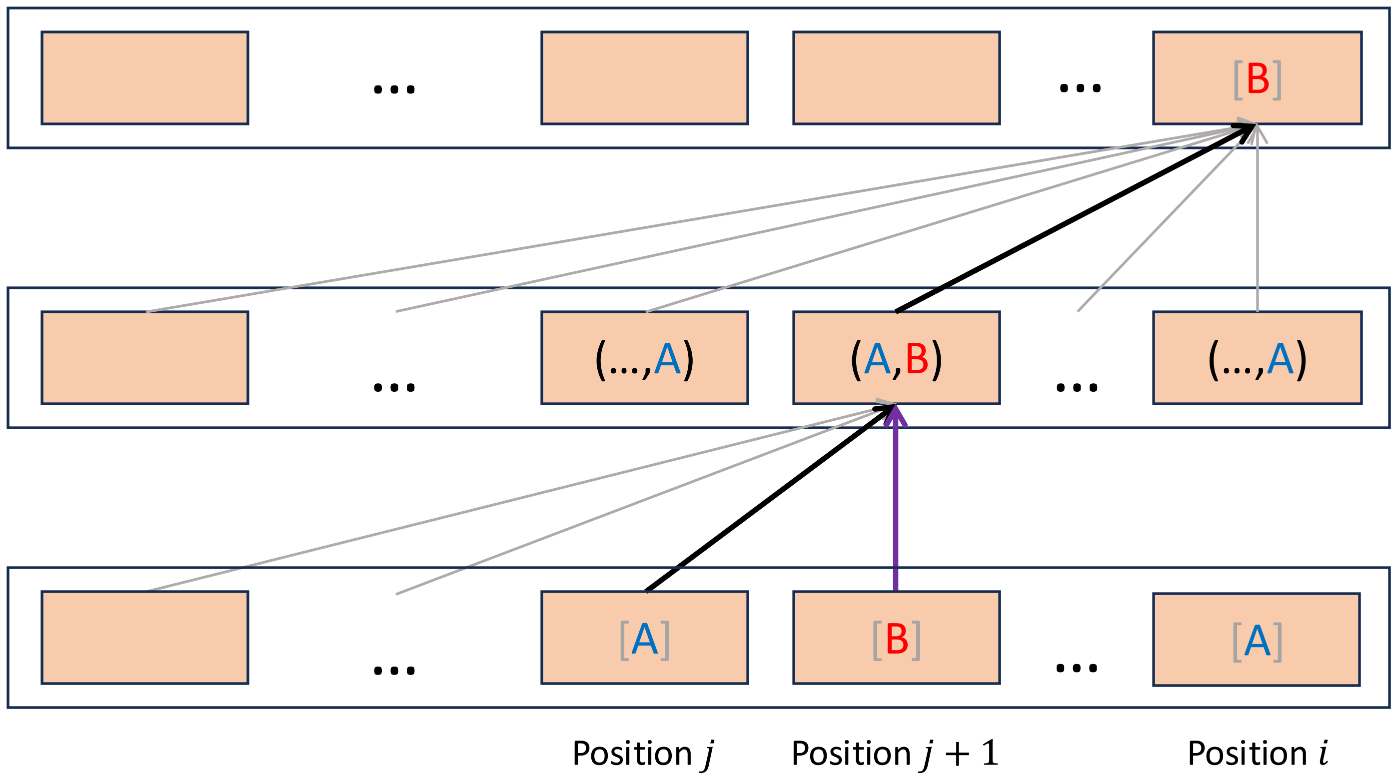
Induction head: abstraction of a salient sub-circuit found in LLMs

- i^{th} output: Find latest time $j < i$ that x_i occurs, output x_{j+1}



INDUCTION HEADS IMPLEMENTATION

Composition of two self-attention heads



Layer 2: find $\langle k, q \rangle$ match

Notation: (KEY, QUERY/VALUE)

Layer 1: move prev. token's key (+ use "skip connection")

Input to induction head

IN-CONTEXT LEARNING [Brown et al, 2020]

Circulation revenue has increased by 5% in Finland. // Positive

Panostaja did not disclose the purchase price. // Neutral

Paying off the national debt will be extremely painful. // Negative

The company anticipated its operating profit to improve. // ________

LM

Circulation revenue has increased by 5% in Finland. // Finance

They defeated … in the NFC Championship Game. // Sports

Apple … development of in-house chips. // Tech

The company anticipated its operating profit to improve. // ________

LM

[Figure from Xie and Min, 2022]

IN-CONTEXT LEARNING VIA INDUCTION HEADS

Prompt:

The mother of Charlotte is Eve. The mother of John is Helen. [...] Who is John's mother?

Sequence after some processing by a few transformer layers (perhaps):

... [Charlotte] [Eve] ... [John] [Helen] ... [John]

"In-context learning" / "meta-learning" / nearest neighbor prediction

E.g., in-context learning n-gram models: [Edelman, Edelman, Goel, Malach, Tsilivis, 2024]

Also Tengyu's talk this afternoon

FUNCTION COMPOSITION

[Peng, Narayanan, Papadimitriou, 2024; Sanford, Hsu, Telgarsky, 2024]

Prompt:

Jane is a teacher. Helen is a doctor. […] The mother of Charlotte is Eve. The mother of John is Helen. […] What is the profession of John's mother?

Function composition = iterated induction head

What are the key primitives in LLMs, and how are they put together?

2. Some theoretical perspectives

SOME (MORE) THEORETICAL PERSPECTIVES

- Transformer as a formal model of computation
- Learning and Chain-of-Thought
- Prediction vs generation
- Associative memories

TRANSFORMER AS FORMAL MODEL OF COMPUTATION

[Liu, Ash, Goel, Krishnamurthy, Zhang, 2023; Merrill & Sabharwal, 2023; Strobl, 2023]

- $O(1)$-layer $\mathrm{poly}(N)$-size transformers ⊆ (Uniform) TC^0
    - Implications: e.g., cannot simulate all finite automata (unless $TC^0 = NC^1$)

[Hahn, 2020; Hao, Angluin, Frank, 2022; Angluin, Chiang, Yang, 2023; …]

- Restrictions on "softmax" and/or masking further limit expressivity

[Sanford, Hsu, Telgarsky, 2024]

- Simulation of/by Massively Parallel Computation algorithms
    - Lower bounds for induction heads and other primitives

What abstraction is relevant for transformers at practical scales?

LEARNING IN PRACTICE

- Transformer maps context (e.g., "the quick brown fox jumped over the lazy") to vector h, which is used in a **log-linear model** $P_\theta(\text{next word} \mid h)$
- **Training:** Tune parameters θ = ((Q, K, V) matrices, feedforward nets, …, log-linear model) to minimize cross-entropy on training data

$$\sum_{t=1}^{T} -\log P_\theta(\text{word } t \mid \text{previous } t-1 \text{ words})$$

May truncate to last N words

- **Equivalent:**
  - Maximize likelihood of θ given data
  - Minimize relative entropy of empirical frequencies w.r.t. P_θ

LEARNING IN THEORY

[Edelman, Goel, Kakade, Zhang, 2022]

- If I manage to find an L-layer transformer with low training error, will its test error also be low?
- Probably YES if:
    - Training/test data are i.i.d. from same distribution over length-N sequences);
    - Token embeddings are computed by "nice" functions and are not too "large";
    - Training data size $\gtrsim \exp(L)\log(N)$

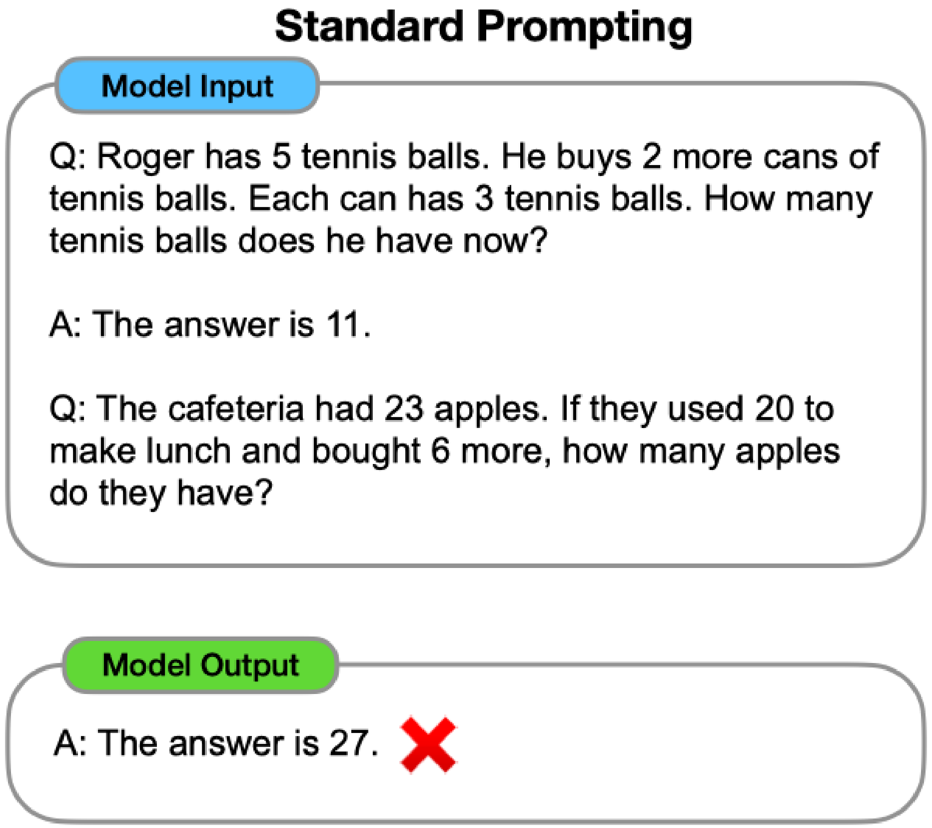
[Chen, Li, 2024; Oymak, Rawat, Soltanolkotabi, Thrampoulidis, 2023; Nichani, Damian, Lee, 2024; …]

- Can I efficiently find a low error transformer? With gradient descent?

Relevant notion of generalization for LLMs?

CHAIN-OF-THOUGHT (CoT)

[Wei, Wang, Schuurmans, Bosma, Xia, Chi, Le, Zhou, 2022; Kojima, Gu, Reid, Matsuo, Iwasawa, 2022; …]



[Figure from Wei et al, 2022]

BENEFITS OF CoT

1. Extra "work space" to compute prediction [Merrill & Sabharwal, 2024; …]
2. Extra "worked steps" available during training

Traditional labeled training example:

Q: Roger has 5 tennis balls. He buys 2 more cans of tennis balls. Each can has 3 tennis balls. How many tennis balls does he have now?

A: The answer is 11.

Labeled training example with worked steps:

Q: Roger has 5 tennis balls. He buys 2 more cans of tennis balls. Each can has 3 tennis balls. How many tennis balls does he have now?

A: Roger started with 5 balls. 2 cans of 3 tennis balls each is 6 tennis balls. 5 + 6 = 11. The answer is 11.

DOES CoT MAKE LEARNING EASIER?

Hard PAC learning problems (e.g., decision trees, DNFs, circuits) become easy with extra "worked steps" / "clues" during training

	Extra "worked steps" / "clues"
[Sloan & Rivest, 1988; Malach, 2023]	Values of all gates in circuit
[Dvir, Rao, Wigderson, Yehudayoff, 2012]	Randomly restricted access to circuit

Where do these "worked steps" come from?

GOALS OF LANGUAGE MODELING

Two roles of a language model $\hat{P}$:

1. **Prediction** **(what comes next?)**

$$\underset{\text{next word}}{\arg\max}\ \hat{P}(\text{next word}|\text{context})$$

2. **Generation** **(write new sentences)**

$$\text{next word} \sim \hat{P}(\cdot\,|\text{context})$$

PREDICTION VS GENERATION

[Kalai and Vempala, 2024]

Even in an "idealized" setting: for any trained language model $\hat{P}$,

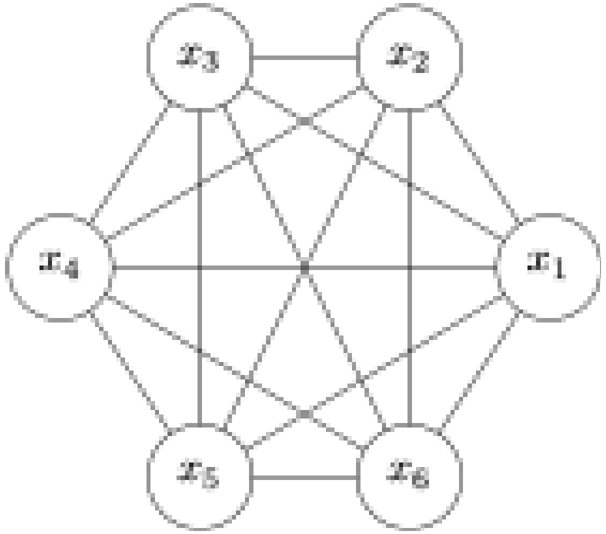
$$\text{Hallucination rate} \geq \widehat{\text{MF}} - \text{miscalibration} - \frac{300|\text{Facts}|}{|\text{Possible hallucinations}|} - \frac{7}{\sqrt{n}}$$

Number of facts seen only once in training / n
≈ "missing mass" of facts not seen in training

ASSOCIATIVE MEMORIES

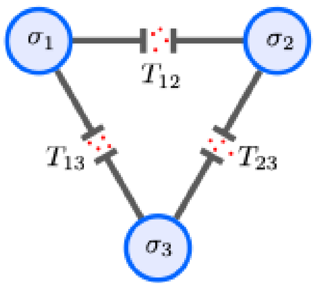
[Hopfield, 1982]

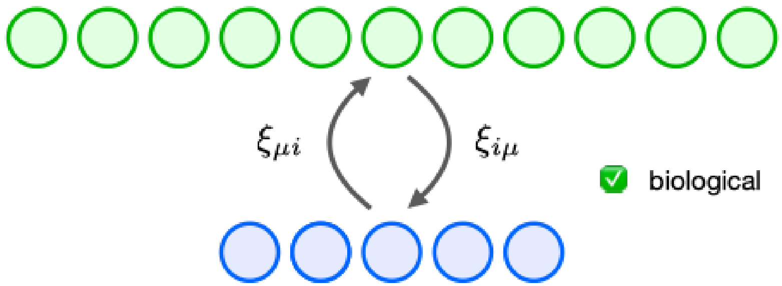
- Hopfield network: Each of d neurons is connected to all others
- State of neurons: $(x_1, \ldots, x_d) \in \{-1,1\}^d$
- How many (random) binary patterns can such a network memorize?



MODERN HOPFIELD NETWORKS

- Hopfield networks: d neurons can memorize $n \sim d$ binary patterns
- "Modern" Hopfield networks: $n \sim \exp(\Omega(d))$ [Demircigil et al, 2017; Ramsauer et al, 2021; Krotov & Hopfield, 2016, 2021]
  - One-step dynamics equivalent to self-attention mechanism in transformers





  - Continuous dynamics [Geshkovski, Letrouit, Polyanskiy, Rigollet, 2023]: related to interacting particle systems and models of opinion dynamics

Implications for capabilities of transformers?

[Figures from Krotov & Hopfield, 2021]

CLOSING

This tutorial:
+ How do transformers work?
+ Some theoretical perspectives

Open question: Which ingredients are essential?

Thank you! Any questions?