Expressivity of Transformers: Logic, Circuits, and Formal Languages

Day 3: Transformers and Turing Machines

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31 July 2024

Main Result (too informal)

Theorem (Pérez et al., 2019, Pérez et al., 2021)

Transformers are Turing-complete!!!1

Main Result (too informal)

▲ tambourine_man on June 15, 2023 | parent | next [–]

Transformers are Turing complete, right?

▲ nyrikki on June 15, 2023 | root | parent | next [–]

The paper from yesterday:

https://news.ycombinator.c...

Showed that attention with positional encodings and arbitrary precision rational activation functions is Turing complete.

Using a finite precision, nonrational activation function and/or without positional encodings is not Turning complete.

▲ canjobear on June 15, 2023 | root | parent | prev | next [–]

No, they are actually very limited formally. For example you can't model a language of nested brackets to arbitrary depth (as you can with an RNN). That makes it all the more interesting that they are so successful.

https://news.ycombinator.com/item?id=36311871

Main Result (informal)

Theorem (Pérez et al., 2019, Pérez et al., 2021)

An average-hard attention transformer decoder using position embeddings and intermediate steps can simulate a Turing machine.

Today's Goals

- **Define** a transformer *decoder* as well as *intermediate steps* and how they relate to *chain of thought*
- **Explain** in what sense a transformer is and isn't Turing-complete
- **Understand** how a transformer, which has no memory, can simulate a Turing machine's tape

Background

Main Result (informal)

Theorem (Pérez et al., 2019, Pérez et al., 2021)

An average-hard attention transformer decoder using position embeddings and intermediate steps can simulate a Turing machine.

Average-Hard Attention

- Like unique-hard attention, attention goes only to highest-scoring positions
- Unlike unique-hard attention, attention is divided equally among highest-scoring positions

scores s	0	1	1
softmax	0.16	0.42	0.42
leftmost-hard	0	1	0
rightmost-hard	0	0	1
average-hard	0	0.5	0.5

Average-Hard Attention

Exercises:

scores s	2	2	0	2	1
average-hard					

scores s	0	0	0	0	0
average-hard					

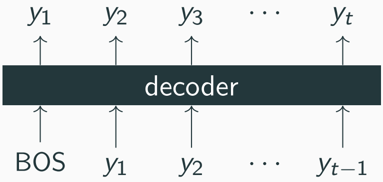
Main Result (informal)

Theorem (Pérez et al., 2019, Pérez et al., 2021)

An average-hard attention transformer decoder using position embeddings and intermediate steps can simulate a Turing machine.

Transformer Decoders

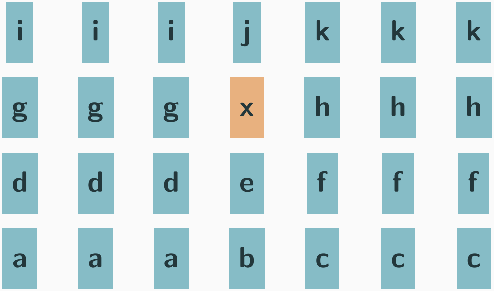
- At each time step, the decoder outputs a word
  - In practice: a probability distribution over words
  - Often in theory: the exact embedding of a word
- The output word becomes the next input word (autoregression)



Future Masking

- At each time step i, attention only attends to positions $j \leq i$
- Optional in encoders, mandatory in decoders

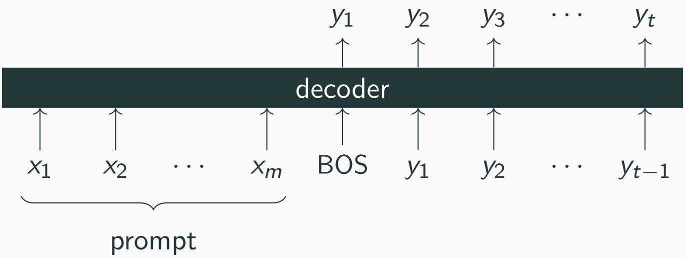
Exercise: Without autoregression, which vectors does vector x depend on?



(How about with autoregression?)

Prompting

- BOS can be preceded by input symbols, known as a *prompt*



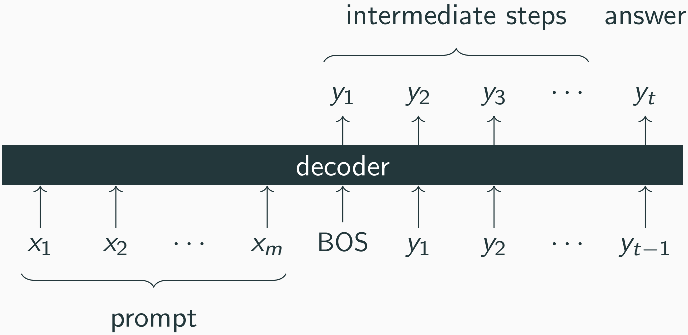
Main Result (informal)

Theorem (Pérez et al., 2019, Pérez et al., 2021)

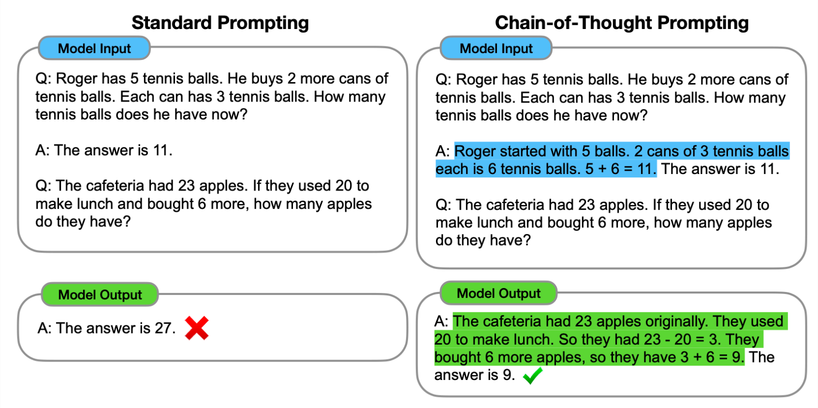
An average-hard attention transformer decoder using position embeddings and intermediate steps can simulate a Turing machine.

Intermediate Steps

- Allow *intermediate* output symbols between BOS and the final output (here, just a single symbol)



Theory Predicts Practice



[Wei et al., 2022]

Main Result (informal)

Theorem (Pérez et al., 2019, Pérez et al., 2021)

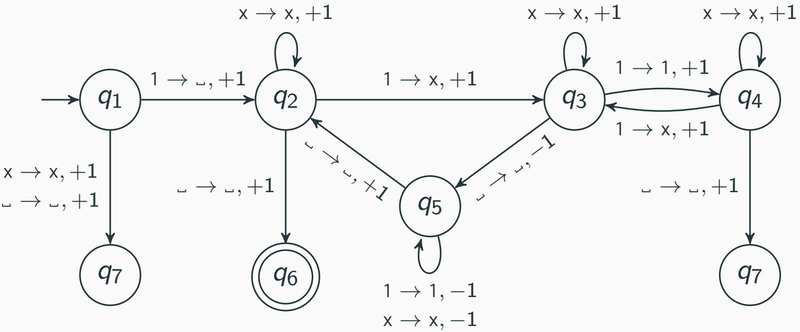
An average-hard attention transformer decoder using position embeddings and intermediate steps can simulate a Turing machine.

Turing Machines

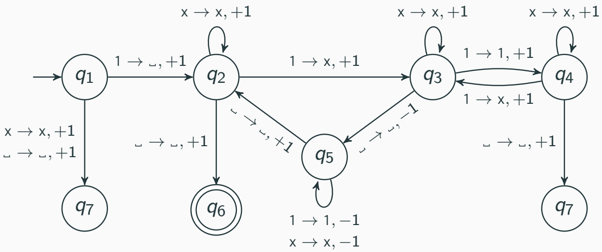
1	1	1	1	␣	␣	␣	␣	$\cdots$
^								

- Semi-infinite tape
- Cells are numbered starting from 0
- At each step, head moves either left (-1) or right ($+1$)

Turing machine for $\{1^{2^m} \mid m \geq 0\}$



Turing Machines



q_1	$\underset{\wedge}{1}1␣\cdots$
q_2	$␣\underset{\wedge}{1}␣\cdots$
q_3	$␣\mathsf{x}\underset{\wedge}{␣}\cdots$
q_5	$␣\underset{\wedge}{\mathsf{x}}␣\cdots$
q_5	$\underset{\wedge}{␣}\mathsf{x}␣\cdots$
q_2	$␣\underset{\wedge}{\mathsf{x}}␣\cdots$
q_6	accept

Turing Machines

Question: What are the inputs and outputs of a Turing machine's transition function?

$$\delta(q, a) = (q', b, m)$$

Simulating Turing Machines

Main Result

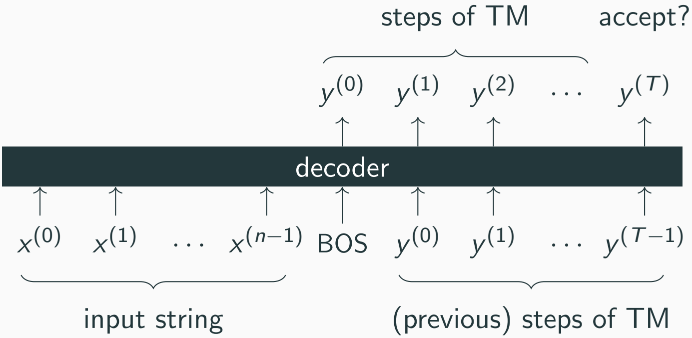
Theorem (Pérez et al., 2019, Pérez et al., 2021)

For any Turing machine M with input alphabet Σ, there is an average-hard attention transformer decoder f with position embedding $i \mapsto (1/(i+1), 1, i, i^2)$ that is equivalent to M in the following sense. For any string $w \in \Sigma^*$:

- *If M halts and accepts on input w, then there is a T such that f, on prompt w, outputs* ACC *after T intermediate steps.*
- *If M halts and rejects on input w, then there is a T such that f, on prompt w, outputs* REJ *after T intermediate steps.*
- *If M does not halt on input w, then there does not exist a T such that f, on prompt w, outputs either* ACC *or* REJ.

Key Idea 1

Use intermediate steps to simulate steps of Turing machine



Key Idea 2

How can a transformer, which has no memory, simulate a Turing machine's head?

Key Idea 2

How can a transformer, which has no memory, simulate a Turing machine's head?

Answer: Sum all the previous moves

previous move $m^{(i-1)}$	$+1$	$+1$	-1	-1	$+1$
current position $h^{(i)}$	1	2	1	0	1

Key Idea 3

How can a transformer, which has no memory, simulate a Turing machine's tape?

Key Idea 3

How can a transformer, which has no memory, simulate a Turing machine's tape?

Answer: Look at the most recent time the head was at current position $h^{(i)}$

- If none, the current symbol is the $h^{(i)}$-th input symbol
- If time j, the current symbol is what was written at time j

Input: $11\text{␣}\cdots$

previous position $h^{(i-1)}$	0	1	2	1	0
previous write $b^{(i-1)}$	␣	x	␣	x	␣
current position $h^{(i)}$	1	2	1	0	1
current symbol $a^{(i)}$	1	␣	x	␣	x

Position Embeddings

Position Embeddings

Adding a few simple elements to the position embeddings enables a very useful set of tricks [Barceló et al., 2024]:

$$\mathrm{PE}(i) = \begin{bmatrix} 1/(i+1) \\ 1 \\ i \\ i^2 \end{bmatrix}.$$

Forward Lookup

Assume that we have computed, for $i \in [n]$,

$$f(i) \in [n]$$
$$g(i) \in \mathbb{R}$$

Forward lookup: Compute $g(f(i))$ for $i \in [n]$

i	0	1	2	3	4
$f(i)$	0	1	1	2	3
$g(i)$	0	1	4	9	16
$g(f(i))$	0	1	1	4	9

Forward Lookup

Assume that we have computed, for $i \in [n]$,

$$f(i) \in [n]$$
$$g(i) \in \mathbb{R}$$

Forward lookup: Compute $g(f(i))$ for $i \in [n]$

$$\text{query}_i = \begin{bmatrix} f(i) \\ 1 \end{bmatrix} \qquad \text{key}_j = \begin{bmatrix} 2j \\ -j^2 \end{bmatrix} \qquad \text{value}_j = \begin{bmatrix} g(j) \end{bmatrix}$$

Exercise: Compute $\text{score}_{ij} = \text{query}_i \cdot \text{key}_j$ and maximize with respect to j.

Forward Lookup

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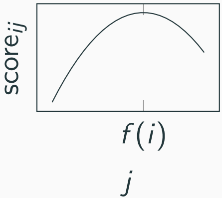
$$\begin{aligned} \text{score}_{ij} &= \text{query}_i \cdot \text{key}_j \\ &= -j^2 + 2f(i)j \\ \operatorname*{argmax}_j \text{score}_{ij} &= f(i). \end{aligned}$$



Backward Lookup

Assume that we have computed, for $i \in [n]$,

$$f(i) \in \mathbb{R}$$
$$g(i) \in \mathbb{R}$$

Backward lookup: compute $g^{-1}(f(i))$ for $i \in [n]$. That is, find j such that $g(j) = f(i)$.

i	0	1	2	3	4
$f(i)$	0	1	1	4	9
$g(i)$	0	1	4	9	16
$g^{-1}(f(i))$	0	1	1	2	3

Backward Lookup

Assume that we have computed, for $i \in [n]$,

$$f(i) \in \mathbb{R}$$

$$g(i) \in \mathbb{R}$$

Backward lookup: compute $g^{-1}(f(i))$ for $i \in [n]$. That is, find j such that $g(j) = f(i)$.

$$\text{query}_i = \begin{bmatrix} f(i) \\ 1 \end{bmatrix} \qquad \text{key}_j = \begin{bmatrix} 2g(j) \\ -g(j)^2 \end{bmatrix} \qquad \text{value}_j = \begin{bmatrix} j \end{bmatrix}$$

$$\begin{aligned} \text{score}_{ij} &= \text{query}_i \cdot \text{key}_j \\ &= -g(j)^2 + 2f(i)g(j) \\ \operatorname*{argmax}_j \text{score}_{ij} &= g^{-1}(f(i)). \end{aligned}$$

Backward Lookup

Assume that we have computed, for $i \in [n]$,

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$$g(i) \in \mathbb{R}$$

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forward lookup

$$\begin{aligned} \text{score}_{ij} &= \text{query}_i \cdot \text{key}_j \\ &= -g(j)^2 + 2f(i)g(j) \\ \operatorname*{argmax}_j \text{score}_{ij} &= g^{-1}(f(i)). \end{aligned}$$

Multiplication and Division

Assume that we have computed, for $i \in [n]$,

$$f(i) \in \mathbb{R}$$
$$g(i) \in \mathbb{R}$$

and we want to compute $f(i)/g(i) \in [n]$.

i	0	1	2	3	4
$f(i)$	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{3}{4}$	$\frac{2}{5}$
$g(i)$	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$
$g(f(i))$	1	1	1	3	2

Multiplication and Division

Assume that we have computed, for $i \in [n]$,

$$f(i) \in \mathbb{R}$$
$$g(i) \in \mathbb{R}$$

and we want to compute $f(i)/g(i) \in [n]$.

$$\text{query}_i = \begin{bmatrix} f(i) \\ g(i) \end{bmatrix} \qquad \text{key}_j = \begin{bmatrix} 2j \\ -j^2 \end{bmatrix} \qquad \text{value}_j = \begin{bmatrix} j \end{bmatrix}$$

$$\begin{aligned} \text{score}_{ij} &= \text{query}_i \cdot \text{key}_j \\ &= -g(i)j^2 + 2f(i)j \\ \operatorname*{argmax}_j \text{score}_{ij} &= f(i)/g(i). \end{aligned}$$

Exercise: How would you compute $f(i)\,g(i)$?

Simulating Turing Machines: In More Detail

Detailed Overview

i	tape	$x^{(i)}$	$q^{(i)}$	$b^{(i-1)}$	$m^{(i-1)}$	$h^{(i)}$	$a^{(i)}$	$y^{(i)}$	
0	$\underset{\wedge}{1}1\textvisiblespace\cdots$	1	$\perp$	$\perp$	0	0	1	1	wait
1	$\underset{\wedge}{1}1\textvisiblespace\cdots$	1	$\perp$	$\perp$	0	0	1	1	
2	$\underset{\wedge}{1}1\textvisiblespace\cdots$	BOS	$\perp$	$\perp$	0	0	1	$(q_1, 1, 0)$	
3	$\underset{\wedge}{1}1\textvisiblespace\cdots$	$(q_1, 1, 0)$	q_1	1	0	0	1	$(q_2, \textvisiblespace, +1)$	
4	$\textvisiblespace\underset{\wedge}{1}\textvisiblespace\cdots$	$(q_2, \textvisiblespace, +1)$	q_2	$\textvisiblespace$	$+1$	1	1	$(q_3, \mathrm{x}, +1)$	
5	$\textvisiblespace\mathrm{x}\underset{\wedge}{\textvisiblespace}\cdots$	$(q_3, \mathrm{x}, +1)$	q_3	x	$+1$	2	$\textvisiblespace$	$(q_5, \textvisiblespace, -1)$	
6	$\textvisiblespace\underset{\wedge}{\mathrm{x}}\textvisiblespace\cdots$	$(q_5, \textvisiblespace, -1)$	q_5	$\textvisiblespace$	-1	1	x	$(q_5, \mathrm{x}, -1)$	
7	$\underset{\wedge}{\textvisiblespace}\mathrm{x}\textvisiblespace\cdots$	$(q_5, \mathrm{x}, -1)$	q_5	x	-1	0	$\textvisiblespace$	$(q_2, \textvisiblespace, +1)$	
8	$\textvisiblespace\underset{\wedge}{\mathrm{x}}\textvisiblespace\cdots$	$(q_2, \textvisiblespace, +1)$	q_2	$\textvisiblespace$	$+1$	1	x	ACC	

Transformer reads in input string, simulated TM does nothing

Detailed Overview

i	tape	$x^{(i)}$	$q^{(i)}$	$b^{(i-1)}$	$m^{(i-1)}$	$h^{(i)}$	$a^{(i)}$	$y^{(i)}$	
0	$\underset{\wedge}{1}1\textvisiblespace\cdots$	1	$\perp$	$\perp$	0	0	1	1	
1	$\underset{\wedge}{1}1\textvisiblespace\cdots$	1	$\perp$	$\perp$	0	0	1	1	
2	$\underset{\wedge}{1}1\textvisiblespace\cdots$	BOS	$\perp$	$\perp$	0	0	1	$(q_1, 1, 0)$	init
3	$\underset{\wedge}{1}1\textvisiblespace\cdots$	$(q_1, 1, 0)$	q_1	1	0	0	1	$(q_2, \textvisiblespace, +1)$	
4	$\textvisiblespace\underset{\wedge}{1}\textvisiblespace\cdots$	$(q_2, \textvisiblespace, +1)$	q_2	$\textvisiblespace$	$+1$	1	1	$(q_3, \mathrm{x}, +1)$	
5	$\textvisiblespace\mathrm{x}\underset{\wedge}{\textvisiblespace}\cdots$	$(q_3, \mathrm{x}, +1)$	q_3	x	$+1$	2	$\textvisiblespace$	$(q_5, \textvisiblespace, -1)$	
6	$\textvisiblespace\underset{\wedge}{\mathrm{x}}\textvisiblespace\cdots$	$(q_5, \textvisiblespace, -1)$	q_5	$\textvisiblespace$	-1	1	x	$(q_5, \mathrm{x}, -1)$	
7	$\underset{\wedge}{\textvisiblespace}\mathrm{x}\textvisiblespace\cdots$	$(q_5, \mathrm{x}, -1)$	q_5	x	-1	0	$\textvisiblespace$	$(q_2, \textvisiblespace, +1)$	
8	$\textvisiblespace\underset{\wedge}{\mathrm{x}}\textvisiblespace\cdots$	$(q_2, \textvisiblespace, +1)$	q_2	$\textvisiblespace$	$+1$	1	x	ACC	

Transformer outputs fake action, simulated TM enters start state

Detailed Overview

i	tape	$x^{(i)}$	$q^{(i)}$	$b^{(i-1)}$	$m^{(i-1)}$	$h^{(i)}$	$a^{(i)}$	$y^{(i)}$
0	$\underset{\wedge}{1}1\text{␣}\cdots$	1	$\perp$	$\perp$	0	0	1	1
1	$\underset{\wedge}{1}1\text{␣}\cdots$	1	$\perp$	$\perp$	0	0	1	1
2	$\underset{\wedge}{1}1\text{␣}\cdots$	BOS	$\perp$	$\perp$	0	0	1	$(q_1, 1, 0)$
3	$\underset{\wedge}{1}1\text{␣}\cdots$	$(q_1, 1, 0)$	q_1	1	0	0	1	$(q_2, \text{␣}, +1)$
4	$\text{␣}\underset{\wedge}{1}\text{␣}\cdots$	$(q_2, \text{␣}, +1)$	q_2	␣	$+1$	1	1	$(q_3, \text{x}, +1)$
5	$\text{␣x}\underset{\wedge}{\text{␣}}\cdots$	$(q_3, \text{x}, +1)$	q_3	x	$+1$	2	␣	$(q_5, \text{␣}, -1)$
6	$\text{␣}\underset{\wedge}{\text{x}}\text{␣}\cdots$	$(q_5, \text{␣}, -1)$	q_5	␣	-1	1	x	$(q_5, \text{x}, -1)$
7	$\underset{\wedge}{\text{␣}}\text{x␣}\cdots$	$(q_5, \text{x}, -1)$	q_5	x	-1	0	␣	$(q_2, \text{␣}, +1)$
8	$\text{␣}\underset{\wedge}{\text{x}}\text{␣}\cdots$	$(q_2, \text{␣}, +1)$	q_2	␣	$+1$	1	x	ACC

run

Transformer outputs the actions of the simulated TM one by one

Detailed Overview

i	tape	$x^{(i)}$	$q^{(i)}$	$b^{(i-1)}$	$m^{(i-1)}$	$h^{(i)}$	$a^{(i)}$	$y^{(i)}$
0	$\underset{\wedge}{1}1␣\cdots$	1	$\perp$	$\perp$	0	0	1	1
1	$\underset{\wedge}{1}1␣\cdots$	1	$\perp$	$\perp$	0	0	1	1
2	$\underset{\wedge}{1}1␣\cdots$	BOS	$\perp$	$\perp$	0	0	1	$(q_1, 1, 0)$
3	$\underset{\wedge}{1}1␣\cdots$	$(q_1, 1, 0)$	q_1	1	0	0	1	$(q_2, ␣, +1)$
4	$␣\underset{\wedge}{1}␣\cdots$	$(q_2, ␣, +1)$	q_2	␣	$+1$	1	1	$(q_3, \mathrm{x}, +1)$
5	$␣\mathrm{x}\underset{\wedge}{␣}\cdots$	$(q_3, \mathrm{x}, +1)$	q_3	x	$+1$	2	␣	$(q_5, ␣, -1)$
6	$␣\underset{\wedge}{\mathrm{x}}␣\cdots$	$(q_5, ␣, -1)$	q_5	␣	-1	1	x	$(q_5, \mathrm{x}, -1)$
7	$\underset{\wedge}{␣}\mathrm{x}␣\cdots$	$(q_5, \mathrm{x}, -1)$	q_5	x	-1	0	␣	$(q_2, ␣, +1)$
8	$␣\underset{\wedge}{\mathrm{x}}␣\cdots$	$(q_2, ␣, +1)$	q_2	␣	$+1$	1	x	ACC
		input						

Detailed Overview

i	tape	$x^{(i)}$	$q^{(i)}$	$b^{(i-1)}$	$m^{(i-1)}$	$h^{(i)}$	$a^{(i)}$	$y^{(i)}$
0	$\underset{\wedge}{1}1\textvisiblespace\cdots$	1	$\perp$	$\perp$	0	0	1	1
1	$\underset{\wedge}{1}1\textvisiblespace\cdots$	1	$\perp$	$\perp$	0	0	1	1
2	$\underset{\wedge}{1}1\textvisiblespace\cdots$	BOS	$\perp$	$\perp$	0	0	1	$(q_1, 1, 0)$
3	$\underset{\wedge}{1}1\textvisiblespace\cdots$	$(q_1, 1, 0)$	q_1	1	0	0	1	$(q_2, \textvisiblespace, +1)$
4	$\textvisiblespace\underset{\wedge}{1}\textvisiblespace\cdots$	$(q_2, \textvisiblespace, +1)$	q_2	$\textvisiblespace$	$+1$	1	1	$(q_3, \text{x}, +1)$
5	$\textvisiblespace\text{x}\underset{\wedge}{\textvisiblespace}\cdots$	$(q_3, \text{x}, +1)$	q_3	x	$+1$	2	$\textvisiblespace$	$(q_5, \textvisiblespace, -1)$
6	$\textvisiblespace\underset{\wedge}{\text{x}}\textvisiblespace\cdots$	$(q_5, \textvisiblespace, -1)$	q_5	$\textvisiblespace$	-1	1	x	$(q_5, \text{x}, -1)$
7	$\underset{\wedge}{\textvisiblespace}\text{x}\textvisiblespace\cdots$	$(q_5, \text{x}, -1)$	q_5	x	-1	0	$\textvisiblespace$	$(q_2, \textvisiblespace, +1)$
8	$\textvisiblespace\underset{\wedge}{\text{x}}\textvisiblespace\cdots$	$(q_2, \textvisiblespace, +1)$	q_2	$\textvisiblespace$	$+1$	1	x	ACC

step 1

Unpack previous action into state (q), write (b), and move (m)

Detailed Overview

i	tape	$x^{(i)}$	$q^{(i)}$	$b^{(i-1)}$	$m^{(i-1)}$	$h^{(i)}$	$a^{(i)}$	$y^{(i)}$
0	$\underset{\wedge}{1}1\sqcup\cdots$	1	$\perp$	$\perp$	0	0	1	1
1	$\underset{\wedge}{1}1\sqcup\cdots$	1	$\perp$	$\perp$	0	0	1	1
2	$\underset{\wedge}{1}1\sqcup\cdots$	BOS	$\perp$	$\perp$	0	0	1	$(q_1, 1, 0)$
3	$\underset{\wedge}{1}1\sqcup\cdots$	$(q_1, 1, 0)$	q_1	1	0	0	1	$(q_2, \sqcup, +1)$
4	$\sqcup\underset{\wedge}{1}\sqcup\cdots$	$(q_2, \sqcup, +1)$	q_2	$\sqcup$	$+1$	1	1	$(q_3, \mathrm{x}, +1)$
5	$\sqcup\mathrm{x}\underset{\wedge}{\sqcup}\cdots$	$(q_3, \mathrm{x}, +1)$	q_3	x	$+1$	2	$\sqcup$	$(q_5, \sqcup, -1)$
6	$\sqcup\underset{\wedge}{\mathrm{x}}\sqcup\cdots$	$(q_5, \sqcup, -1)$	q_5	$\sqcup$	-1	1	x	$(q_5, \mathrm{x}, -1)$
7	$\underset{\wedge}{\sqcup}\mathrm{x}\sqcup\cdots$	$(q_5, \mathrm{x}, -1)$	q_5	x	-1	0	$\sqcup$	$(q_2, \sqcup, +1)$
8	$\sqcup\underset{\wedge}{\mathrm{x}}\sqcup\cdots$	$(q_2, \sqcup, +1)$	q_2	$\sqcup$	$+1$	1	x	ACC
						step 2		

Compute head position (h) by summing previous moves

Detailed Overview

i	tape	$x^{(i)}$	$q^{(i)}$	$b^{(i-1)}$	$m^{(i-1)}$	$h^{(i)}$	$a^{(i)}$	$y^{(i)}$
0	$\underset{\wedge}{1}1␣\cdots$	1	$\bot$	$\bot$	0	0	1	1
1	$\underset{\wedge}{1}1␣\cdots$	1	$\bot$	$\bot$	0	0	1	1
2	$\underset{\wedge}{1}1␣\cdots$	BOS	$\bot$	$\bot$	0	0	1	$(q_1, 1, 0)$
3	$\underset{\wedge}{1}1␣\cdots$	$(q_1, 1, 0)$	q_1	1	0	0	1	$(q_2, ␣, +1)$
4	$␣\underset{\wedge}{1}␣\cdots$	$(q_2, ␣, +1)$	q_2	␣	$+1$	1	1	$(q_3, \mathrm{x}, +1)$
5	$␣\mathrm{x}\underset{\wedge}{␣}\cdots$	$(q_3, \mathrm{x}, +1)$	q_3	x	$+1$	2	␣	$(q_5, ␣, -1)$
6	$␣\underset{\wedge}{\mathrm{x}}␣\cdots$	$(q_5, ␣, -1)$	q_5	␣	-1	1	x	$(q_5, \mathrm{x}, -1)$
7	$\underset{\wedge}{␣}\mathrm{x}␣\cdots$	$(q_5, \mathrm{x}, -1)$	q_5	x	-1	0	␣	$(q_2, ␣, +1)$
8	$␣\underset{\wedge}{\mathrm{x}}␣\cdots$	$(q_2, ␣, +1)$	q_2	␣	$+1$	1	x	ACC

step 3

Compute current tape symbol (a)

Detailed Overview

i	tape	$x^{(i)}$	$q^{(i)}$	$b^{(i-1)}$	$m^{(i-1)}$	$h^{(i)}$	$a^{(i)}$	$y^{(i)}$
0	$\underset{\wedge}{1}1\textvisiblespace\cdots$	1	$\perp$	$\perp$	0	0	1	1
1	$\underset{\wedge}{1}1\textvisiblespace\cdots$	1	$\perp$	$\perp$	0	0	1	1
2	$\underset{\wedge}{1}1\textvisiblespace\cdots$	BOS	$\perp$	$\perp$	0	0	1	$(q_1, 1, 0)$
3	$\underset{\wedge}{1}1\textvisiblespace\cdots$	$(q_1, 1, 0)$	q_1	1	0	0	1	$(q_2, \textvisiblespace, +1)$
4	$\textvisiblespace\underset{\wedge}{1}\textvisiblespace\cdots$	$(q_2, \textvisiblespace, +1)$	q_2	$\textvisiblespace$	$+1$	1	1	$(q_3, \mathrm{x}, +1)$
5	$\textvisiblespace\mathrm{x}\underset{\wedge}{\textvisiblespace}\cdots$	$(q_3, \mathrm{x}, +1)$	q_3	x	$+1$	2	$\textvisiblespace$	$(q_5, \textvisiblespace, -1)$
6	$\textvisiblespace\underset{\wedge}{\mathrm{x}}\textvisiblespace\cdots$	$(q_5, \textvisiblespace, -1)$	q_5	$\textvisiblespace$	-1	1	x	$(q_5, \mathrm{x}, -1)$
7	$\underset{\wedge}{\textvisiblespace}\mathrm{x}\textvisiblespace\cdots$	$(q_5, \mathrm{x}, -1)$	q_5	x	-1	0	$\textvisiblespace$	$(q_2, \textvisiblespace, +1)$
8	$\textvisiblespace\underset{\wedge}{\mathrm{x}}\textvisiblespace\cdots$	$(q_2, \textvisiblespace, +1)$	q_2	$\textvisiblespace$	$+1$	1	x	ACC

step 4

Output next action

Step 1: Unpack Input Symbol

...into current state, previously written symbol, and previous move.

phase	$x^{(i)}$	$q^{(i)}$	$b^{(i-1)}$	$m^{(i-1)}$
wait	$\in \Sigma$	$\perp$	$\perp$	0
init	BOS	$\perp$	$\perp$	0
run	(r, b, m)	r	b	m

Use a FFN to compute the function

$$x^{(i)} \mapsto \begin{bmatrix} q^{(i)} \\ b^{(i-1)} \\ m^{(i-1)} \end{bmatrix}$$

Step 2a: Compute Head Position

The current head position is just the sum of all previous moves:

$$h^{(i)} = \sum_{j=0}^{i} m^{(j-1)}$$

Using uniform self-attention, we can compute

$$h^{(i)}/(i+1) = \frac{1}{i+1} \sum_{j=0}^{i} m^{(j-1)}$$

Question: How do we get rid of the $\cdot/(i+1)$?

Step 3: Compute Tape Symbol

Find most recent $j < i$ such that $h^{(j)} = h^{(i)}$ and return $b^{(j)}$; if none, return $x^{h^{(i)}}$.

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We can't do this because we only have non-strict masking ($j \leq i$).

Step 3: Compute Tape Symbol

~~Find most recent $j < i$ such that $h^{(j)} = h^{(i)}$ and return $b^{(j)}$; if none, return $x^{h^{(i)}}$.~~

Find most recent $j \leq i$ such that $h^{(j-1)} = h^{(i)}$ and return $b^{(j-1)}$; if none, return $x^{h^{(i)}}$.

This is a reverse table lookup of $h^{(i)}$ in $j \mapsto h^{(j-1)}$. But finding the *most recent* will require some extra care.

Step 3b: Compute Tape Symbol

Find most recent $j \leq i$ such that $h^{(j-1)} = h^{(i)}$ and return $b^{(j-1)}$; if none, return $x^{h^{(i)}}$.

Reverse table lookup with tie-breaking:

$$\text{query}_i = \begin{bmatrix} h^{(i)} \\ 1 \\ \frac{1}{2(i+1)} \end{bmatrix} \quad \text{key}_j = \begin{bmatrix} 2h^{(j-1)} \\ -(h^{(j-1)})^2 \\ j \end{bmatrix} \quad \text{value}_j = \begin{bmatrix} h^{(j-1)} \\ b^{(j-1)} \end{bmatrix}$$

Attention scores are:

$$\text{score}_{i,j} = \underbrace{-(h^{(j-1)})^2 + 2h^{(i)}h^{(j-1)}}_{\text{find } h^{(j-1)} = h^{(i)}} + \underbrace{\frac{j}{2(i+1)}}_{\text{find rightmost}}$$

Step 3b: Compute Tape Symbol

Find most recent $j \leq i$ such that $h^{(j-1)} = h^{(i)}$ and return $b^{(j-1)}$; if none, return $x^{h^{(i)}}$.

Reverse table lookup with tie-breaking: $= h^{(j)} - m^{(j-1)}$

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forward lookup

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Step 3b: Compute Tape Symbol

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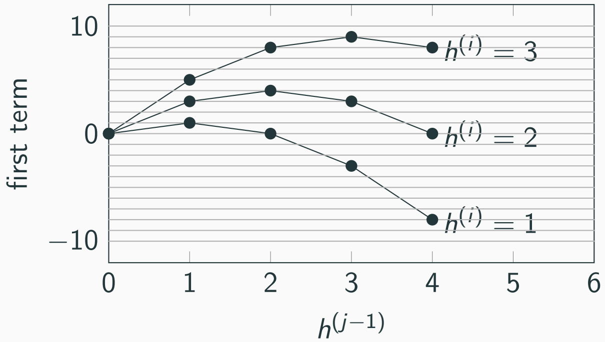
In first term, difference between best and second-best score is 1:



So we make the second term $\frac{j}{2(i+1)} \leq \frac{1}{2} < 1$.

Step 3b: Compute Tape Symbol

Find most recent $j \leq i$ such that $h^{(j-1)} = h^{(i)}$ and return $b^{(j-1)}$; if none, return $x^{h^{(j-1)}}$.

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FFN:

$$\text{if } h^{(j-1)} = h^{(i)} \text{ and } b^{(j-1)} \neq \perp \rightsquigarrow a^{(i)} := b^{(j-1)}$$
$$\text{else} \rightsquigarrow a^{(i)} := x^{(h^{(i)})}$$

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forward lookup

Step 4: Compute Transition

Given $x^{(i)}$ = current input symbol and $a^{(i)}$ = current tape symbol:

$$\begin{aligned} \text{if } x^{(i)} \in \Sigma &\rightsquigarrow \text{output } x^{(i)} \\ \text{if } x^{(i)} = \text{BOS} &\rightsquigarrow \text{let } (r, b, m) = (q_{\text{start}}, a^{(i)}, 0) \\ \text{else} &\rightsquigarrow \text{let } (r, b, m) = \delta(q^{(i)}, a^{(i)}) \end{aligned}$$

$$\begin{aligned} \text{if } r = q_{\text{accept}} &\rightsquigarrow \text{output ACC} \\ \text{if } r = q_{\text{reject}} &\rightsquigarrow \text{output REJ} \\ \text{else} &\rightsquigarrow \text{output } (r, b, m) \end{aligned}$$

Recap

- Transformer decoders generate strings; they may be allowed to generate *intermediate steps* (a.k.a. chain of thought).
- A transformer decoder can simulate a Turing machine by generating the steps of the Turing machine as intermediate steps. But not if the answer is required immediately.
- Even though it has no memory, a transformer can use attention to reconstruct what it needs to know about the Turing machine configuration.

References i

Pablo Barceló, Alexander Kozachinskiy, Anthony Widjaja Lin, and Vladimir Podolskii. Logical languages accepted by transformer encoders with hard attention. In *Proceedings of the Twelfth International Conference on Learning Representations (ICLR)*, 2024. URL https://openreview.net/forum?id=gbrHZq07mq.

Jorge Pérez, Pablo Barceló, and Javier Marinkovic. Attention is Turing-complete. *Journal of Machine Learning Research*, 22:75:1–75:35, 2021. URL http://jmlr.org/papers/v22/20-302.html.

Jorge Pérez, Javier Marinković, and Pablo Barceló. On the Turing completeness of modern neural network architectures. In *Proceedings of the Seventh International Conference on Learning Representations (ICLR)*, 2019. URL https://openreview.net/forum?id=HyGBdo0qFm.

Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, Brian Ichter, Fei Xia, Ed H. Chi, Quoc V. Le, and Denny Zhou. Chain-of-thought prompting elicits reasoning in large language models. In *Advances in Neural Information Processing Systems 35 (NeurIPS)*, pages 24824–24837, 2022. URL https://proceedings.neurips.cc/paper_files/paper/2022/hash/9d5609613524ecf4f15af0f7b31abca4-Abstract-Conference.html.