Thinking Like Transformers

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July 26, 2021

How does a transformer think, intuitively?

> Intuitively, transformers' computations are applied to their entire input in parallel, using attention to draw on and combine tokens from several positions at a time as they make their calculations (Vaswani et al., 2017; Bahdanau et al., 2015; Luong et al., 2015). The iterative process of a transformer is then not along the length of the input sequence but rather the depth of the computation: the number of layers it applies to its input as it works towards its final result.
>
> –Weiss, Goldberg & Yahav

What purpose does the RASP language serve?

We find RASP a natural tool for conveying transformer solutions to [...] tasks for which a human can encode a solution: we do not expect any researcher to implement, e.g., a strong language model or machine-translation system in RASP...we focus on programs that convey concepts people can encode in "traditional" programming languages, and the way they relate to the expressive power of the transformer...

Considering computation problems and their implementation in RASP allows us to "think like a transformer" while abstracting away the technical details of a neural network in favor of symbolic programs.

–Weiss, Goldberg & Yahav

RASP: Restricted Access Sequence Processing

If transformers are a series of operators applied to an input sequence in parallel, what operations could they be performing?

Not saying transformers are RASPs, but *for problems with known solutions*, they often share a curiously similar representation...

How do we do pack useful compute into matrix/vector arithmetic? Array programming seems to be a surprisingly good fit.

- Data types: $\{\mathbb{R}, \mathbb{N}, \mathbb{B}, \Sigma\}^n, \mathbb{B}^{n \times n}$
- Elementwise ops: $\{+, \times, \texttt{pow}\} : \mathbb{N}^n \to \mathbb{N}^n$ (e.g. $\mathbf{x} + \mathbf{1}$)
- Predicates: $\{\mathbb{R}, \mathbb{N}, \Sigma\}^n \to \mathbb{B}^n$
- Standard functions: `indices`: $\Sigma^n \to \mathbb{N}^n$, `tokens`: $\mathbb{N}^n \to \Sigma^n$,

Selection operator

Takes a key, query and predicate, and returns a selection matrix:

$$\texttt{select} : \Big(\underbrace{\mathbb{N}^n}_{key} \times \underbrace{\mathbb{N}^n}_{query} \times \underbrace{(\mathbb{N} \times \mathbb{N} \to \mathbb{B})}_{predicate} \Big) \to \mathbb{B}^{n \times n}$$

$$\texttt{select}(\underbrace{[0,1,2]}_{key}, \underbrace{\begin{bmatrix}1\\2\\3\end{bmatrix}}_{query}, <) = \begin{array}{c} \\ 1 \\ 2 \\ 3 \end{array} \begin{array}{c} \begin{array}{ccc} 0 & 1 & 2 \end{array} \\ \begin{bmatrix} 0<1 & 1<1 & 2<1 \\ 0<2 & 1<2 & 2<2 \\ 0<3 & 1<3 & 2<3 \end{bmatrix} \end{array}$$

$$= \begin{bmatrix} \mathbf{T} & F & F \\ \mathbf{T} & \mathbf{T} & F \\ \mathbf{T} & \mathbf{T} & \mathbf{T} \end{bmatrix}$$

Aggregate

Takes a selection matrix, a list, and averages the selected values:

$$\texttt{aggregate} : (\mathbb{B}^{n \times n} \times \underbrace{\mathbb{N}^n}_{list}) \rightarrow \mathbb{R}^n$$

$$\texttt{aggregate}\left(\begin{bmatrix} \mathbf{T} & F & F \\ \mathbf{T} & \mathbf{T} & F \\ \mathbf{T} & \mathbf{T} & \mathbf{T} \end{bmatrix}, \begin{bmatrix} 10 & 20 & 30 \end{bmatrix} \right) = \begin{bmatrix} \frac{10}{1} & \frac{10+20}{2} & \frac{10+20+30}{3} \end{bmatrix}$$

$$= \begin{bmatrix} 10 & 15 & 20 \end{bmatrix}$$

Selector width

Takes a selection matrix, a string and returns the histogram:

$$\texttt{selector\_width} : \mathbb{B}^{n\times n} \to \Sigma^n \to \mathbb{N}^n$$

$$\texttt{selector\_width(same\_token)(}\begin{bmatrix}\texttt{h} & \texttt{e} & \texttt{l} & \texttt{l} & \texttt{o}\end{bmatrix}\texttt{)}$$

$$= \begin{bmatrix} \mathbf{T} & F & F & F & F \\ F & \mathbf{T} & F & F & F \\ F & F & \mathbf{T} & \mathbf{T} & F \\ F & F & \mathbf{T} & \mathbf{T} & F \\ F & F & F & F & \mathbf{T} \end{bmatrix} \begin{bmatrix}\texttt{h} & \texttt{e} & \texttt{l} & \texttt{l} & \texttt{o}\end{bmatrix}$$

$$= \begin{bmatrix} 1 & 1 & 2 & 2 & 1 \end{bmatrix}$$

Dyck words and languages

Definition

A **Dyck-1 word** is a string containing the same number of (’s and)’s, where the number of)’s in every prefix is less than or equal to the number of (’s.

✓ `((()))`, `(())()`, `()(())`, `(()())`, `()()()`

✗ `)))(((`, `))(()(`, `)())((`, `))()((`, `)()()(`, `(((()(`,…

Definition

A **Dyck-n word** is a Dyck word with n bracket types.

✓ `()[]{}`, `([]{})`, `[(){}]`, `{()[]}`, `([]){}`, `[()]{}`, …

✗ `([)]{}`, `[{]}()`, `[{](})`, `([){]}`, `...` , `}{()]]`

shuffle Dyck-3

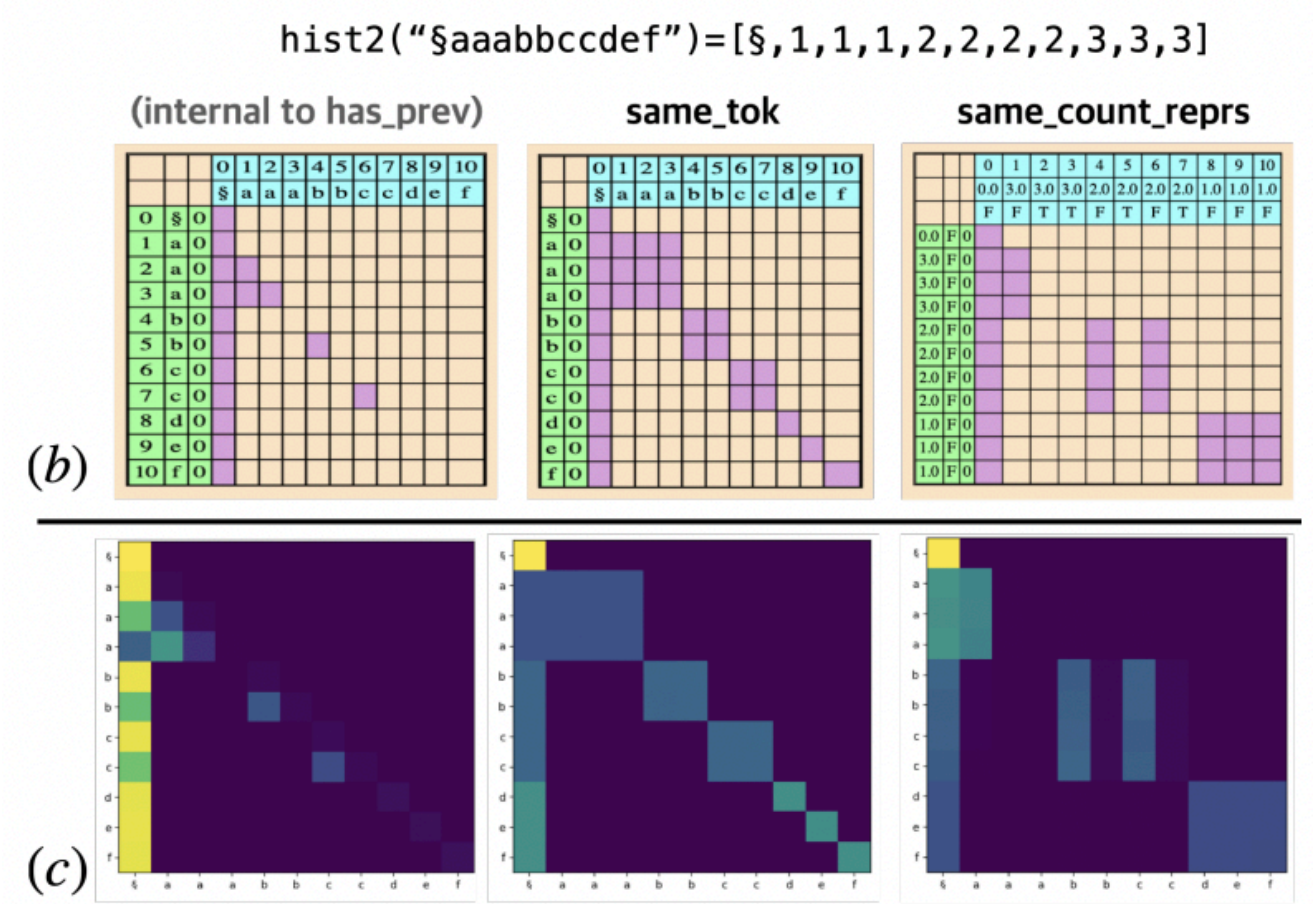
Experiments

Three sets of experiments:

- With attention supervision: assuming the solution could be learned, would it even work in the first place?
- Without attention supervision: does standard supervision (i.e. cross-entropy loss on the target without teacher forcing) recover the same (or similar) solution?
- How tight are the RASP-implied bounds for the minimum number of layers and maximum attention heads? Compile the RASP to a transformer: there exists a transformer which can solve the task! But can we recover it via learning?

Experiment 1: Compiling RASP to transformers

Can we force a transformer to implement RASP selectors?



Experiment 2: Can it be learned / does it learn the same thing?

So there exists a feasible solution. Can it be learned from scratch?

Language	Layers	Heads	Test Acc.	Attn. Matches?
Reverse	2	1	99.99%	✓✗
Hist BOS	1	1	100%	✓
Hist no BOS	1	2	99.97%	✓✗
Double Hist	2	2	99.58%	✓✗
Sort	2	1	99.96%	✗
Most Freq	3	2	95.99%	✗
Dyck-1 PTF	2	1	99.67%	✓✗
Dyck-2 PTF [8]	3	1	99.85%	✗

Experiment 3: How tight are the L, H bounds?

Is the RASP-implied depth/width necessary and/or sufficient?

Language	RASP	Average test accuracy (%) with...			
	L, H	L, H	$H-1$	$L-1$	$L-1, 2H$
Reverse	$2, 1$	**99.9**	-	23.1	41.2
Hist	$1, 2$	**99.9**	91.9	-	-
2-Hist	$2, 2$	**99.0**	73.5	40.5	83.5
Sort	$2, 1$	99.8	-	99.0	**99.9**
Most Freq	$3, 2$	**93.9**	92.1	84.0	90.2
Dyck-1	$2, 1$	**99.3**	-	96.9	96.4
Dyck-2	$3, 1$	**99.7**	-	98.8	94.1

What is this paper trying to say?

- Array programming provides an intuitive model for thinking about transformer reasoning
- Can logical matrices be interpreted as the fixed points of self attention (for certain problems)?
- The [optimal?] RASP solution a human constructs often matches the solution a transformer discovers
- Given a known solution, we can predict sufficient hyperparameters (e.g. depth, width) needed to learn it

Threats to validity

- How do we know whether RASP solutions are learnable? What do the L, H bounds tell us?
- Do transformers really think this way? Or are we just selecting problems which we can force a transformer to reproduce that are relatively "learnable"?
- Are there "unlearnable" tasks for which the RASP-implied bounds do not predict learnability in practice?
- What other evidence could be shown to demonstrate transformers actually think this way?
- What does these results really mean if we need to know a RASP solution exists a priori? If we knew it to begin with, would we really need a transformer to find it?
- Still, not a huge leap to think, *if* a human solution might exist and could be learned, maybe it could be decoded...

Unanswered questions/Future work

- How does ordering work? If selectors can be merged, how do you align attention heatmaps with selectors?
- What can we say (if anything) about uniqueness? Is there a way to canonicalize attention/selector order?
- Is there a way to "scale up" to longer sequences? How do/can you "upsample" a RASP heatmap?
- Would it be possible to extract RASP source code from a pretrained transformer?
- What other evidence could be shown to demonstrate transformers actually think this way?

References on Formal Language Induction / Recognition

- Weiss et al., Thinking Like Transformers (2021)
- Weiss et al., On the Practical Computational Power of Finite Precision RNNs for Language Recognition (2018)
- Weiss et al., Learning Deterministic Weighted Automata with Queries and Counterexamples (2019)
- Weiss et al., Extracting Automata from Recurrent Neural Networks Using Queries and Counterexamples (2018)
- Bhattamishra et al., On the Ability and Limitations of Transformers to Recognize Formal Languages (2020)
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