



# Thinking Like Transformers









Gail Weiss, Yoav Goldberg, Eran Yahav





### **Attention Is All You Need**

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, Illia Polosukhin





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What are they doing?

We're figuring out all kinds of things...



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Are Transformers universal approximators of sequence-to-sequence functions?

Chulhee Yun, Srinadh Bhojanapalli, Ankit Singh Rawat, Sashank J. Reddi, Sanjiv Kumar





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### **Theoretical Limitations of Self-Attention in Neural Sequence Models**

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### On the Ability and Limitations of Transformers to Recognize Formal Languages

Satwik Bhattamishra, Kabir Ahuja, Navin Goyal





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### **Attention is Turing-Complete**

Jorge Pérez, Pablo Barceló, Javier Marinkovic; 22(75):1-35, 2021.

### Statistically Meaningful Approximation: a Case Study on Approximating Turing Machines with Transformers

Colin Wei, Yining Chen, Tengyu Ma





L-star variants

Computational Model(s)!



**Deterministic** Finite Automata (DFAs)





RNNs to WFAs

DFA extraction: Clustering

DFA and WDFA extraction: L-star variants

LSTMs are counter machines

GRUs are DFAs

Computational Model(s)!



**Deterministic** Finite Automata (DFAs)





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RNNs to WFAs

DFA extraction: Clustering

DFA and WDFA extraction: L-star variants

LSTMs are counter machines

GRUs are DFAs

Stack-RNNs



Transformer Oct 16, 2012 god i wish that were me





## (References for the Interested)



Explaining Black Boxes on Sequential Data using Weighted Automata

> Extraction of Rules from Discrete-**Time Recurrent Neural Networks**

**Extracting Automata from Recurrent** Neural Networks Using Queries and Counterexamples

Connecting Weighted Automata and **Recurrent Neural Networks through** Spectral Learning

On the Practical Computational Power of Finite Precision RNNs for Language Recognition

Sequential Neural Networks as Automata

A Formal Hierarchy of RNN Architectures

Inferring Algorithmic Patterns with **Stack-Augmented Recurrent Nets** 

Learning to Transduce with **Unbounded Memory** 



### But what are Transformer-Encoders?











### Any ideas?

### **Transformer Encoders**



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### **Transformer Encoders**



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• Receive their entire input 'at once', processing all tokens in parallel

### **Transformer Encoders**



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- Receive their entire input 'at once', processing all tokens in parallel
- Have a fixed number of layers, where the output of one is the input of the next

### The Transformer-Encoder





### The Transformer-Encoder







Does this thing have "states"? What does it have?









The layers themselves are "operations"

# So... a programming language?

### **RASP (Restricted Access Sequence Processing)**

- Its layers apply operations to the sequence
- RASP describes the input sequences and what the layers can do with them



• A transformer-encoder is a sequence to sequence function ("sequence operator", or, "s-op")

The layers themselves are "operations"



### **RASP (Restricted Access Sequence Processing)**

- Its layers apply operations to the sequence
- RASP describes the **input sequences** and what the layers can do with them



• A transformer-encoder is a sequence to sequence function ("sequence operator", or, "s-op")

The layers themselves are "operations"



# **RASP base s-ops**



The information before a transformer has done anything ("0 layer transformer")





### **RASP base s-ops**

The information before a transformer has done anything ("0 layer transformer")

tokens and indices are RASP built-ins:

# **RASP base s-ops**



### The information before a transformer has done anything ("0 layer transformer")

tokens and indices are RASP built-ins:

Example: tokens("hello") = [h, e, l, l, o] (strings) s-op: indices Example: indices("hello") = [0, 1, 2, 3, 4] (ints)

> The RASP REPL gives you examples (until you ask it not to)





## Okay, now what?

>> tokens;

s-op: tokens

Example: tokens("hello") = [h, e, l, l, o] (strings)

### >> indices;

s-op: indices

Example: indices("hello") = [0, 1, 2, 3, 4] (ints)

To know what operations RASP may have, we must inspect the transformer-encoder layers!

### **Transformer-Encoder Layer**







### Feed-Forward Sublayer





### Feed-Forward Sublayer





### Feed-Forward gives us (Many) Elementwise Operations



>> indices+1; s-op: out Example: out("hello") >> tokens=="e" or tokens=="o"; s-op: out Example: out("hello")

### Multilayer Feedforward Networks are Universal Approximators

KURT HORNIK

Technische Universität Wien

MAXWELL STINCHCOMBE AND HALBERT WHITE

University of California, San Diego

(Received 16 September 1988; revised and accepted 9 March 1989)

**Abstract**—This paper rigorously establishes that standard multilayer feedforward networks with as few as one hidden layer using arbitrary squashing functions are capable of approximating any Borel measurable function from one finite dimensional space to another to any desired degree of accuracy, provided sufficiently many hidden units are available. In this sense, multilayer feedforward networks are a class of universal approximators.

### Example: out("hello") = [1, 2, 3, 4, 5] (ints) =="e" or tokens=="o";

Example: out("hello") = [F, T, F, F, T] (bools)



### So far

Are we all-powerful (well, transformer-powerful) yet?





## **Transformer-Encoder Layer**

# **Attention Sublayer**


## **Background - Multi Head Attention**

### Starting from single-head attention...

#### input



































scores



#### input



 $\mathbf{X}$ 

 $d_{v}$ 









### **Background - Multi-Headed Self Attention**



## The multi-headed attention lets one layer do multiple operations

It does not in itself add new power

# So, how do we present one head?



## Single Head: Scoring ↔ Selecting





Decision: RASP abstracts to binary choose/don't choose decisions



#### sel = select([2,0,0],[0,1,2],==)

2 0 0 0 F T T 1 F F F 2 T F F

Decision: RASP abstracts to binary choose/don't choose decisions



#### sel = select [2,0,0], [0,1,2], ==) 2 0 0 0 F T T 1 F F F 2 T F F

Decision: RASP abstracts to binary choose/don't choose decisions



## sel = select([2,0,0][0,1,2]]==)

2 0 0 0 F T T 1 F F F 2 T F F

Decision: RASP abstracts to binary choose/don't choose decisions



sel = select([2,0,0],[0,1,2],==)

2 0 0 0 F T T 1 F F F 2 T F F

Decision: RASP abstracts to binary choose/don't choose decisions



#### sel = select([2,0,0],[0,1,2],==)

200 0FTT 1FFF 2TFF

Decision: RASP abstracts to binary choose/don't choose decisions



#### sel = select([2,0,0],[0,1,2],==)

2 0 0 0 F T T 1 F F F 2 T F F

Decision: RASP abstracts to binary choose/don't choose decisions



#### sel = select([2,0,0],[0,1,2],==)

200 0FTT 1FFF 2TFF

Decision: RASP abstracts to binary choose/don't choose decisions



#### sel = select([2,0,0],[0,1,2],==)

2 0 0 0 F T T 1 F F F 2 T F F

## Single Head: Scoring ↔ Selecting

Decision: RASP abstracts to binary choose/don't choose decisions



#### sel = select([2,0,0],[0,1,2],==)

200 2 T F F

Another example:

sel2 = select([2,0,0],[0,1,2] 200 ΟΤΤΤ **1 T** F F **2 T F F** 

Is this "reasonable"? What does it mean with respect to Q and K?





### Single Head: Weighted Average $\leftrightarrow$ Aggregation



### Single Head: Weighted Average $\leftrightarrow$ Aggregation



new=aggregate(sel, [1,2,4])

# 124F T T 124 => 3 F F F 124 => 0 => [3,0,1] T F F 124 => 1

### Single Head: Weighted Average ↔ Aggregation



new=aggregate(sel, [1,2,4])



### Single Head: Weighted Average ↔ Aggregation



#### new=aggregate(sel, [1,2,4])



### Single Head: Weighted Average ↔ Aggregation



#### new=aggregate(sel, [1,2,4])



### Single Head: Weighted Average $\leftrightarrow$ Aggregation



new=aggregate(sel, [1,2,4])

# 124F T T 124 => 3 F F F 124 => 0 => [3,0,1] T F F 124 => 1

### Single Head: Weighted Average $\leftrightarrow$ Aggregation



#### new=aggregate(sel, [1,2,4])

# 124F T T 124 => 3 F F F 124 => 0 => [3,0,1] T F F 124 => 1

Symbolic language + no averaging when only one position selected allows (for example):

flip = select([2,1,0],[0,1,2],==)	reverse=aggregate(flip, [A,E			
210	ABC			
<b>0</b> F F <b>T</b>	F F T ABC => C			
1 F T F	F T F ABC => B =>			
2 T F F	T F F A B C => A			





## Single Head: Select/Aggregate in RASP



**Example from before: reverse in RASP** 

>>	fl	.ip =	select(	length-in	dice	s-1,	indices	,==);
		sele	ctor: fl	.ip				
			Example:					
					h	e l	.lo	
				h			1	
				е			1	
				1	i i	1		
				l	i .	1		
				0	j 1			

The select decisions are pairwise!! What would happen if they weren't?

## Single Head: Select/Aggregate in RASP



**Example from before: reverse in RASP** 



#### The select decisions are pairwise!! What would happen if they weren't?

## Single Head: Select/Aggregate in RASP



#### See anything suspicious in the example?

**Example from before: reverse in RASP** 



#### The select decisions are pairwise!! What would happen if they weren't?

## Okay, that's our parts!
### **The Initial Sequences**



### **The Initial Sequences**

### **Feed-Forward Sublayers**





### **The Initial Sequences**

### **Feed-Forward Sublayers**





### **Attention Heads**



## **The Initial Sequences**

### **Feed-Forward Sublayers**





### **Attention Heads**



## But also ...

## **The Initial Sequences**

### **Feed-Forward Sublayers**





### **Attention Heads**



### **Skip connection**

## $\bigcirc$

Deep Residual Learning for Image Recognition Kaiming He, Xiangyu Zhang, Shaoqing Ren, Jian Sun

Encourages idea that information can be retained through many layers...

## **The Initial Sequences**

### **Feed-Forward Sublayers**





### **Attention Heads**





### Layernorms

Skip connection

## LayerNorm

### Parameters

- a\_2 (vector)
- b\_2 (vector)
- (small constant) • E



## So the components are:

### **The Initial Sequences**

**Feed-Forward Sublayers** 





### **Attention Heads**



### Skip connection

## $\bigcirc$

**Deep Residual Learning for Image Recognition** Kaiming He, Xiangyu Zhang, Shaoqing Ren, Jian Sun

Encourages idea that information can be retained through many layers...



Layernorms

**Powerful** 

elementwise

operations

## **RASP (Restricted Access Sequence Processing)**

### **Initial Sequences**



















## Small Example



(On an example of length 4:)

### frac\_0=aggregate(full\_s, [1,0,0,0])

```
1000
T T T T 1000 => 0.25
T T T T 1000 => 0.25 => [0.25, 0.25, 0.25, 0.25]
T T T T 1000 => 0.25
T T T T 1000 => 0.25
```









```
>> full_s = select(1,1,==);
     selector: full_s
         Example:
                             hello
                         h
                             1 1 1
                                   1 1
                         е
                             1 1 1
                         0
                             1 1 1
> frac_0=aggregate(full_s, indicator(indices==0));
     s-op: frac_0
         Example: frac_0("hello") = [0.2]*5 (floats)
>> round(1/frac_0);
     s-op: out
         Example: out("hello") = [5]*5 (ints)
```





- *indices* and *tokens* : require zero layers

- select-aggregate pairs:

must be at least one layer after all of their dependencies can have multiple pairs in one layer (multi-headed attention)

 local (feed-forward) operations: don't add layers (attached to earliest layer after dependencies are finished)

Can draw head/layer analysis, eg:





Can draw head/layer analysis, eg:





Can draw head/layer analysis, eg:



![](_page_92_Figure_4.jpeg)

![](_page_92_Figure_5.jpeg)

Can draw head/layer analysis, eg:

![](_page_93_Figure_3.jpeg)

![](_page_93_Figure_4.jpeg)

Can draw head/layer analysis, eg:

![](_page_94_Figure_3.jpeg)

![](_page_94_Figure_4.jpeg)

Can draw head/layer analysis, eg:

![](_page_95_Figure_3.jpeg)

![](_page_95_Figure_4.jpeg)

Are our RASP programs predicting relevant selector patterns?

Are our RASP programs predicting the right number of layers?

## Example 1: reverse

![](_page_97_Figure_2.jpeg)

## Example 1: reverse

![](_page_98_Figure_2.jpeg)

## **RASP** analysis:

- First, *length* is computed (1 layer, uniform attention)
- Then, *length* is used to create *flip\_s* (necessarily in next layer, 'flipped' attention)

![](_page_98_Picture_6.jpeg)

## Example 1: reverse

![](_page_99_Figure_2.jpeg)

## **RASP** analysis:

- First, *length* is computed (1 layer, uniform attention)
- Then, *length* is used to create *flip\_s* (necessarily in next layer, 'flipped' attention)

hypothesis: reverse requires 2 layers?

![](_page_99_Picture_7.jpeg)

### [>> draw(reverse,"abcdeabcde")

![](_page_100_Figure_2.jpeg)

RASP expects 2 layers for arbitrary-length reverse

### [>> draw(reverse,"abcdeabcde")

![](_page_101_Figure_2.jpeg)

RASP expects 2 layers for arbitrary-length reverse

### Test:

Training small transformers on lengths 0-100:

2 layers: 99.6% accuracy after 20 epochs 1 layer: 39.6% accuracy after 50 epochs

Even with compensation for number of heads and parameters!

### [>> draw(reverse,"abcdeabcde")

![](_page_102_Figure_2.jpeg)

RASP expects 2 layers for arbitrary-length reverse

Test:

Training small transformers on lengths 0-100:

2 layers: **99.6**% accuracy after 20 epochs 1 layer: **39.6**% accuracy after 50 epochs

**Bonus**: the 2 layer transformer's attention patterns:

![](_page_102_Figure_8.jpeg)

![](_page_102_Figure_9.jpeg)

## **Connection to Reality?** Example 2: *histogram* (assuming BOS)

Eg:

 $[\$,h,e,l,l,o] \mapsto [0,1,1,2,2,1]$  $[\$,a,b,c,c,c] \mapsto [0,1,1,3,3,3]$  $[\S,a,b,a] \mapsto [0,2,1,2]$ 

## Example 2: histogram (assuming BOS)

Eg:

 $\begin{array}{ll} [\S,h,e,l,l,o] &\mapsto & [0,1,1,2,2,1] \\ \\ [\S,a,b,c,c,c] &\mapsto & [0,1,1,3,3,3] \\ \\ & & [\S,a,b,a] &\mapsto & [0,2,1,2] \end{array}$ 

Reminder: computing length

frac\_0=aggregate(full\_s, [1,0,0,0])

1000T T T T T 1000 => 0.25 T T T T 1000 => 0.25 => [0.25,0.25,0.25,0.25] T T T T 1000 => 0.25 T T T T 1000 => 0.25 T T T T 1000 => 0.25

## Example 2: histogram (assuming BOS)

Eg:

 $\begin{array}{ll} [\S,h,e,l,l,o] &\mapsto & [0,1,1,2,2,1] \\ \\ [\S,a,b,c,c,c] &\mapsto & [0,1,1,3,3,3] \\ \\ & & [\S,a,b,a] &\mapsto & [0,2,1,2] \end{array}$ 

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frac\_0=aggregate(full\_s, [1,0,0,0])

1000T T T T T 1000 => 0.25
T T T T 1000 => 0.25 => [0.25,0.25,0.25,0.25]
T T T T 1000 => 0.25
T T T T 1000 => 0.25

Trick was: send 1 from exactly one position, and then use weighted average to compute inverse of number of selected positions (for length, this was all positions)

## Example 2: histogram (assuming BOS)

Eg:

 $\begin{array}{ll} [\S,h,e,l,l,o] &\mapsto & [0,1,1,2,2,1] \\ \\ [\S,a,b,c,c,c] &\mapsto & [0,1,1,3,3,3] \\ \\ & & [\S,a,b,a] &\mapsto & [0,2,1,2] \end{array}$ 

Reminder: computing length

```
frac_0=aggregate(full_s, [1,0,0,0])
```

```
1000
T T T T T 1000 => 0.25
T T T T 1000 => 0.25 => [0.25,0.25,0.25,0.25]
T T T T 1000 => 0.25
T T T T 1000 => 0.25
```

Trick was: send 1 from exactly one position, and then use weighted average to compute inverse of number of selected positions (for length, this was all positions)

Can we use a similar trick for histograms?

## Example 2: histogram (assuming BOS)

Eg:

 $\begin{array}{ll} [\S,h,e,l,l,o] &\mapsto & [0,1,1,2,2,1] \\ \\ [\S,a,b,c,c,c] &\mapsto & [0,1,1,3,3,3] \\ \\ & & [\S,a,b,a] &\mapsto & [0,2,1,2] \end{array}$ 

Reminder: computing length

```
frac_0=aggregate(full_s, [1,0,0,0])
```

```
1000
T T T T T 1000 => 0.25
T T T T 1000 => 0.25 => [0.25,0.25,0.25,0.25]
T T T T 1000 => 0.25
T T T T 1000 => 0.25
T T T T 1000 => 0.25
```

Trick was: send 1 from exactly one position, and then use weighted average to compute inverse of number of selected positions (for length, this was all positions)

Can we use a similar trick for histograms?

Specifically, what's the challenge for histograms?
#### Example 2: histogram (assuming BOS)

Eg:

 $\begin{array}{ll} [\S,h,e,l,l,o] &\mapsto & [0,1,1,2,2,1] \\ \\ [\S,a,b,c,c,c] &\mapsto & [0,1,1,3,3,3] \\ \\ & & [\S,a,b,a] &\mapsto & [0,2,1,2] \end{array}$ 

Reminder: computing length

```
frac_0=aggregate(full_s, [1,0,0,0])
```

```
1000
T T T T T 1000 => 0.25
T T T T 1000 => 0.25 => [0.25,0.25,0.25,0.25]
T T T T 1000 => 0.25
T T T T 1000 => 0.25
T T T T 1000 => 0.25
```

Trick was: send 1 from exactly one position, and then use weighted average to compute inverse of number of selected positions (for length, this was all positions)

Can we use a similar trick for histograms?



Specifically, what's the challenge for histograms?

Need a known position to send 1 from!

- - - - - - - -

### **Connection to Reality?** Example 2: *histogram* (assuming BOS)

>> set example "§hello"

Example 2: histogram (assuming BOS)



### **Connection to Reality? Example 2:** *histogram* (assuming BOS)



### **Connection to Reality? Example 2:** *histogram* (assuming BOS)



```
Example: frac_with_0("§hello") = [1, 0.5, 0.5, 0.333, 0.333, 0.5] (floats)
Example: histogram_assuming_bos("§hello") = [0, 1, 1, 2, 2, 1] (ints)
```

### **Example 2:** *histogram* (assuming BOS)



### Example 2: *histogram* (assuming BOS)



#### **RASP** analysis:

- Just one attention head
- It focuses on:
  - 1. All positions with same token, and:
  - 2. Position 0 (regardless of content)

### **Example 2:** *histogram* (assuming BOS)



Selector pattern vs trained transformer's attention for same input sequence:



#### **RASP** analysis:

- Just one attention head
- It focuses on:
  - 1. All positions with same token, and:
  - 2. Position 0 (regardless of content)

§ -	0.8	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.1		- 1.0
j-	0.3	0.4	0.0	0.0	0.0	0.0	0.0	0.3	0.0	0.0		
i -	0.2	0.0	0.3	0.0	0.0	0.3	0.0	0.0	0.2	0.0		- 0.8
b -	0.4	0.0	0.0	0.3	0.3	0.0	0.0	0.0	0.0	0.0		0.6
b -	0.4	0.0	0.0	0.3	0.3	0.0	0.0	0.0	0.0	0.0		- 0.0
i -	0.2	0.0	0.3	0.0	0.0	0.2	0.0	0.0	0.2	0.0		- 0.4
e -	0.6	0.0	0.0	0.0	0.0	0.0	0.4	0.0	0.0	0.0		0.4
j -	0.3	0.4	0.0	0.0	0.0	0.0	0.0	0.3	0.0	0.0		- 0.2
i -	0.2	0.0	0.3	0.0	0.0	0.3	0.0	0.0	0.2	0.0		0.2
g -	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3		- 0.0
	5	j	i	b	b	i	e	j	i	ģ		0.0

#### 1. Further motivates the Universal Transformer



#### Universal Transformers

Mostafa Dehghani, Stephan Gouws, Oriol Vinyals, Jakob Uszkoreit, Łukasz Kaiser

#### Recurrent blocks are like allowing loops in RASP!

#### 2. Explains results of the Sandwich Transformer

#### Improving Transformer Models by Reordering their Sublayers

Ofir Press, Noah A. Smith, Omer Levy

If re-ordering and switching attention and feedforward layers of a transformer (while adjusting) to keep same number of parameters):

- 1. Better to have attention earlier, and feedforward later
- 2. Only attention not enough

#### self-attention

feed-forward

Model					
sfffssfsfsfsffffsfffff	2				
sffssfssssssssssfsfsfssffsssffsssf	2				
sssss <mark>ff</mark> s <mark>ffff</mark> ss <mark>fffffsssfsf</mark> sssssssss	2				
fffffffffsffssffssffsssfsfssf	2				
fssfsssffffffssfsssfsffssssfss	2				
s f f s f f f f f f s f s s f s s s f s f s f s s f s s f s	2				
s f f s s f f s f f f s f s s s s s f f f f f f s s s s f f	2				
fsffsfssfffsfsfffsffssfffssfffss	1				
sffsffssffsffsfssssfsssfsssfffsss	1				
ssfffffffssffssfsffsfsfsf	1				
sfsfsfffsfffssfffsffssffsfsfss	1				
sfsffsssffsffsssffssfffffssssf	1				
sffsfssffsffsffsfssssffsffffsfsss	1				
sffffsffssssfsssffssfffsssfsssfssf	1				
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sssfsffsfssfssffsfffffssfff	1				
sssfsfsffsssfffffsfsfffssff	1				
sfsfsfsfsfsfsfsfsfsfsfsfsfsfsf	1				
sssssfssffffsfsfffffffff	1				



#### 3. Transformers can "use" at least $n \log(n)$ of the $n^2$ computational cost they have:

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**Open Question**: is there something that "uses" all  $n^2$  of the attention head cost?





### End



"Thinking Like Transformers" - ICML 2021 (Available on Arxiv)

### **Optional Talking Points**

- Bhattamishra et al (2020) note that, unlike LSTMs, transformers struggle with some regular languages. Why might that be? (What would a general method for encoding a DFA in a transformer be?)
- Hahn (2019) proves that transformers with hard attention cannot compute Parity with hard attention. RASP can compute parity. What is the difference?
- How should we convert a RASP program to 'real' transformers? How big does our head-dimension need to be for "select(indices,indices,<)"? How do we implement *and*, *or*, and *not* between selectors?
- Do our selectors cover all the possible attention patterns? What is missing?

