Expressivity of Transformers: Logic, Circuits, and Formal Languages

Day 4: Encoders with Soft Attention

David Chiang (Univ. of Notre Dame, USA) Jon Rawski (MIT/San Jose State Univ., USA) Lena Strobl (Umeå University, Sweden) Andy Yang (Univ. of Notre Dame, USA) 1 August 2024

- **Describe** the concept of soft attention and its role in transformer encoders.
- **Explain** the upper and lower bounds of computational expressivity in soft attention models.
- **Identify** key arithmetic predicates, counting quantifiers, and their relevance in soft attention encoders.

In the previous two days, we gave exact equivalences:

masked $\mathsf{UHATs} = \mathsf{star-free}$

AHAT decoders with intermediate steps = Turing-complete

Today, we turn to softmax-attention transformers (SMATs), which we don't have an exact characterization of.

Instead, we have upper bounds and lower bounds.

Upper bound

We saw already that FO is equivalent to UHATs, but FO is not powerful enough for SMATs. It's not hard to write a SMAT for:

 $\mathsf{MAJORITY} = \{ \mathbf{w} \in \{0,1\}^* \mid \mathbf{w} \text{ has more 1's than 0's} \}.$

We need to extend FO with:

- Arithmetic predicates
- Majority or counting quantifiers

 We can increase the expressivity of FO by adding more predicates besides <. The logic FO[+, ×] extends FO with predicates:

$$w, I \models x + y = z \quad \text{if } I(x) + I(y) = I(z)$$
$$w, I \models x \times y = z \quad \text{if } I(x)I(y) = I(z)$$

• $\mathsf{FO}[+,\times]$ is also called $\mathsf{FO}[\mathrm{BIT}]$

Exercise

Write a formula ODD(x) that tests whether x is odd.

Things that can be defined in $FO[+, \times]$:

- The sum of $O(\log n)$ numbers with $O(\log n)$ bits each [Immerman, 1999]
- The product of $O(\log n)$ numbers with $O(\log n)$ bits each [Hesse et al., 2002]
- x^y (special case of above)

Theorem (Barrington et al., 1990)

 $\mathsf{FO}[+,\times]$ defines exactly the languages in <code>DLOGTIME-uniform</code> $\mathsf{AC}^0.$

Definition (TC^k)

 TC^k is the class of languages that can be recognized by families of circuits with

- 1. unbounded fan-in,
- 2. O(poly(n)) size,
- 3. $O((\log n)^k)$ depth, and
- 4. MAJORITY gates, which output 1 iff at least half of their inputs are 1.

Definition (TC^0)

 TC^0 is the class of languages that can be recognized by families of circuits with unbounded fan-in, O(poly(n)) size, O(1) depth, and MAJORITY gates.



Definition (NC¹)

 NC^1 is the class of languages that can be recognized by families of circuits with fan-in at most 2, O(poly(n)) size, and $O((\log n))$ depth.



Circuit Complexity Classes

We will show that transformers (with $O(\log n)$ precision) are in TC⁰. It's widely believed that TC⁰ \neq NC¹ (as in the figure). If so, then NC¹-complete languages do not belong to TC⁰. Consequently, we don't think that transformers can recognize them either.



Let's look at two examples.

Circuit Complexity Classes

Example (Boolean Formula Value Problem (BFVP))

The BFVP is to decide whether a Boolean formula (with constants 0 and 1, no variables) is true or not. This problem is context-free and NC^1 -complete.



Uniform TC^0 and NC^1 Languages

Example (Boolean Formula Value Problem (BFVP)) The BFVP is to decide whether a Boolean formula (with constants 0 and 1, no variables) is true or not. Examples:

 $\begin{array}{ccc} 1 \in \mathsf{BFVP} & 0 \not\in \mathsf{BFVP} \\ 1 \wedge 1 \in \mathsf{BFVP} & 1 \wedge 0 \not\in \mathsf{BFVP} \\ 0 \lor (1 \wedge 1) \in \mathsf{BFVP} & 1 \land (1 \land 0) \not\in \mathsf{BFVP} \end{array}$

This problem is context-free and NC¹-complete.

Boolean Formulas and Compositional Semantics

- Evaluating Boolean formulas is crucial for computations in compositional semantics.
- Boole's work on logical descriptions aimed to codify a "language of thought."
- Modern semantic theory, influenced by lambda calculus (Montague, Partee), builds on this foundation.
- The relationship between neural networks and compositional behavior has been debated for decades (Fodor, Pylyshyn, Smolensky).

Example (Word Problem for S_5)

 S_5 is the set of all permutations of $\{1, 2, 3, 4, 5\}$. The word problem for S_5 is regular and NC¹-complete.



Uniform TC^0 and NC^1 Languages

Example (Word Problem for S_5)

 S_5 is the set of all permutations of $\{1,2,3,4,5\}.$ For simplicity, let's just consider

$$s = (12)$$
swap 1 and 2 $c = (12345)$ cycle $1 \mapsto 2, 2 \mapsto 3, \dots, 5 \mapsto 1$

Does a sequence of permutations equal the identity permutation?

$$arepsilon \in \mathsf{W}(S_5)$$

 $\mathrm{ss} \in \mathsf{W}(S_5)$ $\mathrm{s}
ot\in \mathsf{W}(S_5)$
 $\mathrm{ccccc} \in \mathsf{W}(S_5)$ $\mathrm{cccc}
ot\in \mathsf{W}(S_5)$
 $\mathrm{scccccs} \in \mathsf{W}(S_5)$

This problem is regular and NC¹-complete.

GPT 3.5 and $W(S_5)$

I have five cups, labeled A through E. When I say "S", swap the first two cups. When I say "C", move the first cup to the last position. When I saw "P", don't move any cups. Then please tell me if the cups are in order. Do not write anything except for a yes or no answer. Ready?



Ready.

SS



GPT 3.5 and $W(S_5)$



GPT 3.5 and $W(S_5)$



The languages $W(S_k)$ have some relevance to natural language:

- They resemble expressions like *the child of the enemy of Ann* where the interpretation of *the child of* is (roughly) a permutation of possible referents [Paperno, 2022].
- They have been used to benchmark transformers' state-tracking abilities [Kim and Schuster, 2023].

FOC is first order logic with *counting terms* [van Benthem and Icard, 2023].

Example (Majority Language)

The majority language,

 $\mathsf{MAJORITY} = \{ \mathbf{w} \in \{0,1\}^* \mid \mathbf{w} \text{ has more 1's than 0's} \}$

can be defined by the FOC formula

$$\underbrace{(\#z,Q_0(z))}_{\text{number of }0\text{'s}} < \underbrace{(\#z,Q_1(z))}_{\text{number of }1\text{'s}}$$

Exercise (Parity) Write a FOC[+] formula for the language

 $\mathsf{PARITY} = \{ \textbf{w} \in \{0,1\}^* \mid \textbf{w} \text{ has an odd number of } 1's \}.$

Equivalences:

- $FOC[+, \times] = FOC[\times]$ [Lange, 2004]
- FOC = FOM (FO with *majority quantifiers*) and is more commonly called that
- $FOC[+, \times] = DLOGTIME$ -uniform TC^0

Things they can do:

- The sum of O(poly(n)) numbers with O(poly(n)) bits each
- The product of O(poly(n)) numbers with O(poly(n)) bits each [Hesse et al., 2002]
- Division and remainder of two O(poly(n))-bit numbers [Hesse et al., 2002]

Precision in transformers

- UHATs and AHATs only produce rational numbers, while soft attention produces real numbers.
- Upper bounds on the expressivity of SMATs involve limiting the precision of the numbers involved.





- UHATs and AHATs only produce rational numbers, while soft attention produces real numbers.
- Upper bounds on the expressivity of SMATs involve limiting the precision of the numbers involved.
- Merrill and Sabharwal [2023] argue that O(1) precision is too small. You need log n bits just to store the number n or 1/n!
- Instead, they use $O(\log n)$ bits of precision.



The significand and exponent combined have $p \in O(\log n)$ bits Details aren't very important:

- How to apportion bits between the significand and exponent
- Does the sign bit count as a bit
- And so on.

Theorem (Merrill and Sabharwal, 2023)

For any $O(\log n)$ -bit floating-point transformer encoder T that recognizes a language L, there is a formula of FOC[+, \times] that defines L.

Merrill and Sabharwal [2023]'s proof converted T to a family of threshold circuits, but we show how to go straight to FOC[+,×].

What's in a Transformer?

- Addition (+), multiplication, comparison (<) of two numbers
- Exponential function (exp)
- Addition of *n* numbers (\sum)
- If layer normalization: division (÷), square root (\swarrow

We just need to show that these can be done on $O(\log n)$ -bit floating point numbers. Most of these operations can be reduced to operations on $O(\log n)$ -bit integers.

Exercise

Explain why multiplication of two $O(\log n)$ -bit floating point numbers is definable in FOC[+, ×]. How about addition?

Summation of $n O(\log n)$ -bit floating point numbers: just convert every summand into a fixed-point number

$1.011 \cdot 2^{0}$		1.011
$1.100\cdot2^{-5}$		0.00001100
$1.111\cdot2^{-10}$	\rightsquigarrow	0.000000001111
$+ 1.101 \cdot 2^{-15}$		+ 0.0000000000001101
$?.??? \cdot 2^{?}$		1.011011000111101101

Each number has $2^{O(\log n)} = O(\operatorname{poly}(n))$ bits, and the sum of *n* numbers with $O(\operatorname{poly}(n))$ bits is still in FOC[+, ×].

Compute first *p* terms of Taylor series:

$$\exp x = \sum_{i=0}^{p-1} \frac{x^i}{i!}$$
$$= 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots + \frac{x^{p-1}}{(p-1)!}$$

If $p \in O(\log n)$:

- The error will be less than 2^{-p+1} .
- Each term in the series is an iterated product of O(log n) numbers, expressible in FO[+, ×].
- Summation of the terms can also be expressed in $FO[+, \times]$.

- O(log n)-precision transformer encoders only recognize languages in FOC[+, ×] = DLOGTIME-uniform TC⁰.
- Assuming that TC⁰ ≠ NC¹, this implies that O(log n)-precision transformer encoders cannot solve many interesting problems:
 - deciding whether a Boolean formula is true
 - deciding whether a sequence of permutations is the identity
 - reconstructing a chess board from chess moves [Merrill et al., 2024]

- Are O(1)-precision transformers equivalent to FO = LTL?
- At O(log n) precision, every operation except summation is in FO[+, ×]. Is there a tighter bound than FOC[+, ×]?
- At infinite precision, is it possible to find an upper bound?



Softmax Attention and Related Work

- Bhattamishra et al. [2020] showed that one-state Parikh automata can be simulated by SMATs.
- Chiang et al. [2023] defined a logic called FOC[+; MOD] and showed that it can be simulated by SMATs.
- Barceló et al. [2024] defined an extension of LTL with counting, called LTL[#, +], and showed that it can be simulated by AHATs.
- Perhaps surprisingly, there isn't a published proof that softmax-attention transformers can simulate LTL.

Now, we show that softmax-attention transformers can simulate a temporal logic without **since** but with a counting operator [Yang and Chiang, 2024]. We call this logic $K_t[\#, +]$.

Our proof relies crucially on layer normalization

- Position-wise function $\mathbb{R}^d
 ightarrow \mathbb{R}^d$
- Scales and shifts the components of a vector to have mean β and standard deviation γ



- In practice β and γ are learned; here, we choose them

Set of all strings over $\{(,)\}$ that are balanced and nested. That is

- Total number of (equals total number of)
- At no point in the string is the number of) greater than the number of (

We can test for these constraints using $K_t[\#, +]$.

$\mathsf{K}_t[\#,+]$ Example

$$\phi = (\#[Q_{c}] = \#[Q_{b}]) \land (\#[\#[Q_{b}] > \#[Q_{c}]] = 0$$

$$(((()))) ((b))$$

$$Q_{c} | T T T F F T F F$$

$\mathsf{K}_t[\#,+]$ Example

$$\phi = (\#[Q_{\zeta}] = \#[Q_{\gamma}]) \land (\#[\#[Q_{\gamma}] > \#[Q_{\zeta}]] = 0)$$

$$\phi = (\#[Q_{\zeta}] = \#[Q_{J}]) \land (\#[\#[Q_{J}] > \#[Q_{\zeta}]] = 0)$$



Dyck-1 is the language of nested and balanced parentheses.

	((())	())
$Q_{(}$	т	Т	Т	F	F	Т	F	F
$Q_{ m b}$	F	F	F	Т	Т	F	Т	F
$\#[Q_{\zeta}]$	1	2	3	3	3	4	4	4
$\#[Q_{2}]$	0	0	0	1	2	2	3	4
$\#[\#[Q_{2}] > \#[Q_{1}]]$	0	0	0	0	0	0	0	0

Dyck-1 is the language of nested and balanced parentheses.

	((())	())
$Q_{(}$	Т	Т	Т	F	F	Т	F	F
$Q_{ m b}$	F	F	F	Т	Т	F	Т	F
$\#[Q_{\zeta}]$	1	2	3	3	3	4	4	4
$\#[Q_{2}]$	0	0	0	1	2	2	3	4
$\#[\#[Q_{2}] > \#[Q_{1}]]$	0	0	0	0	0	0	0	0
$\#[Q_{0}] = \#[Q_{0}]$	F	F	F	F	F	F	F	Т

Dyck-1 is the language of nested and balanced parentheses.

((())	())
Т	Т	Т	F	F	Т	F	F
F	F	F	Т	Т	F	Т	F
1	2	3	3	3	4	4	4
0	0	0	1	2	2	3	4
0	0	0	0	0	0	0	0
F	F	F	F	F	F	F	Т
Т	Т	Т	Т	Т	Т	Т	Т
	(T F 1 0 F T	 (T T F F 0 0 0 F F T 	 (((T T T F F F 1 2 3 0 0 0 0 0 0 0 F F F T T 	((() T T T F F F F T 1 2 3 3 0 0 0 1 0 0 0 0 F F F F T T T T	((()) T T T F F F F F T T 1 2 3 3 3 0 0 0 1 2 0 0 0 1 2 0 0 0 1 2 0 0 0 1 2 0 0 F F F T T T T T	(()) (T T T F F T F F F T T F 1 2 3 3 3 4 0 0 0 1 2 2 0 0 0 0 0 0 F F F F F F T T T T T T	(()) () T T T F F T F F F F T T F T F 1 2 3 3 3 4 4 0 0 0 1 2 2 3 0 0 0 0 0 0 0 F F F F F F F T T T T T T T

Dyck-1 is the language of nested and balanced parentheses.

	((())	())
$Q_{(}$	т	Т	Т	F	F	Т	F	F
$Q_{ m b}$	F	F	F	Т	Т	F	Т	F
$\#[Q_{(}]$	1	2	3	3	3	4	4	4
$\#[Q_{2}]$	0	0	0	1	2	2	3	4
$\#[\#[Q_{2}] > \#[Q_{3}]]$	0	0	0	0	0	0	0	0
$\#[Q_1] = \#[Q_2]$	F	F	F	F	F	F	F	Т
$\#[\#[Q_{0}] > \#[Q_{0}]] = 0$	Т	Т	Т	Т	Т	Т	Т	Т
ϕ	F	F	F	F	F	F	F	Т

The syntax of $K_t[\#, +]$ is defined as follows:

$$\begin{array}{l} t ::= \#[\phi_1] \\ & \mid t_1 + t_2 \\ \phi ::= Q_{\sigma} & \sigma \in \Sigma \\ & \mid \phi_1 \land \phi_2 \mid \neg \phi_1 \\ & \mid t_1 = t_2 \mid t_1 < t_2 \end{array}$$

Other operators (\lor , \rightarrow , >, \leq , \geq) can be defined in terms of the ones above.

Language	Formula
a*b*	$\#[\mathcal{Q}_{a} \land (\#[\mathcal{Q}_{b}] \geq 1)] = 0$
a*b*a*	$\#[\mathcal{Q}_{b} \wedge \#[\mathcal{Q}_{a} \wedge (\#[\mathcal{Q}_{b}] \geq 1)] \geq 1] = 0$
Dyck-1	$(\#[Q_{\zeta}] = \#[Q_{\zeta}]) \land (\#[\#[Q_{\zeta}] > \#[Q_{\zeta}]] = 0)$
a ⁿ b ⁿ c ⁿ	$\#[Q_{b} \wedge (\#[Q_{c}] = 0)] = \#[Q_{b}]$
	$\wedge \#[Q_{a} \wedge (\#[Q_{b} \vee Q_{c}] = 0)] = \#[Q_{a}]$
	$\wedge \#[Q_a] = \#[Q_b] \wedge \#[Q_b] = \#[Q_c] \wedge \#[Q_c] = \#[Q_a]$
hello	$\#[\top] = 5 \land Q_{o} \land \#[Q_{1} \land \#[Q_{e} \land \#[Q_{h}] = 1] = 1] = 2$

Theorem (Yang and Chiang, 2024)

For any formula ϕ of $K_t[\#, +]$ that defines a language L, there is a transformer encoder that recognizes L.

Use uniform attention to count.

Problem:

• Uniform attention doesn't count; it averages



how to get rid of this?

- Position embedding tricks (Day 3) require average-hard attention
- Instead: Just keep the $\frac{1}{i+1}$ for now

Key Idea 2

Implement $count_{2,i} > count_{1,i}$ as $\frac{1}{i+1}(count_{2,i} - count_{1,i}) > 0$.

Problem: We need a function like



Slope not bounded (i.e., not Lipschitz continuous) \Rightarrow can't be computed by FFNN

Use layer normalization to make everything $\pm 1.$



Boolean and Count Representations

To represent Boolean values, we use the following representations:

true :
$$\begin{bmatrix} -1\\ 1 \end{bmatrix}$$
false :
$$\begin{bmatrix} 1\\ -1 \end{bmatrix}$$

• To represent the integer count_i in position i, we use:

$$\begin{bmatrix} \frac{\operatorname{count}_i}{i+1} \\ -\frac{\operatorname{count}_i}{i+1} \end{bmatrix}$$

• These representations have zero mean so that layer normalization does not shift them up or down

In the following, we show how to simulate a # term in $K_t[\#, +]$ using a uniform attention layer.

Lemma

Let $\mathbf{A}[*, 2k : 2k + 1]$ store a sequence of Boolean values $\phi(i)$ as defined above. For any *i*, let C(i) be the number of positions $j \leq i$ such that $\mathbf{A}[j, 2k : 2k + 1]$ is true. Then there is a transformer block that computes, at each position *i*, and in two other dimensions 2k', 2k' + 1, the values $-\frac{C(i)}{i+1}$ and $\frac{C(i)}{i+1}$.

We compute in position *i* of dimension *k*, the value $C(i)_k$, which is the average of all values up to position *i* in dimension *k*, The expression reduces to:

$$c_{i,k} = \frac{\sum_{j=0}^{i} \exp(s_{ij}) [W^{(V)} A_{*,j}]_{k}}{\sum_{j=0}^{i} \exp(s_{ij})}$$
$$= \frac{\sum_{j=0}^{i} [W^{(V)} A_{*,j}]_{k}}{\sum_{j=0}^{i} 1}$$
$$= \frac{\sum_{j=0}^{i} A_{k,j}}{i+1}$$

Counting Vector

Since Booleans are stored as ± 1 , the count we compute actually ends up being 2C(i) + 1, which we can easily correct with a FFNN.

$$\begin{bmatrix} \vdots \\ -2\phi(i) - 1 \\ 2\phi(i) + 1 \\ \vdots \\ -\frac{2}{i+1}\sum_{i}\phi(i) - 1 \\ \frac{2}{i+1}\sum_{i}\phi(i) + 1 \\ \vdots \end{bmatrix}$$

Counting Vector

Since Booleans are stored as ± 1 , the count we compute actually ends up being 2C(i) + 1, which we can easily correct with a FFNN.

$$\begin{bmatrix} \vdots \\ -2\phi(i) - 1 \\ 2\phi(i) + 1 \\ \vdots \\ -\frac{2}{i+1}\sum_{i}\phi(i) - 1 \\ \frac{2}{i+1}\sum_{i}\phi(i) + 1 \\ \vdots \end{bmatrix} \xrightarrow{\mathsf{FFNN}} \begin{bmatrix} \vdots \\ -2\phi(i) - 1 \\ 2\phi(i) + 1 \\ \vdots \\ -\frac{1}{i+1}\sum_{i}\phi(i) \\ \frac{1}{i+1}\sum_{i}\phi(i) \\ \vdots \end{bmatrix}$$

 $K_t[\#, +]$ can express any linear constraint on counts, that is, constraints of the form

$$\sum_{k \in K} a_k C_k(i) \ge 0$$

where the C_k are count terms, the a_k are integer coefficients, and K is a finite set of indices.

Recall that a count C_k is stored as a pair of numbers $\frac{C_k}{i+1}$. Thus we need to test if

$$\sum_{k \in K} a_k \frac{C_k(i)}{i+1} \ge 0 \iff \frac{1}{i+1} + \sum_{k \in K} a_k \frac{C_k(i)}{i+1} \ge \frac{1}{i+1}$$

Which boils down to testing if a value is $\geq \frac{1}{i+1}$.

Clipping

To test whether this is nonnegative, we construct a feed-forward layer that computes the function, given any input S(i):

$$\operatorname{gtz}\left(S(i), \frac{1}{i+1}\right) = \min\left(\frac{0.5}{i+1}, \frac{S(i)}{i+1} - \frac{0.5}{i+1}\right) - \min\left(0, \frac{S(i)}{i+1}\right)$$



Returning to Boolean Values

Use layer normalization to make everything ± 1 .



Observe that all count values become $\pm \frac{1}{i+1}$ after clipping and layer normalization. Thus we need to make sure that count values are never needed after a comparison.

It helps to organize the construction by modal depth The *modal* depth of a formula ϕ or term C, which we notate as $md(\phi)$, is the maximum level of nesting of # terms. That is,

$md(Q_\sigma)$	= 0	$md(C_1 + C_2) = max(md(C_1), md(C_2))$
md(1)	= 0	$md(\mathit{C}_1 \leq \mathit{C}_2) = max(md(\mathit{C}_1),md(\mathit{C}_2))$
$md(\neg \phi)$	$= md(\phi)$	$md(\phi_1 \wedge \phi_2) = max(md(\phi_1), md(\phi_2))$
$md(\#[\phi])$	$)=1+md(\phi)$	

$$\phi = (\#[Q_{\mathsf{C}}] = \#[Q_{\mathsf{C}}]) \land (\#[\#[Q_{\mathsf{C}}] > \#[Q_{\mathsf{C}}]] = 0)$$



Observe that the bottommost counts $\#[Q_{(}] \text{ and } \#[Q_{)}]$ are never needed after the comparison <

Theorem

For every $K_t[\#, +]$ formula ϕ , there exists a masked transformer encoder which simulates ϕ .

Proof.

Induct on modal depth of ϕ and apply the constructions described in previous slides! $\hfill \Box$

- While AHATs can simulate LTL[#, +], there is currently no published proof that SMATs can simulate the full LTL logic.
- Uniform attention is used in SMATs to simulate counting operations.
- Layernorm is used to rescale very small values back to Booleans.

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