Limitations and Comparisons of Attention Mechanisms

Based on intership work at Taylor TCS Lab,
joint with Xiaoyu He, Chao Liao, Chen Wu, and Pinyan Lu

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Outline

Motivation

- Transformer core: self-attention, but standard full attention has $O(n^2)$ complexity.

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- Efficient variants: linear attention, log-linear attention, sparse attention, hybrid architectures.
- Key question: Is there any loss in expressive power for these variants?

Table of Results

	Eva	**2-Sum**	***L*-SeqComp**
Full Attention	$O(\text{poly} \log n)$[1,4]	$O(\log n)$[3]	$O(\text{poly} \log n)$[2]
Linear + CoT	$\Omega(n \log n)$[1,4]	$\Omega(n \log n)$[5]	
Log-linear + CoT	$\Omega(n)$[5]	$\Omega(n)$[5]	
Sparse (Block)		$\Omega(B \log n)$[5]	
Hybrid			$\Omega(\text{poly } n)$[5]

1. Bhattamishra, S., Hahn, M., Blunsom, P., Kanade, V. (2024). Separations in the representational capabilities of transformers and recurrent architectures. *NeurIPS*.
2. Chen, L., Peng, B., Wu, H. (2025). Theoretical limitations of multi-layer transformer. *FOCS*.
3. Sanford, C., Hsu, D., Telgarsky, M. (2023). Representational strengths and limitations of transformers. *NeurIPS*.
4. Wen, K., Dang, X., Lyu, K. (2025). RNNs are not Transformers (yet): The key bottleneck on in-context retrieval. *ICLR*.
5. Ye, X., He, X., Liao, C., Wu, C., Lu, P. (2026). A Provable Expressiveness Hierarchy in Hybrid Linear-Full Attention. *ICML*.

Full Attention

- Layer ℓ, head h, position i:

$$y_i^{(\ell,h)} = \sum_{j \le i} \alpha_{i,j}^{(\ell,h)} V^{(\ell,h)} x_j^{(\ell-1)}$$

$$\alpha_{i,j}^{(\ell,h)} = \frac{\exp\left((x_i^{(\ell-1)} Q^{(\ell,h)})^\top K^{(\ell,h)} x_j^{(\ell-1)}\right)}{\sum_{j \le i} \exp\left((x_i^{(\ell-1)} Q^{(\ell,h)})^\top K^{(\ell,h)} x_j^{(\ell-1)}\right)}$$

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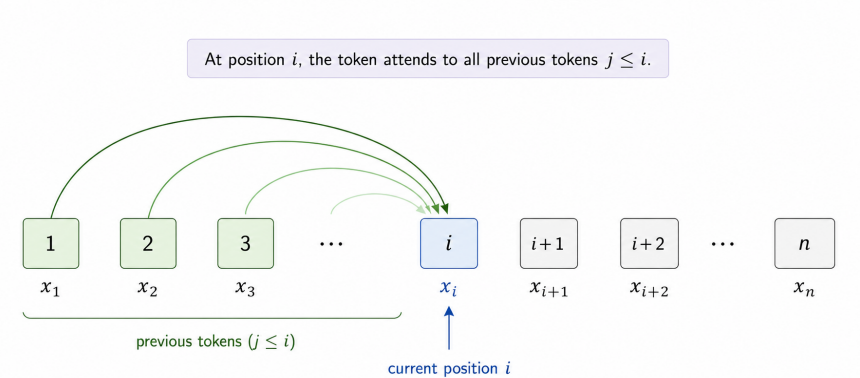
- Complexity $O(n^2)$, but strongest expressive power.

Illustration



Linear Attention $\equiv$ RNN (recurrent neural network)

- Linear attention uses a kernel ϕ:

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with $S_i = S_{i-1} + Vx_i \otimes \phi(Kx_i), \quad Z_i = Z_{i-1} + \phi(Kx_i)$.

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Definition (RNN)

An RNN maintains a **hidden state** $h_t \in \mathbb{R}^m$, updated as:

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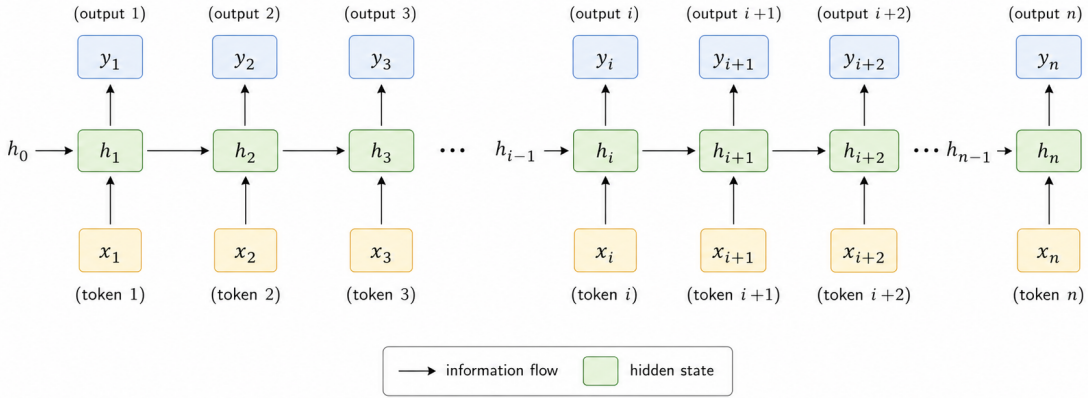
- Hidden state $h_i = (S_i, Z_i) \in \mathbb{R}^{d\times d} \times \mathbb{R}^d \Rightarrow$ linear attention $=$ RNN

Illustration of RNN

RNN: at position i, the hidden state is computed from the previous hidden state (only $i-1$).



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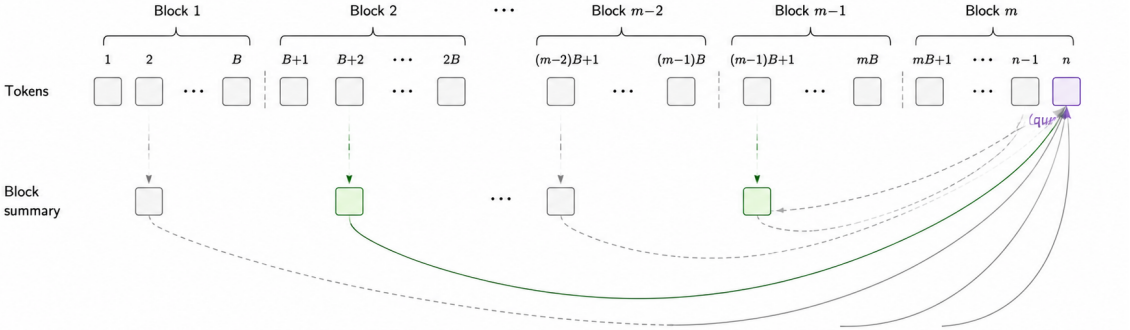

Linear Attention Lower Bound for Function Evaluation

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Input: A function $f : [n] \to [n]$ represented by n tokens $(f(1), \ldots, f(n))$, and an element $x \in [n]$ as a single token. Output: $f(x)$.

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- To distinguish all n^n possible functions, need $2^{LHd(d+1)p} \geq n^n \Rightarrow LHd(d+1)p \geq n \log n$.

Full Attention Construction: Retrieval Head

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Implementation:

- $V_i = b_i, \quad K_i = \log^2(n) \cdot (a_i, \mathbf{1} - a_i), \quad Q_{n+1} = \log^2(n) \cdot (a, \mathbf{1} - a)$.
- $\langle Qx_{n+1}, Kx_i \rangle = \log^2(n) \cdot D$ if $a_i = a$, else $\leq \log^2(n)(D-1)$.

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$$\alpha_{n+1,i} \geq \frac{\exp(\log^2 n)}{\exp(\log^2 n) + n - 1} \geq 1 - \frac{n}{n \log n}, \quad \alpha_{n+1,j} \leq \frac{1}{n \log n} \ (j \neq i).$$

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$p = \Theta(\log n) \Rightarrow$ attention concentrates on position $i \Rightarrow$ retrieving b_i
$\Rightarrow$ solving Eva by setting $a_i = i$, $b_i = f(i)$.

Previous results

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Given a sequence $s_1, \ldots, s_N$ and a position $p \in [N]$, output s_p.

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  - Bounded Dyck languages Recognization: RNNs $>$ 1-layer Transformers.
  - String equality / disjointness: 2-layer Transformers $>$ 1-layer Transformers / RNNs.
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  - String equality / disjointness: 2-layer Transformers $>$ 1-layer Transformers / RNNs.
  - Nearest neighbor algorithm: 2-layer Transformer $>$ RNN.
- **Wen et al. (2025)**:
  - RNN $<$ RNN + CoT $<$ Transformers (associative recall, index, c-gram retrieval, counting, or IsTree).
  - Key bottleneck: RNNs lack *in-context retrieval* capability.
  - Enhancing retrieval (RAG / adding one Transformer layer) closes the gap, allowing RNNs to simulate poly.-time Turing machines with CoT.

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Architecture	Complexity
Full Attention (1-layer)	$Hdp = O(\text{poly} \log n)$
Linear Attention (L layers)	$LHd^2p = \Omega(n \log n)$
Log-Linear Attention (L layers)	$LHd^2p = \Omega(n)$

L-Sequential Function Composition Task

Definition (L-Sequential Function Composition)

Given functions $z_0 \in [m]$, $z_\ell : [N_{\ell-1}] \to [N_{\ell-1}]$ $(\ell = 1, \ldots, L)$ and a query $w = (w_1, \ldots, w_{L-1})$, Compute and output i_L:

$$i_0 = z_0,\ i_1 = z_1(i_0),\ i_2 = z_2(w_1, i_1),\ \ldots,\ i_L = z_L(w_{L-1}, i_{L-1}).$$

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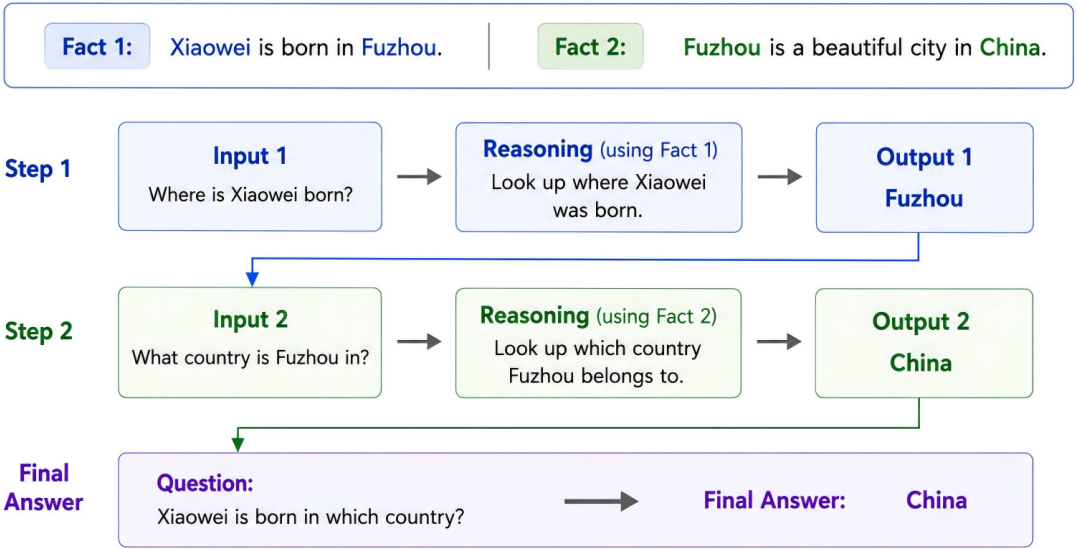
This task captures the essence of real tasks such as multi-step reasoning.

Multi-step Reasoning



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Method: Autoregressive Communication Model
Key Concept: indistinguishable decomposition

Autoregressive Communication Model

Setup:

- $L + 2$ players: $-1, 0, 1, \ldots, L$ (arranged on a line).
- Player ℓ receives input z_ℓ ($\ell \geq 0$) or query w (player -1).
- Communication proceeds in L **epochs** (one per layer).

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After L epochs, player -1 outputs answer.

Indistinguishable Decomposition

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For $\ell \in [2 : L]$, a pair $(R_{\geq \ell}, Z_{<\ell})$ where: $R_{\geq \ell}$ are inputs to players $\ell, \ldots, L$, and $Z_{<\ell} = Z_{-1} \times \cdots \times Z_{\ell-1}$ are inputs to players $-1, \cdots, \ell - 1$.

Such that for every $z_{<\ell} \in Z_{<\ell}$ and any $\alpha_{\geq \ell}, \beta_{\geq \ell} \in R_{\geq \ell}$, all transcripts $\Pi_{j,i}^{(\ell')}$ (for $j \geq \ell$, $i < \ell$, $\ell' \leq \ell$) are identical.

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To prove impossibility: construct $R_{\geq L}, Z_{<L}$ such that:

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Different z_L and i_{L-1} would require different outputs $\Rightarrow$ contradiction.

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Inductive step ($\ell \to \ell + 1$):

1. Extract rectangular subset $S_{\geq \ell+1} \times Z_\ell \subseteq R_{\geq \ell}$ with $S_{\geq \ell+1}$, $\mathcal{I}(Z_\ell)$ large.
2. Use that Z_ℓ is indistinguishable to players $[-1 : \ell - 1]$ after ℓ epochs.
3. Fix transcripts to $[-1 : \ell - 1]$ at epoch $\ell + 1$ via pigeonhole (independent of z_ℓ).
4. Fix transcripts to player ℓ via greedy selection.

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- Therefore, the $(\ell + 1)$-th epoch messages from players $> \ell$ to players $< \ell$ depend only on $z_{<\ell}$, not on the specific z_ℓ.

Hence we can select transcripts that maximize the remaining entropy in $S_{\geq \ell+1}$ without consulting z_ℓ.

Remark: Implications of Chen et al. 2025

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3. **Provable Benefits of Chain-of-Thought**:
   - L-SeqComp solved by 1-layer Transformer with L steps CoT, $\operatorname{poly}\log n$ size, but any L-layer Transformer (no CoT) needs polynomial size.
   - First unconditional proof that CoT strictly increases expressive power.

Lower Bound for Hybrid Attention

Theorem

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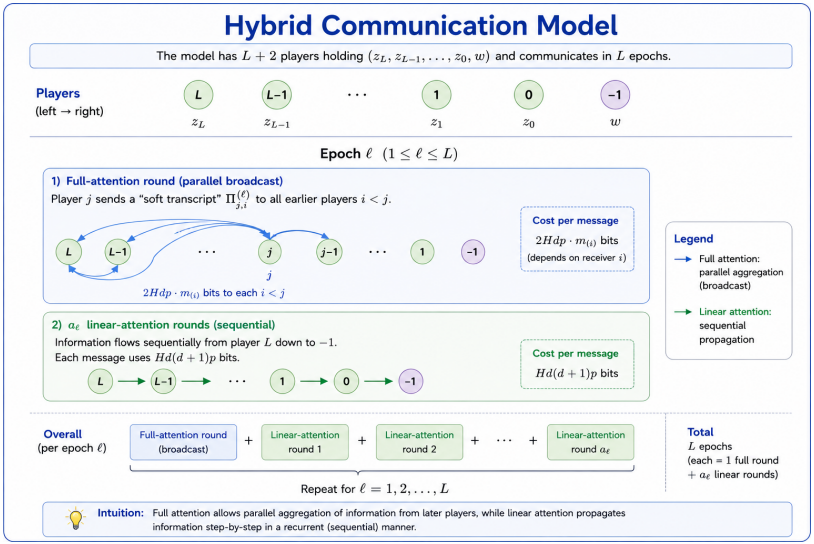
Model	Complexity
Full, L layers	$\Omega(\text{poly } n)$
Full, $L+1$ layers	$O(\text{poly} \log n)$
Hybrid, $L-1$ full layers	$\Omega(\text{poly } n)$

Modified Communication Model

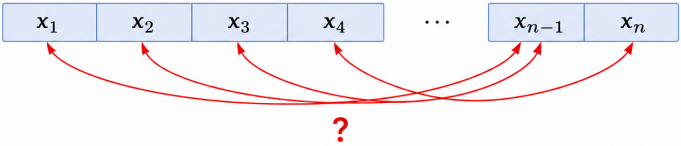


2-Sum Task

Given a sequence of n numbers, determine whether there exist two positions $i \neq j$ such that $x_i + x_j = 0$.

This captures the need for pairwise comparisons across the entire sequence.

Input sequence



Example ($n = 6$)

3	3	0	2	0	5

$0 + 0 = 0 \rightarrow$ **Yes**

Goal: Decide whether any pair (i, j) satisfies $x_i + x_j = 0$.

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Model	**Complexity**
Full	$O(\log n)$
Sparse (Block)	$\Omega(B \log n)$

Full Attention Solves 2-Sum: Trigonometric Construction

Setup: Input $x_1, \ldots, x_{n+1} \in [M]$ with $M = O(n)$. Append a blank token.

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$$\phi(x_i) = \left(\cos \frac{2\pi x_i}{M},\ \sin \frac{2\pi x_i}{M},\ 1 \right) \in \mathbb{R}^3.$$

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$$\langle Q\phi(x_i), K\phi(x_j)\rangle = c\cos\left(\frac{2\pi(x_i + x_j)}{M}\right).$$

This equals c iff $x_i + x_j \equiv 0 \pmod{M}$, otherwise $\leq c(1 - 1/M^2)$.

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This equals c iff $x_i + x_j \equiv 0 \pmod{M}$, otherwise $\leq c(1 - 1/M^2)$.
For $c = \Theta(M^2 \log N)$, the attention concentrates on correct solution.

Other Results of Sanford et al. 2023

- **Sparse Averaging (qSA)**:
  - Input: (y_i, z_i) with $y_i \in \binom{[N]}{q}$, $z_i \in \mathbb{R}^{d'}$, output average of z_j for $j \in y_i$.
  - A single self-attention unit with embedding dimension $m \gtrsim q$ approximates qSA.
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  - A single self-attention unit with embedding dimension $m \gtrsim q$ approximates qSA.
  - RNNs require hidden state $\Omega(N)$ bits.
- **Triple Detection**: 3-Sum **cannot** be solved by a single multi-head attention layer unless $mpH = \Omega(N/\log\log N)$.
  Conjecture: multi-layer transformers cannot solve 3-Sum efficiently.

Lower Bound: Sparse Attention Cannot Solve 2-Sum

Communication Model ($\frac{n}{B} + 1$ players):

- Each of the first $\frac{n}{B}$ players receives B tokens.
- The last player receives a single token (query).
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If selected blocks are $\{b_i\}$, then cannot distinguish remainning blocks $\implies$ contradiction.

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- Expressiveness hierarchy: full attention $>$ hybrid, linear/log-linear, sparse patterns. (Complexity-Expressiveness Trade-offs)

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  - Sparse attention lower bound applies to block compression+selection, not learnable sparse patterns (e.g., DSA).
  - Tasks are synthetic; practical implications require empirical verification.
- **Open Problem**: Can head-wise hybrid attention overcome the current lower bounds? Can lower bounds be proven for multi-layer sparse attention? $\cdots$

Question?

Question? Thank you!