# Limits of Deep Learning: Sequence Modeling through the Lens of Complexity Theory 

Nikola Zubić ${ }^{1}$, Federico Soldá ${ }^{2, *}$, Aurelio Sulser ${ }^{2, *}$, Davide Scaramuzza ${ }^{1}$<br>${ }^{1}$ Robotics and Perception Group, University of Zurich, Switzerland zubic@ifi.uzh.ch, sdavide@ifi.uzh.ch<br>${ }^{2}$ Algorithms and Optimization Group, ETH Zurich, Switzerland<br>federico.solda@inf.ethz.ch, asulser@student.ethz.ch<br>*Equal contribution


#### Abstract

Deep learning models have achieved significant success across various applications but continue to struggle with tasks requiring complex reasoning over sequences, such as function composition and compositional tasks. Despite advancements, models like Structured State Space Models (SSMs) and Transformers underperform in deep compositionality tasks due to inherent architectural and training limitations. Maintaining accuracy over multiple reasoning steps remains a primary challenge, as current models often rely on shortcuts rather than genuine multi-step reasoning, leading to performance degradation as task complexity increases. Existing research highlights these shortcomings but lacks comprehensive theoretical and empirical analysis for SSMs. Our contributions address this gap by providing a theoretical framework based on complexity theory to explain SSMs' limitations. Moreover, we present extensive empirical evidence demonstrating how these limitations impair function composition and algorithmic task performance. Our experiments reveal significant performance drops as task complexity increases, even with Chain-of-Thought (CoT) prompting. Models frequently resort to shortcuts, leading to errors in multi-step reasoning. This underscores the need for innovative solutions beyond current deep learning paradigms to achieve reliable multi-step reasoning and compositional task-solving in practical applications.


## 1 Introduction

Deep learning has achieved remarkable success across various applications, from natural language processing [28, 10, 37] and computer vision [27, 47, 46] to scientific computing [22, 14] and autonomous systems [15, 2]. The new frontier is general artificial intelligence. The goal is to design Large Language Models (LLM) that solve novel and difficult tasks that span mathematics, coding, vision, medicine, law, psychology and more at a close to human-level performance [3]. The mastery of function composition is essential for this objective as mathematical problem solving [17], learning discrete algorithms [35, 39], logical reasoning [20], and dynamic programming [6] are all deeply compositional tasks. However, tasks requiring complex reasoning over sequences, particularly those involving function composition [30] and compositional tasks [6], remain challenging to deep learning models.
These tasks require the breakdown of problems into simpler sub-problems and composing the solutions of the subtasks. Despite their impressive capabilities on various language tasks, current Transformers models [38] like the GPT-4o find it challenging to handle tasks needing deep compositionality [6]. We demonstrate, for instance, that GPT-4o only achieves about $27 \%$ accuracy
on basic tasks like 4-by-3 digit multiplication. One approach at explaining this failure case of the transformer models is by their limitation to express simple kinds of state tracking problems [24]. For this reason, the Structured State Space Models (SSMs) [12, 11] have been introduced as an alternative to transformers, with the goal of achieving similar expressive power to RNNs for handling problems that are naturally sequential and require state-tracking. While SSMs have demonstrated impressive capabilities on various sequential tasks [9, 32], SSMs have similar limitations as Transformer models at solving function composition problems. We observe that for the same 4-by-3 digit multiplication task Jamba [18] (SSM-Attention hybrid model) only achieves 17\% accuracy.

Existing research has experimentally confirmed the inability of Transformers to perform function composition and compositional tasks [6, 45], leading to issues like hallucinations-where responses are incompatible with training data and prompts. Complexity theory analysis further reveals that Transformers belong to a weak complexity class, logspace-uniform TC ${ }^{0}$ [24], just like SSMs [23], emphasizing their limitations. The impossibility of function composition for Transformers has been theoretically studied in [30]. A similar result for SSMs is presented in this paper.

Our contributions are twofold: first, we provide a theoretical framework using complexity theory to explain the limitations of SSMs in sequence modeling. Second, we offer extensive empirical evidence demonstrating these limitations across a variety of tasks. This evidence underscores how the inability to perform function composition critically impairs models in solving compositional and algorithmic tasks, resulting in reasoning errors and hallucinations. Our key insight is the formal proof of SSMs' inability to solve iterated function composition problems without a polynomially growing number of Chain-of-Thought (CoT) [40] steps (Theorems 1]and 2). CoT is a method where a model breaks down complex reasoning tasks into a sequence of intermediate steps or "thoughts," similar to how a human might solve a problem step-by-step. While CoT to some extent can enable complex problem-solving, it introduces a tradeoff between the model's state size and the number of input passes required, leading to increased resource demands, which is not optimal. Our experiments reveal significant performance degradation as task complexity increases, even with CoT prompting. These models often resort to learning shortcuts, leading to errors in multi-step reasoning processes. This behavior highlights their inability to integrate intermediate reasoning steps effectively, resulting in compounded errors, and underscores the need for innovative solutions beyond current deep learning paradigms.

## 2 Background

For two natural numbers $n \leq m$, we denote $[n]=1,2, \ldots n$ and $[n, m]=n, n+1, \ldots, m$, with $[0]=[n, n-1]=\emptyset$. We refer to the number of bits used in each computation as computational precision $p$. Given two domains $B, C$, we denote by $B^{C}$ set of all functions from the $B$ to $C$.
Definition 1 (SSM layer). Given an input sequence $\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{n} \in \mathbb{R}^{m}$, an SSM layer $\mathcal{L}$ is defined in terms of a series of matrices $\boldsymbol{A}_{t} \in \mathbb{R}^{d \times d}, \boldsymbol{B}_{t} \in \mathbb{R}^{d \times m}, \boldsymbol{C}_{t} \in \mathbb{R}^{m \times d}$, and $\boldsymbol{D}_{t} \in \mathbb{R}^{m \times m}$ for $t \in[n]$. $\mathcal{L}$ defines a sequence of states $\boldsymbol{h}_{1}, \ldots, \boldsymbol{h}_{n} \in \mathbb{R}^{d}$ as

$$
\boldsymbol{h}_{t}=\boldsymbol{A}_{t} \boldsymbol{h}_{t-1}+\boldsymbol{B}_{t} \boldsymbol{x}_{t}
$$

and outputs the sequence $\boldsymbol{y}_{1}, \ldots, \boldsymbol{y}_{n} \in \mathbb{R}^{m}$ as

$$
\boldsymbol{y}_{t}=\boldsymbol{C}_{t} \boldsymbol{h}_{t}+\boldsymbol{D}_{t} \boldsymbol{x}_{t} .
$$

Generally, the matrices $\boldsymbol{A}_{t}=\boldsymbol{A}\left(\boldsymbol{x}_{t}\right), \boldsymbol{B}_{t}=\boldsymbol{B}\left(\boldsymbol{x}_{t}\right), \boldsymbol{C}_{t}=\boldsymbol{C}\left(\boldsymbol{x}_{t}\right)$, and $\boldsymbol{D}_{t}=\boldsymbol{D}\left(\boldsymbol{x}_{t}\right)$ are functions of the input vector $\boldsymbol{x}_{t}$ for each $t \in[n]$. In the special case when $\boldsymbol{A}_{t}, \boldsymbol{B}_{t}, \boldsymbol{C}_{t}$, and $\boldsymbol{D}_{t}$ are independent from the input sequence $\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{n}$, we call $\mathcal{L}$ a linear $S S M$ layer. Moreover, we call $d$ the embedding dimension.

## 3 Function Composition Requires Wide Models

The function composition problem has been introduced in [30] to provide a theoretical understanding of the causes for the hallucination of Transformer models. The aim is to evaluate the model's capability to combine relational information in the data to understand language, the core competence of large language models. Indeed to correctly answer questions like 'what is the birthday of Frédéric Chopin's father?' given the information that 'the father of Frédéric Chopin was Nicolas Chopin' and that 'Nicolas Chopin was born on April 15, 1771', the model needs to be able to compose the functions 'birthday-of' and 'father-of' [30], [13].

Next, we give a precise formulation of the function composition problem due to [30]. Consider two functions, $g$ mapping a domain $A$ to a domain $B$, and $f$ mapping $B$ to another domain $C$. These functions will be described in a prompt $X$. The $N$ tokens of $X$ are divided into three parts:

1. the first part describes the function $g$ through $|A|$ sentences in simple, unambiguous language separated by punctuation, e.g. 'the father of Frédéric Chopin is Nicolas Chopin',
2. the second part consists of $|B|$ sentences describing the function $f$, e.g. 'the birthday of Nicolas Chopin is April 15, 1771',
3. the third part is the query question asking for the value of $f(g(x))$ for some specific $x \in A$.

In this section, we discuss the theoretical limitations of SSMs for solving the function composition problem.
Theorem 1. Consider a function composition problem with input domain size $|A|=|B|=n$, and an SSM layer $\mathcal{L}$ with embedding dimension d and computation precision $p$. Let $R=n \log n-\left(d^{2}+d\right) p \geq$ 0 , then the probability that $\mathcal{L}$ answers the query incorrectly is at least $R /(3 n \log n)$ if $f$ is sampled uniformly at random from $B^{C}$.

The proof is based on a reduction to a famous problem in communication complexity [30], [42]. We have three agents dubbed Faye, Grace, and Xavier. We assume that the agents have unbounded computational capabilities but, the only communication allowed is from Faye and Grace to Xavier. Faye knows a function $f:[n] \mapsto[n]$ and the argument $x \in[n]$, Grace knows a function $g:[n] \mapsto[n]$ and the argument $x$, while Xavier only knows the argument $x \in[n]$. The goal is for Xavier to compute the value of $f(g(x))$ minimizing the total number of bits communicated from Faye to Xavier and from Grace to Xavier.
We report here a lemma from [30] which gives a hardness result for the problem above.
Lemma 1 (Lemma 1 from [30]). Consider the problem described above, iffewer than $n \log n$ bits are communicated by Faye to Xavier, then Xavier cannot know the value $f(g(x))$. In particular, if only $n \log n-R$ bits are communicated for some $R \geq 0$, then the probability that the composition is computed incorrectly is at least $R /(3 n \log n)$ if $f$ is sampled uniformly at random from $B^{C}$.

Now we prove the theorem based on the lemma above.
Proof of Theorem 1. In order to establish the bound on $q$, we give a reduction of the communication problem above to the function composition problem. Let $\mathcal{L}$ be a SSM layer that can solve the function composition problem with probability $q$.

Suppose that we have Faye, Grace, and Xavier as in the settings above and Xavier wants to find the value $f(g(x))$. We construct the following prompt: for $i \in[1, n]$ let $\boldsymbol{x}_{i}$ be the token ' $g$ applied to $i$ is $g(i)$ ', where the information is provided by Grace, and for $i \in[n+1,2 n]$ let $\boldsymbol{x}_{i}$ the token string ' $f$ applied to $i$ is $f(i)^{\prime}$, where the information is provided by Faye. Xavier provides the last token string $\boldsymbol{x}_{2 n+1}=$ 'what is the value of $f(g(x))$ '. Since the SSM layer $\mathcal{L}$ can solve the composition task with probability $q$, we have that

$$
\boldsymbol{y}_{2 n+1}=\boldsymbol{C}_{2 n+1} \boldsymbol{h}_{2 n+1}+\boldsymbol{D}_{2 n+1} \boldsymbol{x}_{2 n+1}=f(g(x))
$$

with probability $q$.
But this allows us to construct the following communication protocol. Since Grace knows $g$, she knows the values of $\boldsymbol{x}_{i}$ for $i \in[1, n]$ and she iteratively computes

$$
\boldsymbol{h}_{i}=\boldsymbol{A}_{i} \boldsymbol{h}_{i-1}+\boldsymbol{B} \boldsymbol{x}_{i},
$$

and then sends $\boldsymbol{h}_{n}$ to Xavier. On the other hand, Faye knows $f$ and hence the values of $\boldsymbol{x}_{i}$ for $i \in[n+1,2 n]$, she computes the matrix

$$
\mathcal{A}=\prod_{j=n+1}^{2 n} \boldsymbol{A}_{j}
$$

and the vector

$$
\boldsymbol{b}=\sum_{i=n+1}^{2 n}\left(\prod_{j=n+1}^{2 n-i} \boldsymbol{A}_{j}\right) \boldsymbol{B}_{i} \boldsymbol{x}_{i}
$$

and she sends them to Xavier. At this point, Xavier computes

$$
\boldsymbol{h}_{2 n+1}=\boldsymbol{A}_{2 n+1} \cdot\left(\mathcal{A} \cdot \boldsymbol{h}_{n}+\boldsymbol{b}\right)+\boldsymbol{B}_{2 n+1} \boldsymbol{x}_{2 n+1}
$$

and find the value of $f(g(x))$ with probability $q$ by computing $\boldsymbol{y}_{2 n+1}=\boldsymbol{C}_{2 n+1} \cdot \boldsymbol{h}_{2 n}+\boldsymbol{D}_{2 n+1} \cdot \boldsymbol{x}_{2 n+1}$. The total number of bits of communication between Faye and Xavier is $\left(d^{2}+d\right) \cdot p$. By Lemma 1 , it follows that $q \leq R /(3 n \log n)$.

## 4 Many Thought Steps are Needed

A chain of thought $(\mathrm{CoT})$ is a series of intermediate natural language reasoning steps that lead to the final output. In this section, we focus on language models with the ability to generate a similar chain of thought - a coherent series of intermediate reasoning steps that lead to the final answer for a problem. In [40], it was observed that CoT can mitigate the problem of hallucinations by encouraging the LLM to generate prompts which break down the task into smaller steps eventually leading to the correct answer. In this section, we prove that in general many CoT steps are needed to break down compositional tasks.
We start the discussion with the formal definition of an SSM with $k$ CoT-steps. It adapts the definition for the Transformer model of [25] to the case of SSMs.
Definition 2 (SSM with CoT). Let $\phi:\left(\mathbb{R}^{m}\right)^{*} \rightarrow \mathbb{R}^{m}$ be a function mapping a prefix of tokens to a new token. The function $\phi$ is parametrized by a SSM layer $\mathcal{L}$.
Given an input sequence $\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{n} \in \mathbb{R}^{m}$, we call

$$
\phi_{k}\left(\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{n}\right)=\phi_{k-1}\left(\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{n}\right) \cdot \phi\left(\phi_{k-1}\left(\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{n}\right), \boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{n}\right),
$$

where $\phi_{1}\left(\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{n}\right)=\phi\left(\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{n}\right)$ and $\cdot$ denotes concatenation, the output of the SSM layer $\mathcal{L}$ with $k$ CoT-steps.

In this section, we want to prove that, while this procedure could help SSM layers with compositional tasks, it might require a large number of chain of thought steps in order to be effective. In particular we focus on the iterated function composition problem and show a lower bound on the number of CoT steps needed by a SSM layer in order to solve this problem correctly.

In the iterated function composition problem we are given $k$ functions $f_{1}, f_{2}, \ldots, f_{k}:[n] \mapsto[n]$, and we need to calculate $f_{k}\left(f_{k-1}\left(\ldots f_{2}\left(f_{1}(x)\right) \ldots\right)\right)$ for $x \in[n]$. Here we restrict to the case when $f_{1}=f_{2}=\cdots=f_{k}$, we define $f^{(k)}(x):=f(f(\ldots f(x)))$, and we call this $k$-iterated function composition problem.
Theorem 2. Consider an iterated composition problem with domain size $n$, computation precision $p$, and embedding dimension d. An SSM layer requires $\Omega\left(\frac{\sqrt{n \log n}}{d p}\right)$ CoT steps for answering correctly iterated function composition prompts.

The proof relies on a reduction of the iterated function composition problem to the pointer chasing problem [29], a classical problem in communication complexity. In the $k$-steps pointer chasing problem, we have two agents dubbed Alice and Bob, Alice knows a function $f_{A}:[n] \mapsto[n]$ and Bob knows a function $f_{B}:[n] \mapsto[n]$. We then define the pointers

$$
z_{1}=1, \quad z_{2}=f_{A}\left(z_{1}\right), \quad z_{3}=f_{B}\left(z_{2}\right), \quad z_{4}=f_{A}\left(z_{3}\right), \quad z_{5}=f_{B}\left(z_{4}\right), \quad \ldots
$$

The communication proceeds for $2 k$ rounds, with Alice starting. The goal is for Bob to output the binary value of $z_{2 k+2} \bmod 2$. We prove in the appendix A, that a SSM layer with $R$ CoT steps solving the iterated function composition problem can be used to design a communication protocol for the pointer chasing problem where the number of transmitted bits scales with $R$. The next fundamental Lemma in communication complexity gives a lower bound on the number of bits that need to be communicated in any such communication protocol and thus allows to derive the lower bound on the CoT steps.
Lemma 2 (Theorem 1.1 [43]). Any randomized protocol for the $k$-steps pointer chasing problem with error probability $1 / 3$ under the uniform distribution must involve the transmission of at least $n /(2000 k)-2 k \log n$ bits.

## 5 SSM's Capability to Reason Is Limited by LOGSPACE

In [30], it is suggested to an analyse the computational capability of LLMs on the following three computational problems. In fact, the empirical compositional tasks, studied in later sections, multiplication of multi-digit integers, dynamic programming and logic puzzles such as "Einstein's Riddle" can be expressed in terms of these computational problems[30].
Circuit evaluation: Given the description of a circuit with gates, which can be either Boolean or arithmetic operations, as well as the values of all input gates of the circuit, evaluate the output(s) of the circuit. Multiplying decimal integers with multiple digits is an example of such a circuit.
Derivability: Given a finite domain $S$ and a relation $D \subseteq S \times S$. For a given initial set $I \subseteq S$ and a final set $F \subseteq S$, answer the question whether there are elements $a_{1}, a_{2}, \ldots, a_{k} \in S$ such that (a) $a_{0} \in I$, (b) $a_{k} \in F$, and (c) for all $j$ such that $0<j \leq k,\left(a_{j-1}, a_{j}\right) \in D$.
Logical reasoning: Logic puzzles like 'Einstein's Riddle' can be typically formulated as instances of satisfiability (or SAT). This problem is NP-complete. However, most common-sense reasoning can be expressed by one of the three tractable special cases of SAT: 2-SAT, Horn SAT, Mod 2 SAT.

In [30], it was noted that since derivability, 2-SAT, Horn SAT, and circuit evaluation are all NLcomplete and the Transformer model lies in the complexity class log-uniform $\mathbf{T C}^{0} \subseteq \mathbf{L}$, these problems cannot be solved by a Transformer model provided $\mathbf{N L} \neq \mathbf{L}$ (which is a widely believed hypothesis in computational complexity). For Mod 2 SAT, the result is true provided the weaker statement $\mathbf{L} \neq \operatorname{Mod} 2 \mathbf{L}$. Very recently in [23], it was established that linear and S6- SSMs [11] are also part of the complexity class log-uniform $\mathbf{T C}^{0}$, which yields the following theorem similar to the case of transformers.
Theorem 3. The four problems of Derivability, 2-SAT, Horn SAT, and Circuit evaluation cannot be solved by linear or $S 6-S S M$ s provided $\mathbf{L} \neq \mathbf{N L}$. For Mod 2 SAT, the result is true provided the weaker statement $\mathbf{L} \neq \operatorname{Mod} 2 \mathbf{L}$ holds.

In fact the argument in [23], should also establish that linear and S6- SSMs with $\log (n)$ CoT steps, where $n$ is the size of the input, are still part of the complexity class $\mathbf{L}$. This allows to extend the theorem 3 even to the case of linear and S6- SSMs with $\log (n)$ CoT steps.

## 6 Experiments

To evaluate the inability of various sequence models in addressing function composition tasks (Sec. 6.1a), we examine three axes of composition: spatial, temporal, and relational. This evaluation is conducted using four datasets specifically designed to test function composition (Par. 6.1p). Subsequently, we proceed to compositional tasks involving multi-digit multiplication, dynamic programming, and Einstein's puzzle (Par. 6.1.). We investigate the effects of CoT prompting (Sec. 6.2) and conduct a thorough error analysis to understand the failure points and underlying reasons for this erroneous behaviour (Sec.6.3).
We conduct GPT experiments using the ChatGPT API [28], while evaluations of other models are performed on 2x A100 80 GB GPUs. Each task is evaluated three times with typically 500 test samples per evaluation, unless otherwise specified, to ensure consistency and minimize variance.

### 6.1 Function composition and compositional tasks

In the context of Large Language Models (LLMs), compositional tasks differ from function composition. Function composition $f_{K}\left(f_{K-1}\left(\ldots\left(f_{1}(x)\right)\right)\right)$ is a mathematical process where the output of one function serves as the input for another across multiple functions $f_{1}, f_{2}, \ldots, f_{K}$. Conversely, compositional tasks in LLMs involve breaking down complex inputs into simpler parts and integrating the results to generate an overall output. Examples include: (i) combining linguistic elements to generate coherent text, (ii) solving multi-step reasoning problems, and (iii) decomposing complex tasks (e.g., multi-turn conversations, summarization) into manageable sub-tasks.

Solving compositional tasks necessitates the capability to perform function composition [30, 6] and demands additional competencies such as contextual understanding, multi-step reasoning, and the integration of diverse information types. A model's proficiency in function composition is a critical prerequisite for tackling complex compositional tasks [21]. For instance, if an SSM-powered LLM
cannot evaluate $f(g(x))$, it will be inadequate for tasks involving multi-step arithmetic or logical operations that depend on nested functions.

Composition tasks We begin with three fundamental composition tasks: spatial, temporal, and relationship compositions. These axes are crucial as they encapsulate core aspects of comprehending and interacting with the world. Spatial composition entails integrating information about the positions and orientations of objects. Temporal composition involves reasoning over sequences and durations of events. Relationship composition focuses on understanding the connections between entities, such as those found in a genealogy tree.

Number of Parameters We conducted experiments using Jamba [18] (joint Mamba and Attention) with 7B parameters, Mamba [11] with 2.8B parameters, S4-H3 [12, 7] with 2.7B parameters, GPT-4 [28], and GPT-4o models. Qualitative results are presented in the Fig. 1. As illustrated in Fig. 1, all models failed to correctly answer questions across the three composition axes.
Problem 1 - Spatial axis

Question: Rectangle is to the west of the pen agon. The triangle is to the north of the square The rectangle is to the south of the square. The triangle is to the west of the circle. Wher is the square located in relation to the pentagon?

Jamba: East $X$
Mamba: Northeast $X$
GPT-4: Northeast $\boldsymbol{X}$
GPT-4o: North $\boldsymbol{X}$
Correct: Northwest. $\sqrt{ }$

## Problem 2 - Temporal axis

Question: Anne is the younger sister of Erwin Erwin is the elder brother of Daniel. Is Anne younger than Daniel?

Jamba: Yes $X_{X}$
Mamba: Yes $\boldsymbol{X}$
GPT-4: Yes $\boldsymbol{X}$
GPT-4o: Yes $\boldsymbol{X}$
Correct: Not enough information.

Problem 3 - Relationship axis
Question: Alan is the son of Marco, Joe is the son of Alan. Does Alan have any grandchildren?

Jamba: Yes $X$
Mamba: Yes $\boldsymbol{X}$
GPT-4: No $X$
GPT-4o: No $\boldsymbol{X}$
Correct: Not enough information. $\checkmark$

Figure 1: Qualitative example of zero-shot inference on prominent SSM and Attention-based models. None of the models successfully resolved the problems across any of the composition axes.

To quantitatively assess the limitations of models, including the latest GPT-4o [28], in solving function composition tasks, we evaluate their performance on four datasets specifically designed to test these capabilities. Unless otherwise specified, each model is tested on 500 samples.

Composition datasets Math-QA dataset, derived from [17], includes 25 math topics. We focus on the first 100 samples from Algebra, Calculus, Combinatorics, Game Theory, and Trigonometry. Problems involve solving function compositions and temporal reasoning. BIG-Bench Hard [33] dataset features 250 Boolean expressions that the model must evaluate. In Temporal-NLI [36] dataset each sample consists of a premise (e.g., "They got married on Saturday") and a hypothesis (e.g., "They got married before Friday"), requiring the model to determine if the relationship is entailment, contradiction, or neutral. SpaRTUN [26] dataset is designed for spatial reasoning and it includes stories describing the spatial positions of objects, followed by questions about the orientation of one object relative to another (e.g., left, right, inside, above).

|  | GPT-4o 28] | GPT-4 28 | Jamba 18] | Mamba 11] | S4-H3 12,7] |  | GPT-40 [28] | GPT-4 [28] | Jamba 18] | Mamba 11 | S4-H3 12, 7] |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Math-QA 17 | 51.8\% | 51.0\% | $42.2 \%$ | 35.0\% | $28.6 \%$ | Algebra | 51\% | 47\% | $42 \%$ | $36 \%$ | $29 \%$ |
| BIG-Bench Hard 331 | 56.8\% | 58.4\% | 78.2\% | 67.0\% | 60.6\% | Calculus | 50\% | 48\% | 41\% | 34\% | 28\% |
| Temporal-NLI 36] | 79.4\% | 77.2\% | 69.8\% | 59.2\% | 54.6\% | Combinatorics | 88\% | 70\% | 48\% | 38\% | 33\% |
| SpaRTUN 26] | 80.8\% | $61.4 \%$ | 50.8\% | 42.2\% | $35.2 \%$ | Game theory | 30\% | 40\% | 50\% | $41 \%$ | $32 \%$ |
|  |  |  |  |  |  | Trigonometry | 40\% | 50\% | 30\% | 26\% | 21\% |

Table 1: Performance of Attention, SSM and Attention-SSM based models on various function composition tasks involving logical expressions, temporal reasoning, spatial reasoning, and math tasks

Table 2: Performance of models on various topics within the MathQA [17] dataset. Input dependency consistently improves performance, with Mamba (11] consistently outperforming S4-H3 [12]. 7 .

The results presented in Tables 1 and 2 highlight several key observations regarding the performance of various models across different composition tasks. Notably, Mamba [11] consistently outperforms the S4-H3 [12, 7] model, despite both having almost the same number of parameters. This performance gap underscores the importance of input-dependence in model design, as Mamba's architecture better leverages input information to achieve superior results. Additionally, while GPT-4o is the most performant overall, it struggles with many tasks, including those that seem simple to humans, such as logical expression chaining, as evidenced by its performance on the BIG-Bench Hard [33] benchmark. This indicates that even state-of-the-art models like GPT-4o have limitations in solving complex composition tasks, which numerically justifies our theoretical findings. Accuracy for all models is calculated as the number of correct answers divided by the total number of samples.

Compositional tasks Having demonstrated that models encounter difficulties even with simpler composition tasks, we now examine their performance on more complex compositional tasks. Given their proven inability to perform function composition, as established in Theorem 1, it is entirely anticipated that their performance on these tasks will be suboptimal. We explore three compositional tasks: (i) multi-digit multiplication, (ii) dynamic programming, and (iii) Einstein's puzzle.
For the multi-digit multiplication task, we generate question-answer pairs such as "What is 5 times 90 ?" with the answer being "450". This task involves multiplying two numbers, $x=\left(x_{1}, x_{2}, \ldots, x_{k}\right)$ and $y=\left(y_{1}, y_{2}, \ldots, y_{k}\right)$, where each number can have up to $k$ digits. Consequently, there are $9 \times 10^{(k-1)}$ possible combinations for each number. In our experiments, we set $k$ to 5 and found that both Attention and SSM-based models are unable to solve the 5-by-5 digit multiplication task, even in the case of GPT-4o with CoT prompting (A-12).


Figure 2: Jamba [18] performance on multiplication, DP and puzzle tasks. For DP various models are shown. All struggle with compositional tasks, especially for larger input size.

Dynamic programming ( $D P$ ) recursively decomposes complex problems into simpler sub-problems, making solutions compositional by nature. We consider a classic relaxation of the NP-complete Maximum Weighted Independent Set problem [16]: Given a sequence of integers, find a subsequence with the highest sum such that no two numbers in the subsequence are adjacent in the original sequence. This relaxation can be solved in $O(n)$ time using DP. For our experiments, we restrict each integer to the range $[-5,5]$ and follow the generation steps as in [6], with input list containing from 2 to 6 elements. Prompting details are shown in the A-B. 3

Einstein's puzzle is a well-known logic puzzle commonly used as a benchmark for solving constraint satisfaction problems [31]. It involves a series of houses with various attributes, and the objective is to determine which attributes correspond to each house by interpreting a set of predefined natural language clues or constraints. The solution to the puzzle is represented as a matrix of size $H \times A$, where $H$ denotes the number of houses and $A$ represents the number of attributes. As $H$ and $A$ increase, synthesizing partial solutions that satisfy individual constraints becomes increasingly compositionally complex. Qualitative examples and details about data generation for this task are provided in the $\mathrm{A}, \overline{\mathrm{B} .2}$

### 6.2 CoT experiments

Next, we evaluate how the popular chain-of-thought (CoT) prompting method [40] affects the performance of GPT-4o [28], Jamba [18], Mamba [11] and S4-H3 [12] models on compositional tasks from Sec. 6.1. CoT improves the performance, but does not solve the task. Details of the experiments and examples of full prompts can be found in the $\mathrm{A}-\mathrm{C}$

### 6.3 Error analysis

We focus on graph analysis of errors, with emphasis on multi-digit multiplication, because this problem is easier to interpret and understand. From this analysis we obtain a few interesting conclusions about how errors happen and then propagate inside SSM-based LLMs [7, 11, 26].
Computation Graph To study the propagation of errors and its dependency on input size, we define $A$ as a deterministic algorithm (function), and $\mathcal{F}_{A}$ as the set of primitives (functions) the algorithm employs during execution. Given inputs $\mathbf{x}$ to the algorithm $A$, we define the static computation graph of $A(\mathbf{x})$, denoted as $G_{A(\mathbf{x})}$, as $G_{A(\mathbf{x})}=(V, E, s, o p)$, a directed acyclic graph.
Nodes $V$ represent all variable values during $A$ 's execution, where each node $v \in V$ has an associated value $s(v) \in \mathbb{R}$. Edges $E$ represent function arguments involved in computations: for each non-
source node $v \in V$, let $U=\left\{u_{1}, \ldots, u_{j}\right\} \subset V$ be its parent nodes. Then, $s(v)=f\left(u_{1}, \ldots, u_{j}\right)$ for some $f \in \mathcal{F}_{A}$. Since each node $v$ is uniquely determined by the computation of a single primitive $f$, we define $o p: V \rightarrow \mathcal{F}_{A}, o p(v)=f$ as the operator function that yields $s(v)$. Let $S \subset V$ be the source nodes of $G_{A(\mathbf{x})}$, and without loss of generality, let $o \in V$ be its sole leaf node. By definition, $S \equiv \mathbf{x}$ and $A(\mathbf{x})=s(o)$, representing the input and output of $A$, respectively. To evaluate a language model's ability to follow algorithm $A$, we must linearize $G_{A(\mathrm{x})}$ (arrange the nodes in a linear sequence that respects the dependencies). This means if a node $u$ is a parent of node $v$, the $u$ should appear before $v$ in the sequence. Since we only consider autoregressive models, this linearization must also be a topological ordering. A topological order ensures that every node appears after its parent nodes, maintaining the correct order of computations. This is crucial for correctly following the sequence of operations as defined by the algorithm $A$.

```
Algorithm 1 Multiply two numbers
    function \(\operatorname{MULTIPLY}(x[1 . . p], y[1 . . q]) \quad \triangleright\)
    multiply \(x\) for each \(y[i]\)
        for \(i=q\) to 1 do
            carry \(=0\)
            for \(j=p\) to 1 do
                \(t=x[j] \times y[i]\)
                \(t+=\) carry \(\quad \triangleright\) add carry
                carry \(=t \div 10\)
                digits \([j]=t \bmod 10\)
            end for
            summands \([i]=\) digits
        end for
        product \(=\sum_{i=1}^{q}\) summands \([q+1-i]\).
    \(10^{i-1}\)
        return product
    end function
```



Figure 3: Example of 2-by-1 digit multiplication $(87 \times 9)$. Operations on graph include: inputs, multiply 1 -digit, carry, sum, mod 10 and output.

To instantiate $G_{A(\mathbf{x})}$, let $\mathcal{F}_{A}=\{$ one-digit multiplication, sum, mod 10 , carry over, concatenation $\}$. Source nodes $S$ are digits of input numbers, leaf node $o$ is the final output, and intermediate nodes $v$ are partial results generated during execution of the long-form multiplication algorithm (see Fig. 3). Corresponding algorithm is on the left of the Fig. 3- Alg. 1 .

Error propagation We investigate the types of errors encountered by SSMs. Specifically, Fig. 4 illustrates the errors produced by the $\mathrm{S} 4-\mathrm{H} 3$ model [12, 7]. The figure reveals a prevalence of local errors, where the immediate outputs are incorrect despite the correctness of ancestor outputs. Propagation errors occur when the model generates correct outputs from incorrect ancestor values-e.g., in Fig. 4, the computation $3+4=7$ is correct, but the value 3 results from a local error. Our analysis reveals that propagation errors are 2-4 times more frequent than local errors, consistent with findings by [6] for Transformers. This indicates that SSM-based models, like Transformers, can handle single-step reasoning well due to pretraining memorization but struggle with multi-step reasoning and planning. Consequently, these models excel at local tasks but fail to integrate steps into coherent global reasoning, leading to error propagation.


Figure 4: Error Propagation. Carry operation outputs number 3 instead of 2 from node ' 27 ', and that error is further propagated, yielding incorrect solution in the middle digit, although all other steps were done right.


Figure 5: SSMs and Transformers learn shortcuts that seem to solve function composition but fail with larger inputs and out-of-distribution data.

SSMs learn shortcuts The performance of SSMs provides valuable insights into their behavior. These models often predict partially correct answers even when the overall response is incorrect. For example, using Mamba [11] for 2-by-2 digit multiplication, the first and last digits are usually accurate. In larger multiplications, the first two and last two digits tend to be correct. Using Relative Information Gain (RIG) analysis [6], we find that SSMs learn shortcuts, performing fewer operations (illustrated by the red and green subgraphs in Fig. [5]. This allows them to frequently predict peripheral digits correctly. For instance, to compute the last digit, the model multiplies 8 and 5 , carrying 0 to the end, mimicking human multiplication and easily predicting the last digit accurately. RIG analysis reveals a strong correlation between the first digit (or first two digits) of the output and the first digit (or first two digits) of the input numbers.

These models leverage task distribution shortcuts to guess partial answers without full multi-step reasoning. Increasing the number of Chain-of-Thought (CoT) steps doesn't always improve results, especially for larger input sizes (deeper computation graphs). If the model encounters relevant subgraphs during training, its inference seems highly compositional but is based on shortcuts [8, 19, 34, 5]. These experiments indicate that when an output element heavily relies on a few input features, SSMs recognize this correlation during training and map these features to predict the output during testing. This gives the false impression of performing compositional reasoning while bypassing rigorous multi-hop reasoning [41].

### 6.4 Learning Algorithmic Compositions

Finally, we conduct a comprehensive analysis of the capabilities of SSM-based models, along with GPT-4o [28], to "learn" discrete algorithms. This analysis is performed using two tasks that require the composition of multiple discrete sub-tasks. By empirically examining the models' algorithmic learning through compositionality testing, we observe their inability to effectively perform these tasks, even when provided with few-shot prompts and CoT examples [40]. This suggests that, within the framework of in-context learning, SSM and Transformer-based models fail to attain compositional learning when constrained to a fixed number of samples. Details in the A-D.

## 7 Related work

Limitations in Function Composition and Reasoning Recent studies have underscored the limitations of deep learning models, particularly Transformers in handling tasks requiring deep compositionality and multi-step reasoning [30, 6]. These tasks are crucial in applications like mathematical problem-solving [17], algorithm learning [35], logical reasoning [20], and dynamic programming [6]. Transformers, despite their capabilities, have been shown to struggle with function composition, which is essential for understanding relational information in data [13]. Research has highlighted the architectural and training limitations that prevent these models from maintaining accuracy over multiple reasoning steps, leading to issues like hallucinations [24]. Studies by [23] and [30] have identified that both Transformers and SSMs belong to weak complexity classes, such as logspace-uniform TC ${ }^{0}$, which limits their abilities. However, SSMs were not investigated theoretically and experimentally in terms of ability to perform function composition and compositional tasks, which is our contribution.

Chain-of-Thought (CoT) Prompting The Chain-of-Thought (CoT) prompting method has been proposed as a potential solution to improve reasoning capabilities in large language models by breaking down complex tasks into smaller, intermediate steps [40]. This approach aims to mitigate hallucinations and improve multi-step reasoning. However, our research indicates that even with CoT prompting, current models remain inadequate for solving deeply compositional tasks [25].

## 8 Conclusions

In this paper, we have rigorously explored the limitations of deep learning models, particularly Structured State Space Models (SSMs) and Transformers, in handling tasks requiring deep compositionality and multi-step reasoning. Through a blend of theoretical insights and empirical analysis, we demonstrated that these models inherently struggle with function composition and compositional tasks due to their architectural constraints.

## 9 Limitations

Our study primarily focuses on the theoretical and empirical limitations of SSMs and Transformers in sequence modeling and compositional tasks. While we have demonstrated these inherent limitations, our analysis does not provide a solution but rather establishes the existence of these issues both theoretically and practically. Future research should explore alternative architectures and broader applications to better understand and address these limitations.

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## A Proof of Theorem 2

Before we begin with the actual proof, let us introduce some notation. We note that $\phi_{k}$ is a string of $k$ tokens of $\mathbb{R}^{m}$. Moreover, to compute the new token $\phi\left(\phi_{k-1}\left(\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{n}\right), \boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{n}\right)$ the SSM layer $\mathcal{L}$ computes $n+(k-1)$ hidden states. We denote the $i$-th hidden state by $\phi_{k, i}\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{n}\right)$.

Proof of Theorem 2] The proof is similar to the proof of Theorem 2 in [30]. We reduce the pointer chasing problem to the iterated composition problem with CoT prompts. In particular, we show that if the SSM $\mathcal{L}$ can solve the $k$-iterated function composition problem with $R$ CoT steps, then we can construct a protocol solving the $(k-1)$-steps pointer chasing problem using $2 R d p$ bits of communication.

Fix a $(k-1)$-steps pointer chasing problem for the function $f_{A}, f_{B}:[n] \mapsto[n]$. Define the function $f:[2 n] \mapsto[2 n]$ as

$$
f(i)= \begin{cases}f_{A}(i)+n, & i \in[1, n] ; \\ f_{B}(i-n), & i \in[n+1,2 n] .\end{cases}
$$

We point out that $f^{(k)}(i)=\left(f_{B} \circ f_{A}\right)^{(k)}(i)$. Consider the $k$-iterated function composition problem for $f$ and suppose that there exists a SSM $\mathcal{L}$ that solves it using $R \operatorname{CoT}$ steps.
We construct the following prompt: for $i \in[1, n]$ let $\boldsymbol{x}_{i}$ be the token ' $f$ applied to $i$ is $f(i)$ ', where the information $f(i)$ is provided by Alice, and for $i \in[n+1,2 n]$ let $\boldsymbol{x}_{i}$ the token string 'f applied to $i$ is $f(i)$ ', where the information $f(i)$ is provided by Bob. The last token string $\boldsymbol{x}_{2 n+1}$ is given by 'what is the value of $f^{(k)}$ applied to $x$ '. Since the SSM layer $\mathcal{L}$ can solve the $k$-iterated function composition task with $R$ CoT steps, we have that $\phi_{R}\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{2 n}\right)$ is the right answer for $f^{k}(x)$. We will use this fact to construct a communication protocol transmitting at most $2 \cdot R d p$ bits. The communication protocol lasts for $R$ rounds.
In the r-th round Alice computes $\phi_{r, n+k}\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{2 n}\right)$ from $\phi_{r-1}\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{2 n}\right)$ (where $\phi_{0}\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{2 n}\right)$ is the empty string of tokens) and $\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{n}$ and communicates it with Bob. Bob on the other hand computes $\phi_{r}\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{2 n}\right)$ from $\phi_{r, n+k}\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{2 n}\right)$ and $\boldsymbol{x}_{n+1}, \ldots, \boldsymbol{x}_{2 n}$ and transmits it to Alice. In each iteration at most $d p$ bits are communicated from Alice to Bob and from Bob to Alice.
After $R$ rounds, Bob knows the value of $\phi_{R}\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{2 n}\right)$. By hypothesis, this is the solution to the $(k-1)$-steps pointer chasing problem. Notice that, the total number of bits communicated by the protocol are $2 R d p$. In conclusion, we fix $k=\frac{1}{100} \sqrt{\frac{n}{\log n}}+1$ and by Lemma 2 we get that $2 R d p \geq n /(2000 k)-2 k \log n$ which gives $R \geq \frac{3}{100} \frac{\sqrt{n \log n}}{d p}$

## B Compositional Tasks Details

## B. 1 Multiplication

We show examples of few-shot and CoT prompting methods for multiplication task (Figs. 6\& 7).

```
To multiply two numbers, start by multiplying the rightmost digit of the
multiplicand by each digit of the multiplier, writing down the products and
carrying over any remainders. Repeat this process for each digit of the
multiplicand, and then add up all the partial products to obtain the final result.
Here are examples:
Question: what's 32 times 8? Answer 256.
Question: what's 69 times 3? Answer 207.
Question: what's 93 times 6? Answer 558.
Question: what's 76 times 8? Answer:
```

Figure 6: Example prompt for the multiplication task used for the few-shot prompting.

```
Question: What is 904 times 74?
Scratchpad: Let's perform the multiplication step by step:
Let's multiply }904\mathrm{ by the digit in the ones place of 74, which is 4.
1. Multiply 4 by the digit in the ones place of 904, which is 4. This gives 4 x }
= 16. Write down the result 6 and carry over the 1 to the next step.
2. Multiply }4\mathrm{ by the digit in the tens place of 904, which is 0. Add the
carryover from the previous step to account for this. This gives (0 x 4) + 1 = 1.
Write down the result 1.
3. Multiply 4 by the digit in the hundreds place of 904, which is 9. This gives }
x 4 = 36. Write down the result 36.
4. The partial product for this step is A=3616 which is the concatenation of the
digits we found in each step.
Now, let's multiply 904 by the digit in the tens place of 74, which is 7.
5. Multiply }7\mathrm{ by the digit in the ones place of 904, which is 4. This gives 4 x 7
= 28. Write down the result }8\mathrm{ and carry over the 2 to the next step.
6. Multiply }7\mathrm{ by the digit in the tens place of 904, which is 0. Add the
carryover from the previous step to account for this. This gives (0 x 7) + 2 = 2.
Write down the result 2.
7. Multiply }7\mathrm{ by the digit in the hundreds place of 904, which is 9. This gives }
x 7 = 63. Write down the result 63.
8. The partial product for this step is B=6328 which is the concatenation of the
digits we found in each step.
Now, let's sum the 2 partial products A and B, and take into account the position
of each digit: A=3616 (from multiplication by 4) and B=6328 (from multiplication
by }7\mathrm{ but shifted one place to the left, so it becomes 63280). The final answer is
3616 x 1 + 6328 x 10=3616 + 63280 = 66896.
```

Figure 7: A sample scratchpad for the multiplication task.

## B. 2 Einstein's Puzzle

Data Construction Following [6], we first define a set of properties such as "Color", "PhoneModel", and "Pet", along with their corresponding values in natural language templates (e.g., "The house has a red color."). We then create a basic and clear set of clue types:

1. found_at: For example, "Alice lives in House 2."
2. same_house: For example, "The person who is a cat lover lives in the house that has a red color."
3. direct_left: For example, "The person who has a dog as a pet lives to the left of the person who lives in a red house."
4. besides: For example, "The person who has a dog as a pet and the person who has a red house live next to each other."

Additionally, we introduce more challenging clue types for auxiliary experiments, such as not_at, left_of (not necessarily directly left), and two_house_between. These harder clues are used to test the robustness and versatility of our models.

Graph Construction To address the complex compositional reasoning required for a logical grid puzzle, we utilize existing puzzle solvers [4] to generate the computation graph. Our algorithm follows a basic greedy principle: it applies the minimum number of rules necessary to solve any cell. Specifically, if a single rule can solve a cell, that rule is applied.

The algorithm iterates through all clues in the clue set, seeking combinations that can solve any cell in the table. Although this approach may not be the most efficient, it enables models to have explicit scratchpad verbalization via an intuitive computation graph. Fig 8 shows an example of a scratchpad.

```
This is a logic puzzle. There are 3 houses (numbered 1 on the left, 3 on the
right). Each has a different person in them. They have different characteristics:
- Each person has a unique name: peter, eric, arnold
- People have different favorite sports: soccer, tennis, basketball
- People own different car models: tesla model 3, ford f150, toyota camry
1. The person who owns a Ford F-150 is the person who loves tennis.
2. Arnold is in the third house.
3. The person who owns a Toyota Camry is directly left of the person who owns a
Ford F-150.
4. Eric is the person who owns a Toyota Camry.
5. The person who loves basketball is Eric.
6. The person who loves tennis and the person who loves soccer are next to each
other.
Let's think step by step. Please first briefly talk about your reasoning and show
your final solution by filling the blanks in the below table.
$ House: _-_ $ Name: _-_ $ Sports: _-_ $ Car: _-_ $ Sports: _-- $ Car: _-- 
Reasoning:
Step 1: First apply clue <Arnold is in the third house.> We know that The Name in
house 3 is arnold.
Step 2: Then combine clues: <The person who loves tennis and the person who loves
soccer are next to each other.> <The person who loves basketball is Eric.>
Unique Values Rules and the fixed table structure. We know that The Name in house
1 is eric. The FavoriteSport in house 1 is basketball. The Name in house 2 is
peter.
Step 3: Then apply clue <Eric is the person who owns a Toyota Camry.> We know
that The CarModel in house 1 is toyota camry.
Step 4: Then apply clue <The person who owns a Toyota Camry is directly left of
the person who owns a Ford F-150.> and Unique Values We know that The CarModel in
house 2 is ford f150. The CarModel in house 3 is tesla model }3
Step 5: Then apply clue <The person who owns a Ford F-150 is the person who loves
tennis.> and Unique Values We know that The FavoriteSport in house 2 is tennis.
The FavoriteSport in house 3 is soccer.
The puzzle is solved.
Final solution:
$ House: 1 $ Name: Eric $ Sports: Basketball $ Car: Camry
$ House: 2 $ Name: Peter $ Sports: Tennis $ Car: Ford
$ House: 3 $ Name: Arnold $ Sports: Soccer $ Car: Tesla
```

Figure 8: A sample scratchpad for the Einstein's puzzle task.

## B. 3 Dynamic Programming

We show examples of zero/few-shot and CoT prompting methods for dynamic programming task (Figs. 9 \& 10), following [6].

```
Given a sequence of integers, find a subsequence with the highest sum, such that
no two numbers in the subsequence are adjacent in the original sequence.
Output a list with "1" for chosen numbers and "2" for unchosen ones. If multiple
solutions exist, select the lexicographically smallest. input = [3, 2, 1, 5, 2].
```

Figure 9: Example prompt for the DP task, used for zero-shot and few-shot settings.

```
Question: Let's solve input = [3, 2, 1, 5, 2].
Scratchpad: dp[4] = max(input[4], 0) = max (2, 0) = 2
dp[3] = max(input [3], input[4], 0) = max(5, 2, 0) = 5
dp[2] = max (dp[3], input[2] + dp[4], 0) = max (5, 1 + 2, 0) = 5
dp[1] = max (dp[2], input[1] + dp[3], 0) = max (5, 2 + 5, 0) = 7
dp[0] = max (dp[1], input[0] + dp[2], 0) = max (7, 3 + 5, 0) = 8
Finally, we reconstruct the lexicographically smallest subsequence that fulfills
the task objective by selecting numbers as follows. We store the result on a list
named "output".
Let can_use_next_item = True.
Since dp[0] == input[0] + dp[2] (8 == 3 + 5) and can_use_next_item == True, we
store output[0] = 1. We update can_use_next_item = False.
Since dp[1] != input[1] + dp[3] (7 != 2 + 5) or can_use_next_item == False, we
store output[1] = 2. We update can_use_next_item = True.
Since dp[2] != input[2] + dp[4] (5 != 1 + 2) or can_use_next_item == False, we
store output[2] = 2. We update can_use_next_item = True.
Since dp[3] == input[3] (5 == 5) and can_use_next_item == True, we store
output[3] = 1. We update can_use_next_item = False.
Since dp[4] != input[4] (2 != 2) or can_use_next_item == False, we store
output[4] = 2.
Reconstructing all together, output=[1, 2, 2, 1, 2].
```

Figure 10: A sample scratchpad for the DP task.

## C Details of CoT experiments

## C. 1 Main CoT experiments

We plot the performance of Jamba [18] on multiplication and puzzle tasks, and various models on DP task after using CoT.


Figure 11: Jamba's [18] performance on multiplication and puzzle tasks improves with CoT, though not fully solved. Other models were tested on the DP task, where they failed at higher input sizes, despite CoT.

The leftmost heatmap on Fig. 11 represents the Jamba [18] model's multiplication performance, showing a consistent high performance for multipliers of 1 and 2, but a noticeable decline as the multipliers increase, particularly beyond 3. The middle heatmap compares the performance of four models-GPT-4o [28], Jamba [18], Mamba [11], and S4-H3 [12] 7]-on dynamic programming tasks with CoT prompting [40]. GPT-4o [28] consistently outperforms the other models, maintaining high performance even for larger problem list sizes, while the performance of the other models decreases more rapidly. The rightmost heatmap displays Jamba's puzzle-solving performance, indicating high accuracy for simpler puzzles with fewer attributes but a steep decline as the complexity increases. These visualizations highlight that while CoT prompting [40] generally enhances model performance, its effectiveness varies significantly across different models and task complexities.

## C. 2 Performance of other models on multiplication and puzzle tasks

We observe the same pattern on both tasks, for all the models - Figs. 12 \& 13 GPT-4o [28] is always the best model, followed by Jamba [18], then Mamba [11], then S4-H3 [7, 12]. While CoT helps, it is not enough to solve the task.


Figure 12: Comparison of different models on multiplication task using CoT.


Figure 13: Comparison of different models on puzzle task using CoT.

## C. 3 Few-shot prompting multiplication results

We investigate whether few-show prompting (giving a model few input/output pairs) and then asking for the answer to the new problem helps. Fig. 14 shows the results, and consistently CoT outperforms Few-shot prompting, and Few-shot prompting outperforms Zero-shot prompting.


Figure 14: Comparison of different models on multiplication task using few-shot prompting.

## D Algorithmic Compositions

Following [35], we evaluate the models using the PE's Neighbour (PEN) task. This task involves navigating from one word to the next based on a specified matching criterion and outputting all the neighbours encountered along the way. The PEN task, inspired by [1] and rooted in the Pointer Value Retrieval framework [44], is particularly compelling due to its four sub-tasks, which test the necessary sub-operations for PEN. These sub-tasks are: (i) Copy words, (ii) Reverse Copy (copying words in reverse order, where words consist of
multiple tokens), (iii) PE (outputting words in the matching chain instead of neighbours), and (iv) PE Verbose (PEV) - outputting both the words of the matching sequence and their neighbours. These sub-tasks are essential because, to predict the next word, the model must: take the current word in the answer, obtain the left neighbour (learned in Reverse Copy), match it (learned in PE), and then obtain the right neighbour (learned in Copy). PEV is considered a sub-task because it requires solving the same problem as PEN but with the added complexity of providing both matching words and their neighbours. PEN, on the other hand, only requires outputting the neighbours. For accurate next-token prediction the model cannot simply replicate the last matching sequence word from the previous answers, it must first infer it from the neighbour. To increase the task's complexity, "attention traps" or "doppelgangers" are introduced. These traps create additional matching possibilities by allowing each neighbour to match two other words, thus tempting the model to match from the neighbour of a matching sequence instead. This added layer of difficulty further challenges the models' ability to learn and compose discrete algorithms effectively. Pointer Execution Reverse Multicount (PER Multi) shares conceptual similarities with the PEN task; however, instead of matching forward and predicting the current word or its neighbour, the task involves first outputting the last word in the matching sequence and then proceeding backward. Consequently, to accurately predict the first word, the model must identify the end of the matching sequence and output that word. The model needs to count the total number of matchings and the number of matchings that align to the left in the given word order. The answer requires multiplying these two counts, introducing a non-linearity. For this task, we omit any attention traps, as there are no neighbours involved. In the A-D we show concrete prompt examples and share the code.
We conducted extensive evaluations on 500 test samples using various models under different conditions: zeroshot, few-shot (providing a limited number of input-output pairs), and CoT prompting [40]. Remarkably, none of the models, including the state-of-the-art GPT-4o [28], succeeded in solving the PEN task [35]. Typically, models correctly generated the initial strings but then halted prematurely or produced random strings. The same pattern of failure was observed with the PER Multi task. Specifically, GPT-4o achieved only $1 \%$ and $9 \%$ accuracy using few-shot and CoT prompting, respectively, failing to solve the task. The marginal success of GPT-4o is attributed to its substantially larger parameter count compared to SSM-based models 6.1).

Table 3: Model Accuracy for PEN task

| Model | Prompt Setting | Accuracy [\%] |
| :---: | :---: | :---: |
| GPT-4o [28] | Zero-shot | 0.00 |
|  | Few-shot | 0.00 |
|  | CoT | 0.00 |
| Jamba | Zero-shot | 0.00 |
|  | Few-shot | 0.00 |
|  | CoT | 0.00 |
| Mumba | Zero-shot | 0.00 |
|  | Few-shot | 0.00 |
|  | CoT | 0.00 |
| S4-H3 [12,7 | Zero-shot | 0.00 |
|  | Few-shot | 0.00 |
|  | CoT | 0.00 |

Table 4: Model Accuracy for PER Multi task

| Model | Prompt Setting | Accuracy [\%] |
| :---: | :---: | :---: |
| GPT-4o 28 | Zero-shot | 0.00 |
|  | Few-shot | 0.01 |
|  | CoT | 0.09 |
| Jamba | Zero-shot | 0.00 |
|  | Few-shot | 0.00 |
|  | CoT | 0.00 |
| Mumba | Zero-shot | 0.00 |
|  | Few-shot | 0.00 |
|  | CoT | 0.00 |
| S4-H3 [12,7] | Zero-shot | 0.00 |
|  | Few-shot | 0.00 |
|  | CoT | 0.00 |

In the following subsections we focus on showing the prompts in few-shot and CoT settings for PEN and PER Multi tasks. Moreover, we show the code we used to generate the samples.

## D. 1 Prompts for SSM and Attention-based models for PEN task

```
Example: eg jy vm3zc si2zf nn4ll zf5ka ki7xd ew0si xp3og il5js xn6yx my7ec xu2gb
if2my fy3so ec2il ob5ch kt5if zc4xp ka3mj og1ud zf2ka yh3ux hx2kt vc2pf jy4qd
lj1xu wy5hx bd4xa my4ec at1kb jy3qd ux1fl ew3si ds2qz qd7ew xa1ay si1zf ch4lj
js3rf fl6xn mj7wy zy6rq zh2gu bj3rb if0my pg5ds yv3hs zu3ob ta7qi ji2bj mj1wy
rq7ul mn3fw ay4qu kt2if kr3qb pr0ah tg0at uc1vx xd1pd wy4hx dr6fy mk0vj sm0pg
jl2mo rb1bd il2js vn6kr km4aq eg7nn ka6mj qu4vc hx7kt ll2lb ec6il ud2vn di3xs
pd6ji qd6ew yx7zu rh4qn lb1ki js5rf iv3yh jj0fa kb3sm lh6yk so0iv bx6rs qz1vm
mw7bm gb2xo uyOms qb2zy zm0pz xo4tg zx5jm
Answer: jy ka6mj zf5ka ec6il js5rf ewOsi wy4hx qd6ew mj1wy ifOmy il2js my4ec
si1zf kt2if hx7kt jy4qd
<FEW MORE EXAMPLES>
Your question: ey wt kj5yo jz0aa nu4yw gp2ro mv6kj nk2qz tr3mp ro7rk tu5xj rk0sj
ad2lx up3vd ta7rv qz6ob rc7nt aa4nk mb6mm ob7us jw5wb wt4jz nn4sr wt0jz evOfa
gp1ro sr1nu sj0ku xsOta us5up mp6jw vd1gp xj3cs sj7ku ol3vv vd3gp wd2mv wr4cz
dgOpy ro5rk jt6ev bv0cf yb2qv ch2ss xa3be nb5id lx4jt dz5ht wb5wd fb3ax faOtu
jn5ps rv7qj qa7el rn7ad lz3fk mm1tr yd3lv nt0xs lh4zk mr3ou ja5sn gi5ub rk4sj
wm7zm jz3aa be4mb kw3bh qj4xa cg0mi jl2rn kv1wg qt5mr ye3kg yr5ol nk7qz ub1dg
ob3us cs7so gw4vk ey4wm qz2ob qv4jl xz4hc li0yb oy4qu zm2yr up7vd ou7li rx4wc
yw7gi aa2nk yo3qt yz5cx vv6nn us7up
Clearly mark your answer by writing 'Answer: <your answer>' as last line.
```

Figure 15: Prompt for the PEN task, showcasing few-shot learning examples. Each word's start and end are encoded as distinct tokens, so a model can pattern-match the respective token to do the matching operation.

## Prompt for the PEN task with few-shot CoT examples and a description.

I give you a sequence of words. Each word has four characters plus a middle, words are separated by spaces. Start with the leftmost word. Output its neighbour. Then, match the last two characters of the current word (i.e. not the neighbour) to the word starting with those two characters. Again, output the neighbour. Do this until your current word (not the neighbour) has no match anymore.

Example: xh jz qw4se zs1qh xv4vn me3af vs1nh ok3ks sn6iv qh1va da5gy ks1ew tw7ik em5zs xs5qu ft3me gt3bc em3zs zn5qv ks5ew by7kn me7af je0wt cb0ft pw6hg rk7cb dv2sn ew3rk yg1by va1cq qu7fp qh4va vn5zn ok1ks cc7tw rk0cb bc7qi jz7em qz2cs ew6rk qv6gt ft7me fp1qw sa6ok sd7pn jz3em wi3da cq7sa iv0vl zs7qh vl2kc va5cq fe5wi xl1zh hg0dv cq4sa ja2nb wh5vv ot 4 sh qe0jx yt6xs vc0qx nblam rf2zl kn5hq xg5hk mz7yg aq3uw xh7pw sa7ok wt5ot io6hd pn1je lo6vx hq5cc wp6fc cs7fe yw2ka gy3sd nr0ry am3yt pl0rl ik0tn ub5tq sh0ja ee2it nh6qz xz1ma se0rx is 7 rn kc1xv cb6ft rx2mz wj7qf. The leftmost word is $\mathbf{x h}$. Its right neighbour is $\mathbf{j z}$, so the first output word is $\mathbf{j z}$.
Now, we need to find a word that starts with xh. The word is xh7pw. Its right neighbour is sa7ok, so the next output word is sa7ok.
Now, we need to find a word that starts with pw. The word is pw6hg. Its right neighbour is rk7cb, so the next output word is rk7cb
Now, we need to find a word that starts with hg. The word is hg0dv. Its right neighbour is cq4sa, so the next output word is cq4sa. Now, we need to find a word that starts with $\mathbf{d v}$. The word is dv2sn. Its right neighbour is ew3rk, so the next output word is ew3rk. Now, we need to find a word that starts with sn. The word is sn6iv. Its right neighbour is qh1va, so the next output word is qh1va. Now, we need to find a word that starts with iv. The word is iv0vl. Its right neighbour is $\mathbf{z s} 7 \mathbf{q h}$, so the next output word is $\mathbf{z s} 7 \mathbf{q h}$. Now, we need to find a word that starts with $\mathbf{v l}$. The word is $\mathbf{v} \mathbf{2} \mathbf{k c}$. Its right neighbour is va5cq, so the next output word is va5cq. Now, we need to find a word that starts with $\mathbf{k c}$. The word is $\mathbf{k c} \mathbf{1 x v}$. Its right neighbour is cb6ft, so the next output word is cb6ft. Now, we need to find a word that starts with $\mathbf{x v}$. The word is $\mathbf{x v} 4 \mathrm{vn}$. Its right neighbour is me3af, so the next output word is me3af. Now, we need to find a word that starts with $\mathbf{v n}$. The word is $\mathbf{v n} 5 \mathrm{zn}$. Its right neighbour is $\mathbf{o k} 1 \mathbf{k s}$, so the next output word is $\mathbf{o k} 1 \mathbf{k s}$. Now, we need to find a word that starts with $\mathbf{~ z n}$. The word is $\mathbf{z n 5 q v}$. Its right neighbour is ks5ew, so the next output word is ks5ew Now, we need to find a word that starts with qv. The word is qv6gt. Its right neighbour is $\mathbf{f t 7 m e}$, so the next output word is $\mathbf{f t 7 m e}$. Now, we need to find a word that starts with gt. The word is gt3bc. Its right neighbour is em3zs, so the next output word is em3zs. Now, we need to find a word that starts with bc. The word is bc7qi. Its right neighbour is $\mathbf{j z 7 e m}$, so the next output word is $\mathbf{j z 7 e m}$. There is no word that starts with qi, so we are done with the matching.
Therefore the answer is: jz sa7ok rk7cb cq4sa ew3rk qh1va zs7qh va5cq cb6ft me3af ok1ks ks5ew ft7me em3zs jz7em.
<FEW MORE EXAMPLES>
Your question: ap cb ch5ya gb6lt uu6le vn0pc og0ef md6ki jx0ph md4ki mq5ox vp1rx zp1xj is5am uq5fb te3rz eq3he cb0md he2zp fe2re ef6yp vn5pc ui3yt kb1ji qg2mq am4vp ez3eq lt5fi hw4eg lz2te wn5kd kb2ji le6wk vp3rx yt3lq rx6gb ey 4 dx ji3fe lq1dq lz0te wk7sl am6vp zi0up ki5kb ek7uu re0vq cs3ez vq5lz dx6se lt3fi xp2km fe3re bz7hw rx2gb yp6qg gb4lt at4cs fi7vn ox1nl fi5vn ph3zi rz4is kd2bz jilfe nl3kk ki2kb yo6ey telrz fd5at qb7ia bn2xp cb4md ya2wn gd7sq xj2jg rp6bl aplbn is 4 am se5ui re5vq eg4uq cf6fj fb6jx ll4ic sl4ch qs 3 nf sp5fd qj6bf dq1og rzlis km6yo vq3lz up5sp wc5iv
Reason step by step. Clearly mark your answer by writing 'Answer: <your answer>' as last line.

## D. 2 PEN generation code

```
import itertools
import numpy as np ("abcdefghijklmnopqrstuvwxyz")
big_letter_chars = list("ABCDEFGHIJKLMNOPQRSTUVWXYZ")
number_chars = list("0123456789")
number_chars = lis
    def _-init__(self, min_len,
        selemin_len = min_len
        self.min_hops = min_hops
        self.max_hops = max_hops
        Self.learn_mode = learn_mode
        elf.ambiguous = ambiguous
    self.no_green_confusion = no_green_confusion
    def get(self, key, default):
class PointerExecutionNeighbour:
    def _-init__(self, data_cfg)
        self.length_low = data_cfg.min_len
        self.length_high = data_cfg.max_len
    self.hops_higher = data_cfg.max_hops + 1
    self.all_2tuples = ["".join(t) for t in itertools.product(letter_chars, repeat=2)]
    self.learn_mode = data_cfg.get("learn_mode", "next")
    self.ambiguous = data_cfg.get("ambiguous", False)
    self.ambiguous = data_cfg.get("ambiguous", False)
    generate double pointer execution(self, n_samples)
    lengths = np.arange(self.length_low, self.length_high)
    Mengles = np
    while len(samples) < namps
        length = np.random.choice(lengths)
            n_matching_hops = np.random.choice(np.arange(self.hops_low, min(self.hops_higher, length // 2)))
            tuple_choices = np.random.choice(self.all_2tuples, length * 7, replace=False)
            # select the positions where the green matching sequence will be
            positions = np.random.choice(np.arange(1, length), size=n_matching_hops, replace=False)
            cnt = 0
            question_words1 = ["" for - in range(length)]
            remaining_positions = np.random.permutation([i for i in range(1, length) if i not in positions])
            question_words1[0] = tuple_choices[cnt]
            for pos in positions:
            question_words1[pos] = (tuple_choices[cnt] + np.random.choice(self.data_choices) + tuple_choices[cnt + 1])
            answer_learnseq.append(question_words1[pos])
            cnt += += +=
            cnt_confuse = cnt + length
            positions_next = np.random.permutation(positions)
            question_words2[0] = tuple_choices[cnt]
            answer = [question_words2[0]]
            # select the positions where the doppelgangers of the neighbours will be 
            np.random.shuffle(positions_confuse)
            for i, pos in enumerate(positions_next)
            two_big_letters = np.random.choice(self.data_choices, size=2, replace=self.ambiguous)
            question_words2[pos] = (tuple_choices[cnt] + two_big_letters[0] + tuple_choices[cnt + 1])
            question_words2[positions_confuse[i]] = (tuple_choices[cnt] + two_big_letters[1] + tuple_choices[cnt + 1])
            queswen_words(quostions_conf[ose[1)]
            answer.ap
            cnt_confuse += 1
        cnt = max(cnt, cnt_confuse) +1
        remaining_next_positions = np.random.permutation([i for i in range(1, length) if i not in positions_next and i not in positions_confuse])
            for pos in remaining_positions:
            question_words1[pos] = (tuple_choices[cnt] + np.random.choice(self.data_choices) + tuple_choices[cnt + 1])
            if self.no_green_confusion:
            cnt += 1
        cnt += 1
            for pos in remaining_next_positions:
            question_words2[pos] = (tuple_choices[cnt] + np.random.choice(self.data_choices) + tuple_choices[cnt + 1])
        answer_learnnext = [question_words2[0]]
        for pos in positions:
        answer_learnnext.append (question_words2 [pos])
        answer_seqnext = []
            answer_seqnext.answend_learnseq)):
            answer_seqnext.append (answer_learnnext [i])
        answer.reverse()
        question_words = [] 
            i in range(length):
            question_words.append(question_words2[1]" ".join(["".join(x) for x in question_words]) + " answer: ")
```



```
        answers.append(" ".join(answer_learnseq))
        elif self.learn_mode == "seqnext":
            answers.append(" ".join(answer_seqnext))
            answers.append(" ".join(answer_learnnext))
    return samples, answers
    \mathrm{ return samples, answers }
    samples, answers = self.generate_double_pointer_execution(n_samples)
    return samples, answers
```

Figure 16: Code utilized for generating instances of the PEN task and its associated subtasks. The hyperparameters employed include a length ranging between $[40,50]$ and a number of hops ranging between [10, 20].

## D. 3 PER Multi generation code

```
import itertools
letter_chars = list("abcdefghijklmnopqrstuvwxyz")
class DataConfig:
    def __init__(self, min_len, max_len, logname, learn_mode="seq"):
        self.max_len = max_len
        self.logname = logname
        self.learn_mode = learn_mode
    def get(self, key, default):
class PointerExecutionReverseMulticount:
    def __init__(self, data_cfg):
        self.length_low = data_cfg.min_len
        self.length_higher = data_cfg.max_len +
        self.logname = data_cfg.logname
        elf.all_2tuples = ["".join(t) for t in itertools.product(letter_chars, repeat=2)]
        self.learn_mode = data_cfg.get("learn_mode", "seq")
    assert self.learn_mode in ["seq", "multiseq", "seqrev", "multiseqrev"]
    def generate_samples(self, n_samples)
        lengths = np.arange(self.length_low, self.length_higher)
        samples = []
        for _ in range(n_samples):
            length = np.random.choice(lengths)
            tuple_choices = np.random.choice(self.all_2tuples, length + 3, replace=False)
            last_word = tuple_choices[-3] + tuple_choices[-2]
            shuffled_tuple_choices1 = np.random.permutation(tuple_choices[:-3])
            words = [ch1 + ch2 for ch1, ch2 in zip(shuffled_tuple_choices1, shuffled_tuple_choices2)]
            wtarts np.random.choice(words)
            if "rev" not in self.learn_mode
            answer = self.solve_seqnext(words, start, self.learn_mode)
            else:
                # change the 2tuple of the start of the start word to a random one
                    dx = words.index(start)
                    words[idx] = tuple_choices[-1] + words[idx][2:]
                    answer, answer_n_left = self.solve_seqnext(words, start, self.learn_mode)
                    if self.learn_mode == "seqrev
                    answer = reversed([f"{w}" for i, w in enumerate(answer)])
                    f self.1earn_mode = (multiseqrev
                answer = reverself [w}.{i*n}" for i, (w, n) in enumerate(zip(answer, answer_n_left))])
            samples append(question)
            answers.append (" " join(answer)
    return samples, answers
    ef solve_seqnext(self, words, start, mode):
        answer_next = []
        matching_seq = []
        dx = words.index(current_word)
        n_left = 0
        answer_n_left = []
            matching_seq.append (current_word)
            answer_next.append(words[idx
            next_word = [(w, i) for i, w in enumerate(words) if w.startswith(current_word[-2:])]
            if len(next_word) == 0 and "rev" in mode:
            break
            assert len(next_word) == 1
            if new_idx < idx:
            n_left += 1
            idx = new_idx 
        if "rev" in break
        return matching_seq, answer_n_left
        if "multi" in mode:
            answer = []
            for i, (w, n) in enumerate(zip(matching_seq, answer_n_left))
                answer.append(f"{w}.{i*n}")
            return answer
    ef generate(self, n_samples):
    amples, answers = self.generate_samples(n_samples)
        return samples, answers
```

Figure 17: Code employed for generating instances of the Pointer Execution Reverse Multicount task and its associated subtasks. The hyperparameters employed include a length ranging between [10, 20].

