Towards Revealing the Mystery behind Chain of Thought: a Theoretical Perspective

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Abstract

Recent studies have discovered that Chain-of-Thought prompting (CoT) can dramatically improve the performance of Large Language Models (LLMs), particularly when dealing with complex tasks involving mathematics or reasoning. Despite the enormous empirical success, the underlying mechanisms behind CoT and how it unlocks the potential of LLMs remain elusive. In this paper, we take a first step towards theoretically answering these questions. Specifically, we examine the capacity of LLMs with CoT in solving fundamental mathematical and decisionmaking problems. We start by giving an impossibility result showing that any bounded-depth Transformer cannot directly output correct answers for basic arithmetic/equation tasks unless the model size grows super-polynomially with respect to the input length. In contrast, we then prove by construction that autoregressive Transformers of a constant size suffice to solve both tasks by generating CoT derivations using a commonly-used math language format. Moreover, we show LLMs with CoT are capable of solving a general class of decision-making problems known as Dynamic Programming, thus justifying its power in tackling complex real-world tasks. Finally, extensive experiments on four tasks show that, while Transformers always fail to predict the answers directly, they can consistently learn to generate correct solutions step-by-step given sufficient CoT demonstrations.

1 Introduction

Transformer-based Large Language Models (LLMs) have emerged as a foundation model in natural language processing. Among them, the autoregressive paradigm has gained arguably the most popularity [45, 8, 40, 61, 52, 13, 46, 48], based on the philosophy that all different tasks can be uniformly treated as sequence generation problems. Specifically, for any given task, the input can be encoded together with a sequence of task-dependent tokens, called the *prompt*; the answer is then generated by predicting subsequent tokens conditioned on the prompt in an autoregressive way.

Previous studies highlighted that a carefully-designed prompt greatly matters LLMs' performance [27, 32]. In particular, the so-called *Chain-of-Thought* prompting (CoT) [56] has been found crucial for tasks involving arithmetic or reasoning, where the correctness of generated answers can be dramatically improved via a modified prompt that triggers LLMs to output intermediate derivations. Practically, this can be simply achieved by either adding special phrases such as "*let's think step by step*" or by giving few-shot CoT demonstrations [29, 56, 51, 38, 62]. However, despite the striking performance, the underlying mechanism behind CoT remains largely unclear and mysterious. On one hand, are there indeed *inherent* limitations of LLMs in directly answering math/reasoning questions? On the other hand, why does CoT² boost the power of LLMs on these tasks?

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²Throughout this paper, we use the term CoT to refer to the general framework of the step-by-step generation process rather than a specific prompting technique. In other words, this paper studies why an LLM equipped with CoT can succeed in arithmetic and decision-making tasks rather than which prompt can trigger this process.

This paper takes a step towards theoretically answering the above questions. We begin with studying the capability of LLMs on two basic mathematical tasks: evaluating arithmetic expressions and solving linear equations. Both tasks are extensively employed and serve as elementary building blocks in solving complex real-world math problems [9]. We first provide fundamental impossibility results showing that none of these tasks can be solved using a bounded-depth Transformer model without CoT unless the model size grows super-polynomially with respect to the input length (Theorems 3.1 and 3.2). Remarkably, our proofs provide insights into why this may happen: the reason is not the computational cost of these problems but rather their *parallel complexity* [2]. We next show that the community may largely undervalue the strength of autoregressive generation: we prove by construction that autoregressive Transformer models of constant size can perfectly solve both tasks by generating intermediate derivations in a step-by-step manner using a commonly-used math language format (Theorems 3.3 and 3.4). Intuitively, this result hinges on the recursive nature of CoT, which increases the "effective depth" of the Transformer to be proportional to the generation steps.

Besides mathematics, CoT also exhibits remarkable performance across a wide range of reasoning tasks. To gain a systematic understanding why CoT is beneficial, we turn to a fundamental class of problems known as *Dynamic Programming* (DP) [5]. DP represents a golden framework for solving sequential decision-making tasks: it decomposes a complex problem into a sequence (or chain) of subproblems, and by following the reasoning chain step by step, each subproblem can be solved based on the results of previous subproblems. Our main finding demonstrates that, for general DP problems of the form (5), LLMs with CoT can generate the complete chain and output the correct answer (Theorem 4.7). However, it is impossible to directly generate the answer in general: as a counterexample, we prove that a bounded-depth Transformer with polynomial size cannot solve a classic DP problem known as Context-Free Grammar Membership Testing (Theorem 4.8).

Our theoretical findings are complemented by an extensive set of experiments. We consider the two aforementioned math tasks plus two celebrated DP problems listed in the "Introduction to Algorithms" book [14], known as *longest increasing subsequence* (LIS) and *edit distance* (ED). For all these tasks, our experimental results show that directly predicting the answers without CoT always fails (accuracy mostly below 60%). In contrast, autoregressive Transformers equipped with CoT can learn entire solutions given sufficient training demonstrations. Moreover, they even generalize well to longer input sequences, suggesting that the models have learned the underlying reasoning process rather than statistically memorizing input-output distributions. These results verify our theory and reveal the strength of autoregressive LLMs and the importance of CoT in practical scenarios.

2 Preliminary

An (autoregressive) Transformer [53, 44] is a neural network architecture designed to process a sequence of input tokens and generate tokens for subsequent positions. Given an input sequence s of length n, a Transformer operates the sequence as follows. First, each input token s_i ($i \in [n]$) is converted to a d-dimensional vector $\mathbf{v}_i = \operatorname{Embed}(s_i) \in \mathbb{R}^d$ using an embedding layer. To identify the sequence order, there is also a positional embedding $\mathbf{p}_i \in \mathbb{R}^d$ applied to token s_i . The embedded input can be compactly written into a matrix $\mathbf{X}^{(0)} = [\mathbf{v}_1 + \mathbf{p}_1, \cdots, \mathbf{v}_n + \mathbf{p}_n]^{\top} \in \mathbb{R}^{n \times d}$. Then, L Transformer blocks follow, each of which transforms the input based on the formula below:

$$\boldsymbol{X}^{(l)} = \boldsymbol{X}^{(l-1)} + \operatorname{Attn}^{(l)}(\boldsymbol{X}^{(l-1)}) + \operatorname{FFN}^{(l)}\left(\boldsymbol{X}^{(l-1)} + \operatorname{Attn}^{(l)}(\boldsymbol{X}^{(l-1)})\right), \quad l \in [L], \quad (1)$$

where $\mathrm{Attn}^{(l)}$ and $\mathrm{FFN}^{(l)}$ denote the multi-head self-attention layer and the feed-forward network for the l-th Transformer block, respectively:

$$\operatorname{Attn}^{(l)}(\boldsymbol{X}) = \sum_{h=1}^{H} \operatorname{softmax} \left(\boldsymbol{X} \boldsymbol{W}_{Q}^{(l,h)} (\boldsymbol{X} \boldsymbol{W}_{K}^{(l,h)})^{\top} + \boldsymbol{M} \right) \boldsymbol{X} \boldsymbol{W}_{V}^{(l,h)} \boldsymbol{W}_{O}^{(l,h)}, \tag{2}$$

$$FFN^{(l)}(\boldsymbol{X}) = \sigma(\boldsymbol{X}\boldsymbol{W}_1^{(l)})\boldsymbol{W}_2^{(l)}.$$
(3)

Here, we focus on the standard setting adopted in Vaswani et al. [53], namely, an H-head softmax attention followed by a two-layer pointwise FFN, both with residual connections. The size of the Transformer is determined by three key quantities: its depth L, width d, and the number of heads H. The parameters $\boldsymbol{W}_Q^{(l,h)}, \boldsymbol{W}_K^{(l,h)}, \boldsymbol{W}_V^{(l,h)}, \boldsymbol{W}_O^{(l,h)}$ are query, key, value, output matrices of the h-th head, respectively; and $\boldsymbol{W}_1^{(l)}, \boldsymbol{W}_2^{(l)}$ are two weight matrices in the FFN. The activation σ is

chosen as GeLU [25], following [45, 18]. The matrix $M \in \{-\infty, 0\}^{n \times n}$ is a causal mask defined as $M_{ij} = -\infty$ iff i < j. This ensures that each position i can only attend to preceding positions $j \le i$ and is the core design for autoregressive generation.

After obtaining $X^{(L)} \in \mathbb{R}^{n \times d}$, its last entry $X_{n,:}^{(L)} \in \mathbb{R}^d$ will be used to predict the next token s_{n+1} (e.g., via a softmax classifier). By concatenating s_{n+1} to the end of the input sequence s, the above process can be repeated to generate subsequent token s_{n+2} . The process continues iteratively until a designated End-of-Sentence token is generated, signifying the completion of the process.

Chain-of-Thought prompting. Autoregressive Transformers possess the ability to tackle a wide range of general tasks by encoding the task description into a partial sentence, with the answer being derived by complementing the subsequent sentence [8]. However, for some challenging tasks involving math or general reasoning, a direct generation often struggles to yield a correct answer. To address this shortcoming, researchers proposed the CoT prompting that induces the model to generate intermediate reasoning steps before reaching the answer [56, 29, 51, 38, 62, 10]. In this paper, our primary focus lies in understanding the mechanism behind CoT, while disregarding the aspect of how prompting facilitates its triggering. Specifically, we examine CoT from an *expressivity* perspective: for both mathematical problems and general decision-making tasks studied in Sections 3 and 4, we will investigate whether autoregressive Transformers is expressive for (i) directly generating the answer, and (ii) generating a CoT solution for the tasks.

3 CoT is the Key to Solving Mathematical Problems

Previous studies have observed that Transformer-based LLMs exhibit surprising math abilities in various aspects [40, 9]. In this section, we begin to explore this intriguing phenomenon via two well-chosen tasks: arithmetic and equation. We will give concrete evidence that LLMs are capable of solving both tasks when equipped with CoT, while LLMs without CoT are provably incapable.

3.1 Problem formulation

Arithmetic. The first task focuses on evaluating arithmetic expressions. As shown in Figure 1 (left), the input of this task is a sequence consisting of numbers, addition (+), subtraction (-), multiplication (×), division (÷), and brackets, followed by an equal sign. The goal is to calculate the arithmetic expression and generate the correct result. This task has a natural CoT solution, where each step performs an intermediate computation, gradually reducing one atomic operation at a time while copying down other unrelated items. Figure 1 (left) gives an illustration, and the formal definition of the CoT format is deferred to Appendix C.

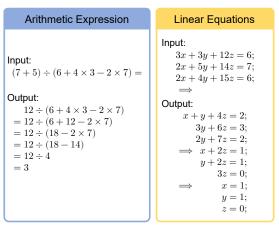


Figure 1: Illustrations of CoT on two math tasks.

Equation. The second task considers solving linear equations. As shown in Figure 1 (right), the input of this task is a sequence consisting of m linear equations, each of which involves m variables. The input ends with a special symbol \Longrightarrow . The goal is to output the value of these variables that satisfies the set of equations (assuming the solution is unique). A natural CoT solution is the Gaussian elimination algorithm: at each step, it eliminates a certain variable in all but one equations. After m-1 steps, all equations will have only one variable and the problem gets solved. Figure 1 (right) gives an illustration, and we defer the formal definition of the CoT format to Appendix C.

Number field. Ideally, for both tasks, the input sequences involve not only symbol tokens but also (infinitely many) floating-point numbers. This complicates the definitions of the model's input/output format and further entails intricate precision considerations when dealing with floating-point divisions. To simplify our subsequent analysis, here we turn to a more convenient setting by transitioning to the *finite field* generated by integers modulo p for a prime number p. Importantly, the finite field contains only p numbers (ranging from 0 to p-1) and thus can be uniformly treated as tokens in a pre-defined dictionary (like other operators or brackets), making the problem setting much cleaner.

Moreover, arithmetic operations $(+, -, \times, \div)$ are well-defined and parallel the real number field (see Appendix B.1 for details). Therefore, this setting does not lose generalities.

In subsequent sections, we denote Arithmetic (n, p) as the arithmetic evaluation task defined on the finite field modulo p, where the input length does not exceed n. Similarly, we denote Equation (m, p) as the linear equation task defined on the finite field modulo p with no more than m variables.

3.2 Theoretical results

We begin by investigating whether Transformers can directly produce answers for the aforementioned problems. This corresponds to generating, for instance, the number "3" or the solution "x = 1; y = 1; z = 0" in Figure 1 immediately after the input sequence (without outputting intermediate steps). This question can be examined via different theoretical perspectives. One natural approach is to employ the classic representation theory, which states that perceptrons with sufficient size (e.g., the depth or width approaches infinity) are already universal function approximators [15, 30, 34]. Recently, such results have been well extended to Transformer models [59]. However, the above results becomes elusive when taking the representation *efficiency* into account, since it says nothing about the required model size for any specific task. Below, we would like to give a more fine-grained analysis on how large the network needs to be by leveraging the tool of complexity theory.

We focus on a *realistic* setting called the **log-precision Transformer** [36, 31]: it refers to a Transformer whose internal neurons can only store floating-point numbers within a finite $O(\log n)$ bit precision where n is the length of the input sequence (see Appendix B.3 for a formal definition). Such an assumption well-resembles practical situations, in which the machine precision (e.g., 16 or 32 bits) is typically much smaller than the input length (e.g., 2048 in GPT), avoiding the unrealistic (but crucial) assumption of infinite precision made in several prior works [43, 17]. Furthermore, log-precision implies that the number of values each neuron can take is *polynomial* in the input length, which is a *necessary* condition for representing important quantities like positional embedding. Equipped with the concept of log-precision, we are ready to present a central impossibility result, showing that the required network width must be prohibitively large for both math problems:

Theorem 3.1. Assume $TC^0 \neq NC^1$. For any prime number p, any integer L, and any polynomial Q, there exists a problem size n such that no log-precision autoregressive Transformer defined in Section 2 with depth L and hidden dimension $d \leq Q(n)$ can solve the problem Arithmetic(n, p).

Theorem 3.2. Assume $TC^0 \neq NC^1$. For any prime number p, any integer L, and any polynomial Q, there exists a problem size m such that no log-precision autoregressive Transformer defined in Section 2 with depth L and hidden dimension $d \leq Q(m)$ can solve the problem Equation(m, p).

Why does this happen? As presented in Appendices E.2 and F.2, the crux of our proof lies in applying circuit complexity theory. By framing the finite-precision Transformer as a computation model, we can precisely delineate its expressivity limitations through an analysis of its circuit complexity. Here, polynomial size log-precision Transformers represent a class of *shallow* circuits with complexity upper bounded by TC^0 [36]. On the other hand, we prove that the circuit complexity of both math problems considered above are lower bounded by NC^1 by applying *reduction* from NC^1 -complete problems. Consequently, they are intrinsically hard to be solved by a well-parallelized Transformer unless the two complexity classes collapse (i.e., $TC^0 = NC^1$), a scenario widely regarded as impossible.

How about generating a CoT solution? We next turn to the setting of generating CoT solutions for these problems. From an expressivity perspective, one might intuitively perceive this problem as more challenging as the model is required to express the entire problem solving process, potentially necessitating a larger model size. However, we show this is not the case: a constant-size autoregressive Transformer already suffices to generate solutions for both math problems.

Theorem 3.3. For any prime p and integer n > 0, there exists an autoregressive Transformer defined in Section 2 with hidden size d = O(poly(p)) (independent of n), depth L = 5, and 5 heads in each layer that can generate the CoT solution defined in Appendix C for all inputs in Arithmetic(n, p). Moreover, all parameter values in the Transformer are bounded by O(poly(n)).

Theorem 3.4. For any prime p and integer m > 0, there exists an autoregressive Transformer defined in Section 2 with hidden size d = O(poly(p)) (independent of m), depth L = 5, and 5 heads in each layer that can generate the CoT solution defined in Appendix C for all inputs in Equation(m, p). Moreover, all parameter values in the Transformer are bounded by O(poly(m)).

Remark 3.5. The polynomial upper bound for parameters in Theorems 3.3 and 3.4 readily implies that these Transformers can be implemented using log-precision without loss of accuracy. See Appendix B.3 for a detailed discussion on how this can be achieved.

The proof of Theorems 3.3 and 3.4 is deferred to Appendices E.1 and F.1, with several discussions made as follows. *Firstly*, the constructions in our proof reveal the significance of several key components in the Transformer design, such as softmax attention, multi-head, and residual connection. We show how these components can be combined to implement basic operations like substring copying and bracket matching, which serve as building blocks for generating a complete CoT solution. *Secondly*, we highlight that these CoT derivations are purely written in a readable math language format, largely resembling how human write solutions. In a broad sense, our findings suggest that LLMs have the potential to convey meaningful human thoughts through *grammatically precise* sentences. *Finally*, one may ask how LLMs equipped with CoT can bypass the impossibility results outlined in Theorems 3.1 and 3.2. Actually, this can be understood via the *effective depth* of the Transformer circuit. By employing CoT, the effective depth is no longer *L* since the generated outputs are repeatedly looped back to the input layer. The dependency between output tokens leads to a significantly deeper circuit with depth proportional to the length of the CoT solution. Even if the recursive procedure is repeated within a fixed Transformer (or circuit), the expressivity can still be far beyond TC⁰.

4 CoT is the Key to Solving Decision-Making Problems

The previous section has delineated the critical role of CoT in solving math problems. In this section, we will switch our attention to a more general setting beyond mathematics. Remarkably, we find that LLMs with CoT are theoretically capable of emulating a powerful decision-making framework called *Dynamic Programming* [5], thus justifying the ability of CoT to solve complex tasks.

4.1 Dynamic Programming

Dynamic programming (DP) is widely regarded as a core technique to solve decision-making problems [50]. The basic idea of DP lies in breaking down a complex problem into a series of small subproblems that can be tackled in a sequential manner. Here, the decomposition ensures that there is a significant interconnection (overlap) among various subproblems, so that each subproblem can be efficiently solved by utilizing the answers (or other relevant information) obtained from previous ones.

Formally, a general DP algorithm can be characterized via three key ingredients: the state space \mathcal{I} , the transition function T, and the aggregation function A. The **state space** \mathcal{I} represents the finite set of decomposed subproblems, where each state $i \in \mathcal{I}$ is an index signifying a specific subproblem. The size of the state space grows with the input size. We denote by $\mathrm{dp}(i)$ the answer of subproblem i (as well as other information stored in the DP process). Furthermore, there is a *partial order* relation between different states: we say state j precedes state i (denoted as $j \prec i$) if subproblem j should be solved before subproblem i, i.e., the value of $\mathrm{dp}(i)$ depends on that of $\mathrm{dp}(j)$. This partial order creates a directed acyclic graph (DAG) within the state space, thereby establishing a reasoning chain where subproblems are resolved in accordance with the topological ordering of the DAG.

The $transition\ T$ characterizes the interconnection among subproblems and defines how a subproblem can be solved based on the results of previous subproblems. It can be generally written as

$$dp(i) = T(i, s, \{(j, dp(j)) : j \prec i\}), \tag{4}$$

where s is the input sequence. In this paper, we focus on a restricted setting where each state i only depends on (i) a finite length of input sequence s and (ii) a finite number of previous states. Under this assumption, we can rewrite (4) into a more concrete form:

$$dp(i) = f(i, s_{g_1(i)}, \dots, s_{g_J(i)}, dp(h_1(i)), \dots, dp(h_K(i))),$$
(5)

where J and K are constant integers. The functions f, g, h fully determine the transition function T and have the form $f: \mathcal{I} \times \mathcal{X}^J \times \mathcal{Y}^K \to \mathcal{Y}, g: \mathcal{I} \to (\mathbb{N} \cup \{\emptyset\})^J, h: \mathcal{I} \to (\mathcal{I} \cup \{\emptyset\})^K$, where the state space \mathcal{I} , input space \mathcal{X} , and DP output space \mathcal{Y} can be arbitrary domains. The special symbol \emptyset denotes a placeholder, such that all terms s_{\emptyset} and $dp(\emptyset)$ are unused in function f.

After solving all subproblems, the **aggregation function** A is used to combine all results to obtain the final answer. We consider a general class of aggregation functions with the following form:

$$A\left(\left\{(i, \mathsf{dp}(i)) : i \in \mathcal{I}\right\}, s\right) = u\left(\Box_{i \in \mathcal{A}} \mathsf{dp}(i)\right),\tag{6}$$

where $\mathcal{A} \subset \mathcal{I}$ is a set of states that need to be aggregated, \square is an aggregation function such as min, max, or Σ , and $u: \mathcal{Y} \to \mathcal{Z}$ is an arbitrary function, where \mathcal{Z} denotes the space of possible answers.

A variety of popular DP problems fits in the above framework. As examples, the longest increasing subsequence (LIS) and the edit distance (ED) are two well-known DP problems presented in the "Introduction to Algorithms" book [14] (see Appendix G.1 for problem descriptions). We list the state space, transition function, and aggregation function of the two problems in the table below.

Problem	Longest increasing subsequence	Edit distance
Input	A string s of length n	Two strings $\mathbf{s}^{(1)}$, $\mathbf{s}^{(2)}$ of length $n_1 = \mathbf{s}^{(1)} $ and $n_2 = \mathbf{s}^{(2)} $, concatenated together
State space	$\{(j,k): j \in [n], k \in \{0,\cdots,j-1\}\}$	$\{0,\cdots,n_1\}\times\{0,\cdots,n_2\}$
Transition function	$dp(j,k) = \begin{cases} 1 & \text{if } k = 0 \\ \max(dp(j,k-1), & dp(k,k-1) \times \\ \mathbb{I}[s_j > s_k] + 1) \end{cases}$	$dp(j,k) = \begin{cases} ak & \text{if } j = 0 \\ bj & \text{if } k = 0 \\ \min(dp(j,k-1) + a, & dp(j-1,k) + b, \\ dp(j-1,k-1) & \text{otherwise} \\ + c\mathbb{I}[s_j^{(1)} \neq s_k^{(2)}]) \end{cases}$
Aggregation function		$dp(n_1,n_2)$

4.2 Theoretical results

We begin by investigating whether CoT can solve the general DP problems defined above. We consider a natural CoT generation process, where the generated output has the following form:

input
$$1 \mid \cdots \mid$$
 input $N \mid (i_1, dp(i_1)) \cdots (i_{|\mathcal{I}|}, dp(i_{|\mathcal{I}|}))$ final answer

Here, the input sequence s consists of N strings separated by special symbols, and their lengths $n:=(n_1,\cdots,n_N)$ determine the size of the state space $\mathcal{I};\,(i_1,\cdots,i_{|\mathcal{I}|})$ is a feasible topological ordering of the state space \mathcal{I} . To simplify our analysis, we consider a regression setting where each element in the output sequence directly corresponds to the output of the last Transformer layer without any additional processing (e.g., using a softmax layer for tokenization). Likewise, we remove the embedding layer so that each generated output is directly looped back to the input layer (unlike Section 3). This setting is convenient for manipulating numerical values and has been extensively adopted in prior works [21, 1]. Furthermore, we assume that the domains $\mathcal{I}, \mathcal{X}, \mathcal{Y}$, and \mathcal{Z} belong to real vector space so that their elements can be effectively represented and handled by a neural network. Likewise, each DP output $(i, \mathrm{dp}(i))$ in the CoT will be represented as a single vector.

Before presenting our main result, we make the following assumptions:

Definition 4.1 (Polynomially-efficient approximation). Given neural network P_{θ} and target function $f: \mathcal{X}^{\text{in}} \to \mathcal{X}^{\text{out}}$ where $\mathcal{X}_{\text{in}} \subset \mathbb{R}^{d_{\text{in}}}$ and $\mathcal{X}_{\text{out}} \subset \mathbb{R}^{d_{\text{out}}}$, we say f can be approximated by P_{θ} with polynomial efficiency if, for any $\epsilon > 0$, there exists parameter θ satisfying that (i) $||f(x) - P_{\theta}(x)|| < \epsilon$ for all $x \in \mathcal{X}^{\text{in}}$; (ii) all elements of parameter θ are bounded by $O(\text{poly}(1/\epsilon))$.

Assumption 4.2. The size of the state space can be polynomially upper bounded by the length of the input sequence, i.e., $|\mathcal{I}| = O(\text{poly}(|s|))$.

Assumption 4.3. Each function f, g, h and u in (5) and (6) can be approximated with polynomial efficiency by a perceptron of constant size (with GeLU activation).

Assumption 4.4. Denote $(i_1, \cdots, i_{|\mathcal{I}|})$ as a feasible topological order of the state space \mathcal{I} . Then, the function $F: \mathbb{N}^N \times \mathcal{I} \to \mathcal{I}$ defined as $F(n, i_k) = i_{k+1}, k \in [|\mathcal{I}| - 1]$ can be approximated with polynomial efficiency by a perceptron of constant size (with GeLU activation).

Assumption 4.5. The function $F: \mathbb{N}^N \times \mathcal{I} \to \{0,1\}$ defined as $F(n,i) = \mathbb{I}[i \in \mathcal{A}]$ (used in (6)) can be approximated with polynomial efficiency by a perceptron of constant size (with GeLU activation).

Remark 4.6. All assumptions above are mild. Assumption 4.2 is necessary to ensure that the state vectors can be represented with log-precision, and Assumptions 4.3 to 4.5 guarantee that all basic functions that determine the DP process can be well-approximated by a composition of finite log-precision Transformer layers of constant size. In Appendix G.1, we show these assumptions are satisfied for both LIS and ED problems described above.

We are now ready to present our main result, which shows that LLMs with CoT can solve all DP problems satisfying the above assumptions. We give a proof in Appendix G.2.

Theorem 4.7. Consider any DP problem that satisfies Assumptions 4.2 to 4.5. For any integer $n \in \mathbb{N}$ and $\epsilon > 0$, there exists an autoregressive Transformer with constant depth L, hidden dimension d and attention heads H (independent of n or ϵ), such that the answer generated by the Transformer can be arbitrary close to the ground truth for all input sequences s of length no more than n, with error uniformly bounded by ϵ . Moreover, all parameter values are bounded by $O(\operatorname{poly}(n, 1/\epsilon))$.

To complete the analysis, we next explore whether Transformers can directly predict the answer of a DP problem without generating intermediate CoT sequences. We show generally the answer is no: many DP problems are intrinsically hard to be solved by a bounded-depth Transformer without CoT. One celebrate example is the Context-Free Grammar (CFG) Membership Testing, which tests whether an input string belongs to a pre-defined context-free language. A formal definition of this problem and a standard DP solution are given in Appendix G.1. We have the following impossibility result:

Theorem 4.8. Assume $TC^0 \neq P$. There exists a context-free language such that for any depth L and any polynomial Q, there exists a sequence length $n \in \mathbb{N}$ where no log-precision autoregressive transformer with depth L and hidden dimension $d \leq Q(n)$ can generate the correct answer for the CFG Membership Testing problem for all input strings of length n.

We give a proof in Appendix G.3. The reason why Theorem 4.8 holds is the same as in Theorems 3.1 and 3.2: the CFG Membership Testing is a P-complete problem, which is intrinsically hard to be solved by a well-parallelized computation model. Combined with the above theoretical results, we conclude that CoT plays a critical role in tackling tasks that are inherently difficult.

5 Experiments

In previous sections, we proved by construction that LLMs exhibit sufficient expressive power to solve mathematical and decision-making tasks. On the other hand, it is still essential to check whether a Transformer model can *learn* such ability from training data. Below, we will complement our theoretical results with experimental evidence, showing that the model can easily learn underlying task solutions when equipped with CoT training demonstrations.

5.1 Experimental Design

Tasks and datasets. We use four tasks for evaluation: Arithmetic, Equation, LIS, and ED. The first two tasks (Arithmetic and Equation) as well as their input/CoT formats have been illustrated in Figure 1. For the LIS task, the goal is to find the length of the longest increasing subsequence of a given integer sequence. For the ED task, the goal is to calculate the minimum cost required (called edit distance) to convert one sequence to another using three basic edit operations: insert, delete and replace. All input sequences, CoT demonstrations, and answers in LIS and ED are bounded-range integers and can therefore be tokenized (similar to the first two tasks). We consider two settings: (i) CoT datasets, which consist of cproblem, CoT steps, answer> samples; (ii) Direct datasets, which are used to train models that directly predict the answer without CoT steps. These datasets are constructed by removing all intermediate derivations from the CoT datasets.

For each task, we construct three datasets with increasing difficulty. For Arithmetic, we build datasets with different number of operators ranging from $\{4,5,6\}$. For Equation, we build datasets with different number of variables ranging from $\{3,4,5\}$. For LIS, we build datasets with different input sequence lengths ranging from $\{50,80,100\}$. For ED, we build datasets with different string lengths, where the average length of the two strings is 12, 16, 20, respectively. We generate 1M samples for each training dataset and 0.1M for testing, while ensuring that duplicate samples between training and testing are removed. More details about the dataset construction can be found in Appendix H.

Model training and inference. For all experiments, we use standard Transformer models with hidden dimension d=256, heads H=4, and different model depths L. We adopt the AdamW optimizer [33] with $\beta_1=0.9, \beta_2=0.999, \text{lr}=10^{-4}$, and weight decay =0.01 in all experiments. We use a fixed dropout ratio of 0.1 for all experiments to improve generalization. For CoT datasets, we optimize the negative log-likelihood loss on all tokens in the CoT steps and answers. For direct datasets, we optimize the negative log-likelihood loss on answer tokens. All models are trained on

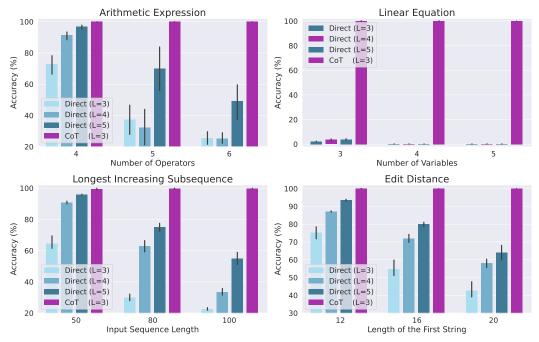


Figure 2: Model performance on different tasks. For all tasks and various difficulty levels, autoregressive Transformers with CoT consistently outperform Transformers trained on direct datasets. In particular, 3-layer Transformers already succeed in these tasks with almost perfect accuracy, while deeper Transformers (L=3,4,5) trained on the direct datasets typically fail.

4 V100 GPUs for 100 epochs. During inference, models trained on the direct datasets are required to output the answer directly, and models trained on CoT datasets will generate the whole CoT process token-by-token (using greedy search) until generating the End-of-Sentence token, where the output in the final step is regard as the answer. We report the accuracy as evaluation metric. Please refer to Appendix H for more training configuration details.

5.2 Experimental Results

All empirical results are shown in Figure 2, where each subfigure corresponds to a task with x-axis representing the difficulty level and y-axis representing the test accuracy (%). We repeat each experiment five times and report the error bars. In each subfigure, the purple bar and blue bars indicate the performance of the model trained on the CoT and direct datasets, respectively. The model depths are specified in the legend. From these results, one can easily see that Transformers with CoT achieve near-perfect performance for all tasks and all difficulty levels. In contrast, models trained on direct datasets perform much worse even when considering larger depths. While increasing the depth usually helps the performance of direct prediction (which is consistent to our theory), it is still poor when the length of the input sequence grows. These empirical findings verify our theoretical results and clearly demonstrate the benefit of CoT with autoregressive generation.

Length extrapolation. We next study whether the learned autoregressive models can further extrapolate to data with longer length. We construct a CoT training dataset for the arithmetic task with the number of operators ranging from 1 to 15, and test the model on expressions with the number of operators $n \in \{16, 17, 18\}$. As shown in Figure 3, our three-layer Transformer model still performs well on longer sequences, suggesting that the model indeed learns the underlying mechanism to some extent. Potentially, we believe models trained on more data with varying lengths can eventually reveal the complete arithmetic rules.

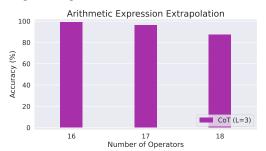


Figure 3: Performance of the length extrapolation experiment, tested on sequences that are longer than those in training.

6 Related Work

Owing to the tremendous success of Transformers and Large Language Models across diverse domains, there has been a substantial body of works dedicated to theoretically comprehending their capabilities and limitations. Initially, researchers primarily focused on exploring the expressive power of Transformers in the context of function approximation. Yun et al. [59] proved that Transformers with sufficient size can universally approximate arbitrary continuous sequence-to-sequence functions on a compact domain. Recently, universality results have been extended to model variants such as Sparse Transformers [60] and Transformers with relative positional encodings (RPE) [35].

More relevant to this paper, another line of works investigated the power of Transformers from a computation perspective. Early results have shown that both standard encoder-decoder Transformers [53] and looped Transformer encoders are Turing-complete [43, 41, 17, 7]. However, these results depend on the unreasonable assumption of *infinite* precision, yielding a quite unrealistic construction that does not match practical scenarios. Recently, Giannou [22] demonstrated that a constant-depth looped Transformer encoder can simulate practical computer programs. Wei et al. [55] showed that finite-precision encoder-decoder Transformers can *approximately* simulate Turing machines with bounded computation time. Liu et al. [31] considered a restricted setting of learning automata, for which a shallow non-recursive Transformer provably suffices. Besides affirmative results, other works characterized the expressivity limitation of Transformers via the perspective of modeling formal languages [23, 6, 57] or simulating circuits [24, 37, 36]. However, none of these works explored the setting of autoregressive Transformers typically adopted in LLMs, which we study in this paper. Moreover, we consider a more practical setting that targets the emergent ability of LLMs in solving basic reasoning problems via a *readable* CoT output, which aligns well with real-world scenarios.

Recently, the power of Transformers has regained attention due to the exceptional in-context learnability exhibited by LLMs [8]. Garg et al. [21] demonstrated that autoregressive Transformers can in-context learn basic function classes (e.g., linear functions, MLPs, and decision trees) via input sample sequences. Subsequent works further revealed that Transformers can implement learning algorithms such as linear regression [1], gradient descent [1, 54, 16], and Bayesian inference [58]. The works of [20, 39] studied in-context learning via the concept of "induction heads". All the above works investigated the power of (autoregressive) Transformer models from an expressivity perspective, which shares similarities to this paper. Here, we focus on the reasoning capability of Transformers and underscore the key role of CoT in improving the power of LLMs.

7 Limitations and Future Directions

In this work, from a model-capacity perspective, we theoretically analyze why Chain-of-Thought prompting is essential in solving mathematical and decision-making problems. Focusing on two basic mathematical problems as well as Dynamic Programming, we show that a bounded-depth Transformer without CoT struggles with these tasks unless its size grows prohibitively large. In contrast to our negative results, we prove by construction that when equipped with CoT, constant-size Transformers are sufficiently capable to address these tasks by generating intermediate derivations sequentially. Extensive experiments show that models trained on CoT datasets can indeed learn solutions almost perfectly, thereby verifying our theoretical findings. We further demonstrate that CoT has the potential to generalize to unseen data with longer length.

Several foundational questions remain to be answered. Firstly, while this paper investigates why CoT enhances the expressivity of LLMs, we do not yet answer how the CoT generation process is triggered by specific prompts. Revealing the relation between prompts and outputs is valuable for better harnessing LLMs. Secondly, it has been empirically observed that scaling the model size significantly improves the CoT ability [56]. Theoretically understanding how model size plays a role in CoT would be an interesting research problem. Thirdly, this paper main studies the expressivity of LLMs in generating CoT solutions, without theoretically thinking about their *generalization* ability. Given our experimental results, we believe it is an important future direction for theoretical studying how LLMs can generalize from CoT demonstrations (even in the out-of-distribution setting, e.g., length extrapolation) [55, 12]. Finally, from a practical perspective, it is interesting to investigate how models can learn CoT solutions when there are only limited CoT demonstrations in training (or even purely from direct datasets). We would like to leave these questions as future work, which we believe are beneficial to better reveal the abilities as well as limitations of LLMs.

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A Organization of Appendices

The Appendix is organized as follows. Appendix B introduces additional mathematical background and useful notations, which will be frequently used in our subsequent proofs. Appendix C presents formal definitions of the arithmetic expression task and the linear equation task. Appendix D gives several useful lemmas, and the formal proofs for the arithmetic expression, the linear equation, and the DP problems are given in Appendices E to G. We finally present experiment details in Appendix H.

B Addition Background and Notation

B.1 Finite field

Intuitively, a *field* is a set \mathcal{F} on which addition, subtraction, multiplication, and division are defined and behave as the corresponding operations on rational and real numbers do. Formally, the two most basic binary operations in a field is the addition (+) and multiplication (×), which satisfy the following properties:

- Associativity: for any $a, b, c \in \mathcal{F}$, (a+b)+c=a+(b+c) and $(a \times b) \times c=a \times (b \times c)$;
- Commutativity: for any a, b, a + b = b + a and $a \times b = b \times a$;
- Identity: there exists two different elements $0, 1 \in \mathcal{F}$ such that a + 0 = a and $a \times 1 = a$ for all $a \in \mathcal{F}$:
- Additive inverses: for any $a \in \mathcal{F}$, there exists an element in \mathcal{F} , denoted as -a, such that a + (-a) = 0;
- Multiplicative inverses: for any $a \in \mathcal{F}$ and $a \neq 0$, there exists an element in \mathcal{F} , denoted as a^{-1} , such that $a \times a^{-1} = 1$;
- Distributivity of multiplication over addition: for any $a, b, c \in \mathcal{F}$, $a \times (b+c) = (a \times b) + (a \times c)$.

Then, subtraction (-) is defined such that a-b=a+(-b) for all $a,b\in\mathcal{F}$; division (\div) can is defined such that $a\div b=a\times b^{-1}$ for all $a,b\in\mathcal{F},b\neq 0$.

Two most widely-used fileds are the rational number field \mathbb{Q} and the real number field \mathbb{R} , both of which satisfy the above properties. However, both fields contains an infinite number of elements. In this paper, we consider a class of fields called finite fields, which contain a *finite* number of elements. Given prime number p, the finite field \mathbb{Z}_p is the field consisting of p elements, which can be denoted as $0,1,\cdots,p-1$. In \mathbb{Z}_p , both addition and multiplication are defined by simply adding/multiplying two input integers and then taking the remainder modulo p. It can be easily checked that the two operations satisfy the six properties described above. Thus, subtraction and division can be defined accordingly. Remarkably, a key result in abstract algebra shows that all finite fields with p elements are *isomorphic*, which means that the above definitions of addition, subtraction, multiplication, and division are unique (up to isomorphism).

As an example, consider the finite field \mathbb{Z}_5 . We have that 2+3 equals 0, since $(2+3) \mod 5 = 0$. Similarly, 2×3 equals 1; 2-3 equals 4; and $2 \div 3$ equals 4.

In Section 3, we utilize the field \mathbb{Z}_p to address the issue of infinite tokens. Both tasks of evaluating arithmetic expressions and solving linear equations (Section 3.1) are well-defined in this field.

B.2 Circuit complexity

In circuit complexity theory, there are several fundamental complexity classes that capture different levels of computation power. Below, we provide a brief overview of these classes; however, for a comprehensive introduction, we recommend readers refer to Arora & Barak [2].

The basic complexity classes we will discuss in this subsection are NC⁰, AC⁰, TC⁰, NC¹, and P. These classes represent increasing levels of computation complexity. The relationships between these classes can be summarized as follows:

$$\mathsf{NC}^0 \subsetneq \mathsf{AC}^0 \subsetneq \mathsf{TC}^0 \subset \mathsf{NC}^1 \subset \mathsf{P}$$

Moreover, in the field of computational theory, it is widely conjectured that all subset relations in the hierarchy are *proper* subset relations. This means that each class is believed to capture a strictly larger

set of computational problems than its predecessor in the hierarchy. However, proving some of these subset relations to be proper subsets remains critical open questions in computational complexity theory. For example, $NC^1 = P$ will imply P = NP, which has long been a celebrated open question in computer science.

Formally, a Boolean circuit with n input bits is a directed acyclic graph (DAG), in which every node is either an input bit or an internal node representing one bit (also called a gate). The value of each internal node depends on its direct predecessors. Furthermore, several internal nodes are designated as output nodes, representing the output of the Boolean circuit. The in-degree of a node is called its fan-in number, and the input nodes have zero fan-in.

A Boolean circuit can only simulate a computation problem of a fixed number of input bits. When the input length varies, a series of distinct Boolean circuits will be required, each designed to process a specific length. Circuit complexity studies how the circuit size (e.g., depth, fan-in number, width) increases with respect to the input length. We now describe each complexity class as follows:

- NC⁰ is the class of constant-depth, constant-fan-in, polynomial-sized circuits consisting of AND, OR, and NOT gates. For example, in [19], the authors considered a restricted version of Transformer with constant depth and a *constant-degree* sparse selection construction, which can be characterized by this complexity class. However, NC⁰ circuits have limited representational power and cannot express functions that depend on a growing number of inputs as the input size increases.
- AC⁰ is the class of constant-depth, unbounded-fan-in, polynomial-sized circuits consisting of AND, OR, and NOT gates, with NOT gates allowed only at the inputs. It is strictly more powerful than NC⁰ mainly because the fan-in number can (polynomially) depend on the input length. However, there are still several fundamental Boolean functions that are not in this complexity class, such as the parity function or the majority function (see below).
- TC⁰ is an extension of AC⁰ that introduces an additional gate called MAJ. The MAJ gate takes an arbitrary number of input bits and evaluates to false when half or more of the input bits are false, and true otherwise. Previous work [36, 37] showed that the log-precision Transformer is in this class.
- NC^1 is a complexity class that consists of constant-fan-in, polynomial size circuits with a logarithmic depth of $O(\log n)$, where n is the input length. Similar to NC^0 , the basic logical gates are AND, OR, and NOT. Allowing the number of layers to depend on the input length significantly increases the expressiveness of the circuit. On the other hand, the logarithmic dependency still enables a descent parallelizability. Indeed, NC^1 is widely recognized as an important complexity class that captures efficiently parallelizable algorithms.
- P is the complexity class that contains problems that can be solved by a Turing machine in polynomial time. It contains a set of problems that do not have an efficient parallel algorithm. For example, the Context-Free-Grammar Membership Testing is in this class and is proved to be P-complete [28].

B.3 Log-precision

In this work, we focus on Transformers whose neuron values are restricted to be floating-point numbers of finite precision, and all computations operated on floating-point numbers will be finally truncated, similar to how computer processes real numbers. Specifically, the log-precision assumption means that we can use $O(\log(n))$ bits to represent a real number, where n is the length of the input sequence. Two most common formats in practice to store real numbers are the fixed-point format and floating-point format (e.g., the IEEE-754 standard [26]). There are also several popular truncation approaches (also called *rounding*), such as round-to-the-nearest, round-to-zero, round-up, and round-down. Our results in this paper hold for both formats and all these truncation approaches.

For any above floating-point format of $O(\log(n))$ bits, an important property is that it can represent all real numbers of magnitude $O(\operatorname{poly}(n))$ within $O(\operatorname{poly}(1/n))$ approximation error. Moreover, since the functions represented by Transformers are continuous, the approximation error in a hidden neuron will *smoothly* influence the approximation error of subsequent neurons in deeper layers. This impact can be bounded by the Lipschitz constant of the Transformer. Given a Transformer of polynomial size, when all parameter values of the Transformer are further bounded by $O(\operatorname{poly}(n))$, it is easy to see that all neuron values in a log-precision Transformer only yield an $O(\operatorname{poly}(1/n))$

approximation error compared to the infinite-precision counterpart³. Therefore, if a problem can be solved by a polynomial-size infinite-precision Transformer with *polynomially-bounded* parameters, it can also be solved by a log-precision Transformer of the same size. This finding is helpful for understanding Theorems 3.3, 3.4 and 4.7.

A key property of log-precision Transformer is that each neuron can only hold $O(\log(n))$ -bit information and thus cannot store the full information of the entire input sequence. Therefore, the log-precision assumption captures the idea that the computation must be somehow distributed on each token, which well-resembles practical situations and the way Transformers work.

C Formal Definitions of CoT in Section 3

In this section, we will formally define the CoT derivation formats for two math problems in Section 3.

Arithmetic expression. In an arithmetic expression that contains operators, there exists at least one pair of neighboring numbers connected by an operator that can be calculated, which we refer to as a *handle*. More precisely, one can represent an arithmetic expression into a (binary) syntax tree where each number is a leaf node and each operator is an internal node that has two children. In this case, a pair of neighboring numbers is a handle if they share the same parent in the syntax tree. For instance, consider the arithmetic formula $7 \times (6+5+4\times5)$. Then, 6+5 and 4×5 are two handles.

An important observation is that we can determine whether a pair of numbers a and b can form a handle with the operator op by examining the token before a and the token after b, where these tokens are either operators, brackets or empty (i.e., approaching the beginning/ending of the sequence). Specifically, given subsequence s_1 a op b s_2 , we have that a op b forms a handle iff one of the following conditions holds:

```
• op \in \{+, -\} and s_1 \in \{ ( ,empty\}, s_2 \notin \{\times, \div\};
• op \in \{\times, \div\} and s_1 \notin \{\times, \div\}.
```

In the proposed chain of thought (CoT), an autoregressive Transformer calculates *one* handle at each step. If there are multiple handles, the leftmost handle is selected. The subsequence a op b is then replaced by the calculated result. For the case of $s_{=}$ (and $s_{=}$), there will be a pair of redundant brackets and thus the two tokens and removed. It is easy to see that the resulting sequence is still a valid arithmetic expression. By following this process, each CoT step reduces one operator and the formula is gradually simplified until there is only one number left, yielding the final answer.

System of linear equations. Assume that we have a system of m linear equations with variables x_1, x_2, \ldots, x_m . Each equation in the input sequence is gramatically written as $a_1x_1 + a_2x_2 + \cdots + a_mx_m = b$, where $a_j \in \{0, \cdots, p-1\}$ and $b \in \{0, \cdots, p-1\}$. For simplicity, we do not omit the token a_j or a_jx_j when $a_j \in \{1, 0\}$. We can construct the following CoT to solve the equations by using the Gaussian elimination algorithm. At each step i, we select an equation k satisfying the following two conditions.

- The coefficient of x_i is nonzero.
- The coefficients of x_1, \dots, x_{i-1} are all zero.

Such an equation must exist, otherwise the solution is not unique or does not exist. If there are multiple equations satisfying the above conditions, we choose the k-th equation with the smallest index k. We then swap it with equation i, so that the i-th equation now satisfy the above conditions.

We then eliminate the variable x_i in all other equations by leveraging equation i. Formally, denote the i-th equation as

$$a_{ii}x_i + a_{i,i+1}x_{i+1} + \dots + a_{im}x_m = b_i, \tag{7}$$

and denote the coefficient of x_i in the j-th equation $(j \neq i)$ as a_{ji} . We can multiply (7) by $-a_{ii}^{-1}a_{ji}$ and add the resulting equation to the j-th equation. This will eliminate the term x_i in the j-th equation. We further normalize equation i so that the coefficient a_{ii} becomes 1. Depending on whether $j \leq i$ or i > i, the resulting equation in the CoT output will have the following grammatical form:

³This result is trivial for constant-depth Transformers. When the depth is also polynomial, the approximation error will scale like $O((1 + \text{poly}(1/n))^{L(n)})$ where the depth L(n) is another polynomial. As long as the inner polynomial has a higher order than L(n) (which can be easily accomplished by using a constant multiples of additional bits), the result can still be upper bounded by O(poly(1/n)).

- If $j \le i$, the j-th equation will be written as $x_j + \tilde{a}_{j,i+1}x_{i+1} + \cdots + \tilde{a}_{jm}x_m = \tilde{b}_j$;
- If j>i, the j-th equation will be written as $\tilde{a}_{j,i+1}x_{i+1}+\cdots+\tilde{a}_{jm}x_m=\tilde{b}_j$.

Note that we remove all zero terms $\tilde{a}_{jk}x_k$ for $k \leq i, k \neq j$ in the CoT output and also remove the coefficient 1 in $\tilde{a}_{kk}x_k$ for $k \leq i$, similar to how human write solutions (see Figure 1 for an illustration). However, to simplify our proof, we reserve the coefficient 0 or 1 (i.e., outputting $0x_k$ or $1x_k$) when k > i since it cannot be easily determined before computing the coefficient. The above process is repeated for m-1 steps, and after the final step, we obtain the solution.

D Useful Lemmas

D.1 Useful lemmas of MLP

In this subsection, we will demonstrate the expressivity and representation efficiency of two-layer MLPs in performing several basic operations, such as multiplication, linear transformation, conditional selection, and look-up table. These operations will serve as building blocks in performing complex tasks.

Firstly, we will show that an MLP with GeLU as its activation function can efficiently approximate the multiplication operation of two scalars, with all weights upper bounded by $O(\text{poly}(1/\epsilon))$, where ϵ is the approximation error.

Lemma D.1. Let $f: \mathbb{R}^2 \to \mathbb{R}$ be a two-layer MLP with GeLU as activation function, and the hidden dimension is 4. Then, for any $\epsilon > 0$ and M > 0, there exists parameters with ℓ_{∞} norm upper bounded by $O(\operatorname{poly}(M, 1/\epsilon))$ such that $|f(a, b) - ab| \le \epsilon$ holds for all $a, b \in [-M, M]$.

Proof. Denote the input vector to the MLP as $(a,b) \in \mathbb{R}^2$. After the first linear layer, it is easy to construct a weight matrix such that the hidden vector is $\frac{1}{\lambda}(a+b,-a-b,a-b,-a+b) \in \mathbb{R}^4$, where λ is an arbitrary scaling factor. Let σ be the GeLU activation. We can similarly construct a weight vector such that the final output of the MLP is

$$f(a,b) = \frac{\sqrt{2\pi}\lambda^2}{8} \left(\sigma\left(\frac{a+b}{\lambda}\right) + \sigma\left(\frac{-a-b}{\lambda}\right) - \sigma\left(\frac{a-b}{\lambda}\right) - \sigma\left(\frac{-a+b}{\lambda}\right) \right).$$

We will prove that the above MLP satisfies the theorem by picking an appropriate λ . By definition of GeLU activation, $\sigma(x)=x\Phi(x)$ where $\Phi(x)$ is the standard Gaussian cumulative distribution function. We thus have $\sigma'(0)=0.5$ and $\sigma''(0)=\sqrt{\frac{2}{\pi}}$. Applying Taylor's formula and assuming $\lambda>2M$, we have

$$\begin{split} & \left| \sigma \left(\frac{a+b}{\lambda} \right) + \sigma \left(\frac{-a-b}{\lambda} \right) - \sigma \left(\frac{a-b}{\lambda} \right) - \sigma \left(\frac{-a+b}{\lambda} \right) - \frac{8ab}{\sqrt{2\pi}\lambda^2} \right| \\ \leq & \left| \frac{1}{2} \sqrt{\frac{2}{\pi}} \left(\left(\frac{a+b}{\lambda} \right)^2 + \left(\frac{-a-b}{\lambda} \right)^2 - \left(\frac{a-b}{\lambda} \right)^2 - \left(\frac{-a+b}{\lambda} \right)^2 \right) - \frac{8ab}{\sqrt{2\pi}\lambda^2} \right| \\ & + \frac{4}{3!} \frac{(2M)^3}{\lambda^3} \left| \max_{x \in [-1,1]} \sigma^{(3)}(x) \right| \\ = & \frac{16M^3}{3\lambda^3} \max_{x \in [-1,1]} \frac{1}{\sqrt{2\pi}} (x^3 - 4x) \exp(-\frac{x^2}{2}) \\ < & \frac{80M^3}{3\sqrt{2\pi}\lambda^3} \end{split}$$

Therefore, $|f(a,b)-ab|<\frac{10M^3}{3\lambda}$. Set $\lambda\geq\frac{10M^3}{3\epsilon}$, and then we can obtain $|f(a,b)-ab|<\epsilon$. Moreover, each weight element in the MLP is upper bounded by $O(\lambda^2)$, which is clearly $O(\operatorname{poly}(M,1/\epsilon))$. \square

Next, we will demonstrate that a two-layer MLP with GeLU activation can efficiently approximate a two-layer MLP with ReLU activation, with all weights upper bounded by $O(\operatorname{poly}(\frac{1}{\epsilon}))$. This result is useful in proving subsequent lemmas.

Lemma D.2. Let $g: \mathbb{R}^{d_1} \to \mathbb{R}^{d_2}$ be a two-layer MLP with ReLU activation and the parameters are upper bounded by M in the ℓ_{∞} norm. Then, for any $\epsilon > 0$, there exists a two-layer MLP f of the same size with ReLU activation and parameters upper bounded by $O(M \operatorname{poly}(1/\epsilon))$ in the ℓ_{∞} norm, such that for all $x \in \mathbb{R}^{d_1}$, we have $\|f(x) - g(x)\|_{\infty} \leq \epsilon$.

Proof. Let $g(x) = W_2 \cdot \text{ReLU}(W_1 x)$. We construct $f(x) = \frac{1}{\lambda} W_2 \cdot \text{GeLU}(\lambda W_1 x)$ where $\lambda > 0$ is a sufficiently large constant. To prove that $||f(x) - g(x)||_{\infty} \le \epsilon$ for all $x \in \mathbb{R}^{d_1}$, it suffices to consider the scalar setting and prove that, for any $\delta > 0$, there exists $\lambda > 0$ such that $|\frac{1}{\lambda} \text{GeLU}(\lambda y) - \text{ReLU}(y)| \le \delta$ for all $y \in \mathbb{R}$.

By definition of ReLU and GeLU, we have

$$\left| \frac{1}{\lambda} \operatorname{GeLU}(\lambda y) - \operatorname{ReLU}(y) \right| = \frac{1}{\lambda} \left| \operatorname{ReLU}(\lambda y) - \int_{-\infty}^{\lambda y} \frac{\lambda y}{\sqrt{2\pi}} \exp\left(-\frac{t^2}{2}\right) dt \right|. \tag{8}$$

When $y \ge 0$, (8) becomes

$$\frac{1}{\lambda} \left| \int_{-\infty}^{+\infty} \frac{\lambda y}{\sqrt{2\pi}} \exp\left(-\frac{t^2}{2}\right) dt - \int_{-\infty}^{\lambda y} \frac{\lambda y}{\sqrt{2\pi}} \exp\left(-\frac{t^2}{2}\right) dt \right| = \frac{1}{\lambda} \int_{\lambda y}^{+\infty} \frac{\lambda y}{\sqrt{2\pi}} \exp\left(-\frac{t^2}{2}\right) dt.$$

Combined with the case of y < 0, (8) can be consistently written as

$$\begin{split} \left| \frac{1}{\lambda} \text{GeLU}(\lambda y) - \text{ReLU}(y) \right| &= \frac{1}{\lambda} \int_{\lambda |y|}^{+\infty} \frac{\lambda |y|}{\sqrt{2\pi}} \exp\left(-\frac{t^2}{2}\right) \text{d}t \\ &\leq \frac{1}{\sqrt{2\pi}\lambda} \int_{\lambda |y|}^{+\infty} t \exp\left(-\frac{t^2}{2}\right) \text{d}t = \frac{1}{\sqrt{2\pi}\lambda} \exp\left(-\frac{\lambda^2 y^2}{2}\right) \\ &\leq \frac{1}{\sqrt{2\pi}\lambda}. \end{split}$$

Picking $\lambda = \frac{1}{\sqrt{2\pi\delta}}$ yields the desired result and completes the proof.

Equipped with the above result, we now prove that a two-layer MLP with GeLU activation can perform linear transformation and conditional selection.

Proposition D.3. Let $f: \mathbb{R}^{d_1} \to \mathbb{R}^{d_2}$ be a two-layer MLP with GeLU activation, and the hidden dimension is $2d_2$. Let $\mathbf{W} \in \mathbb{R}^{d_2 \times d_1}$ be any matrix. Then, for any $\epsilon > 0$, there exists MLP parameters with ℓ_{∞} norm bounded by $O(\text{poly}(1/\epsilon))$, such that for any $\mathbf{x} \in \mathbb{R}^{d_1}$, we have $\|\mathbf{f}(\mathbf{v}) - \mathbf{W}\mathbf{x}\|_{\infty} \leq \epsilon$.

Proof. We can use a two-layer MLP with ReLU activation to implement g(x) = Wx by the following construction:

$$\boldsymbol{W}\boldsymbol{x} = \text{ReLU}(\boldsymbol{W}\boldsymbol{x}) + \text{ReLU}(-\boldsymbol{W}\boldsymbol{x})$$

Combined with Lemma D.2, we can also implement g(x) by a two-layer MLP with GeLU activation.

Lemma D.4. Define the selection function $g: \mathbb{R}^{d_1} \times \mathbb{R}^{d_2} \times \mathbb{R} \to \mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$ as follows:

$$g(x, y, t) = \begin{cases} (x, 0) & \text{if } t \ge 0, \\ (0, y) & \text{if } t < 0. \end{cases}$$

$$(9)$$

Let $f: \mathbb{R}^{d_1} \times \mathbb{R}^{d_2} \times \mathbb{R} \to \mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$ be a two-layer MLP with GeLU as activation function, and the hidden dimension is $d_1 + d_2 + 2$. Then, for any $\epsilon > 0$ and M > 0, there exists MLP parameters with ℓ_{∞} norm bounded by $O(\operatorname{poly}(M, 1/\epsilon))$, such that for all $\mathbf{x} \in [-M, M]^{d_1}$, $\mathbf{y} \in [-M, M]^{d_2}$, and $t \in [-1, -1/2] \cup [1/2, 1]$, we have $\|\mathbf{f}(\mathbf{x}, \mathbf{y}, t) - \mathbf{g}(\mathbf{x}, \mathbf{y}, t)\|_{\infty} \leq \epsilon$.

Proof. We can simply use a two-layer MLP with ReLU activation to implement g by the following construction:

$$h(x, y, t) = (h_1, h_2, h_3, h_4) = (x + 2Mt\mathbf{1}_{d_1}, y - 2Mt\mathbf{1}_{d_2}, 2Mt, -2Mt) \in \mathbb{R}^{d_1 + d_2 + 2}$$

 $f(x, y, t) = (\text{ReLU}(h_1) - \text{ReLU}(h_3)\mathbf{1}_{d_1}, \text{ReLU}(h_2) - \text{ReLU}(h_4)\mathbf{1}_{d_2})$

where $\mathbf{1}_d$ is the all-one vector of d dimension. It is easy to check that, for all $\mathbf{x} \in [-M, M]^{d_1}$, $\mathbf{y} \in [-M, M]^{d_2}$, and $t \in [-1, -1/2] \cup [1/2, 1]$, we have $\mathbf{f}(\mathbf{x}, \mathbf{y}, t) = \mathbf{g}(\mathbf{x}, \mathbf{y}, t)$. Moreover, all parameters are bounded by O(M). Therefore, by using Lemma D.2, we can also implement $\mathbf{g}(\mathbf{x})$ by a two-layer MLP with GeLU activation and all parameters are bounded by $O(\text{poly}(M, 1/\epsilon))$.

We final show that a two-layer MLP can efficiently represent a look-up table. Consider a k-dimensional table of size d^k , where each element in the table is an integer ranging from 1 to d. Denote the set $\mathcal{D} = \{e_i : i \in [d]\}$, where e_i is a d-dimensional one-hot vector with the i-th element being 1. The above look-up table can thus be represented as a discrete function $g: \mathcal{D}^k \to \mathcal{D}$. The following lemma shows that g can be implemented by a two-layer MLP with GeLU activation.

Lemma D.5. Let $g: \mathcal{D}^k \to \mathcal{D}$ be any function defined above, and let $f: \mathbb{R}^{d \times k} \to \mathbb{R}^d$ be a two-layer MLP with GeLU as activation, and the hidden dimension is d^k . Then, for any $\epsilon > 0$, there exists MLP parameters with ℓ_{∞} norm bounded by $O(\operatorname{poly}(k, 1/\epsilon))$, such that for all $x \in \mathcal{D}^k \subset \mathbb{R}^{dk}$ and all perturbation $y \in [-1/2k, 1/2k]^{dk}$, we have $||f(x+y) - g(x)||_{\infty} \le \epsilon + 2k||y||_{\infty}$.

Proof. We can simply use a two-layer MLP with ReLU as the activation function to implement g by the following construction. Denote the index of the MLP hidden layer as $(i_1, \dots, i_k) \in [d]^k$. We can construct the weights of the first MLP layer such that

$$h_{(i_1,\dots,i_k)}(\mathbf{x}) = 2(x_{1,i_1} + \dots + x_{k,i_k}) - 2k + 1.$$

We can then construct the weights of the second layer such that the final output of the MLP is

$$f_j(\boldsymbol{x}) = \sum_{g_j(\boldsymbol{e}_{i_1}, \dots, \boldsymbol{e}_{i_k}) = 1} \text{ReLU}(h_{(i_1, \dots, i_k)}(\boldsymbol{x})).$$

One can check that f(x) = g(x) holds for all $x \in \mathcal{D}^k \subset \mathbb{R}^{dk}$. Furthermore, for all perturbation $y \in [-1/2k, 1/2k]^{dk}$, we have

$$\begin{split} \| \boldsymbol{f}(\boldsymbol{x} + \boldsymbol{y}) - \boldsymbol{g}(\boldsymbol{x}) \|_{\infty} &= \| \boldsymbol{f}(\boldsymbol{x} + \boldsymbol{y}) - \boldsymbol{f}(\boldsymbol{x}) \|_{\infty} \\ &= \max_{j \in [d]} \left| \sum_{g_{j}(\boldsymbol{e}_{i_{1}}, \cdots, \boldsymbol{e}_{i_{k}}) = 1} \left(\operatorname{ReLU}(h_{(i_{1}, \cdots, i_{k})}(\boldsymbol{x} + \boldsymbol{y})) - \operatorname{ReLU}(h_{(i_{1}, \cdots, i_{k})}(\boldsymbol{x}) \right) \right| \\ &\leq \max_{(i_{1}, \cdots, i_{k}) \in [d]^{k}} \left| h_{(i_{1}, \cdots, i_{k})}(\boldsymbol{x} + \boldsymbol{y}) - h_{(i_{1}, \cdots, i_{k})}(\boldsymbol{x}) \right| \leq 2k \| \boldsymbol{y} \|_{\infty}. \end{split}$$

Therefore, by using Lemma D.2, we can also implement g(x) by a two-layer MLP with GeLU activation and all parameters are bounded by $O(\text{poly}(k, 1/\epsilon))$.

D.2 Useful lemmas for the attention layer

In this subsection, we will introduce two special operations that can be performed by the attention layer (with causal mask). Below, we denote by x_1, x_2, \cdots, x_n a sequence of vectors where $x_i = (v_i, r_i, i, 1) \in [-M, M]^{d+1} \times [n] \times \{1\}$. Here, v_i is a d-dimensional vector and r_i is a scalar, both of which are bounded by M. Let $K, Q \in \mathbb{R}^{d \times d}$ be arbitrary matrices, and let $\rho > 0$, $\delta > 0$ be any real numbers. We further define the *matching set* $S_i = \{j \leq i : |k_i \cdot q_j| \leq \rho\}$ where $k_i = Kx_i$ and $q_j = Qx_j$. Equipped with these notations, we define two basic operations as follows:

- COPY: The output is a sequence of vectors u_1, \dots, u_n with $u_i = v_{pos(i)}$, where $pos(i) = \underset{i \in S_i}{\operatorname{argmax}}_{i \in S_i} r_i$.
- MEAN: The output is a sequence of vectors u_1, \dots, u_n with $u_i = \text{mean}_{i \in S_i} v_i$.

We make the following assumption:

Assumption D.6. The matrices K, Q and ρ, δ satisfy that for all considered sequences x_1, x_2, \dots, x_n , the following hold:

- For any $i \in [n]$, S_i is not empty.
- For any $i, j \in [n]$, either $|\mathbf{k}_i \cdot \mathbf{q}_j| \le \rho$ or $\mathbf{k}_i \cdot \mathbf{q}_j \le -\delta$.
- For any $i, j \in [n]$, either $r_i = r_j$ or $|r_i r_j| \ge \delta$.

Assumption D.6 says that there are sufficient gaps between the attended position (e.g., pos(i)) and other positions. The two lemmas below show that the attention layer with casual mask can implement both COPY operation and MEAN operation efficiently.

Lemma D.7. Assume Assumption D.6 holds with $\rho \leq \frac{\delta^2}{8M}$. For any $\epsilon > 0$, there exists an attention layer with embedding size O(d) and one causal attention head that can approximate the COPY operation defined above. Formally, for any considered sequence of vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$, denote the attention output as $\mathbf{o}_1, \mathbf{o}_2, \dots, \mathbf{o}_n$. Then, we have $\|\mathbf{o}_i - \mathbf{u}_i\|_{\infty} \leq \epsilon$ for all $i \in [n]$. Moreover, the ℓ_{∞} norm of attention parameters is bounded by $O(\operatorname{poly}(M, 1/\delta, \log(n), \log(1/\epsilon)))$.

Proof. The purpose of the attention head is to focus only on the vector that needs to be copied. The key, query, and value components are constructed as follows:

• Query: $(\lambda \boldsymbol{q}_i, \mu) \in \mathbb{R}^{d+1}$

• Key: $(\lambda \mathbf{k}_i, r_i) \in \mathbb{R}^{d+1}$

• Value: $oldsymbol{v}_i \in \mathbb{R}^d$

where λ and μ are constants which will be defined later. Denote a_{ij} as the attention score, then

$$a_{i,j} = \frac{\exp(\lambda(\mathbf{k}_i \cdot \mathbf{q}_j) + \mu r_j)}{\sum_j \exp(\lambda(\mathbf{k}_i \cdot \mathbf{q}_j) + \mu r_j)} = \frac{\exp(\lambda(\mathbf{k}_i \cdot \mathbf{q}_j))}{\sum_j \exp(\lambda(\mathbf{k}_i \cdot \mathbf{q}_j) + \mu(r_j - r_i))}.$$

Since $\rho \leq \frac{\delta^2}{8M}$ and $M \geq \delta$, we have $\delta - \rho \geq \frac{7}{8}\delta$. By setting $\lambda = \frac{8M\ln(\frac{4nM}{\epsilon})}{\delta^2}$ and $\mu = \frac{3\ln(\frac{4nM}{\epsilon})}{\delta}$ (which are bounded by $O(\operatorname{poly}(M, 1/\delta, \log(n), \log(1/\epsilon)))$), we have

$$\begin{split} a_{i,\text{pos}(i)} &\geq \frac{\exp(-\lambda\rho)}{\exp(-\lambda\rho) + (n-1)\exp(\max(-\lambda\delta + 2M\mu, \lambda\rho - \mu\delta))} \\ &= \frac{1}{1 + (n-1)\exp(\max(-\lambda(\delta-\rho) + 2M\mu, 2\lambda\rho - \mu\delta))} \\ &\geq 1 - n\exp(\max(-\lambda(\delta-\rho) + 2M\mu, 2\lambda\rho - \mu\delta)) \\ &\geq 1 - n\exp\left(\max\left(-\frac{M}{\delta}\ln\left(\frac{4nM}{\epsilon}\right), -\ln\left(\frac{4nM}{\epsilon}\right)\right)\right) \\ &\geq 1 - n\exp\left(-\ln\left(\frac{4nM}{\epsilon}\right)\right) \\ &= 1 - \frac{\epsilon}{4M}. \end{split}$$

Therefore,

$$\|\boldsymbol{o}_i - \boldsymbol{u}_i\|_{\infty} \le 2M \cdot \left(1 - a_{i,pos(i)} + \sum_{j \neq pos(i)} a_{i,j}\right)$$

= $2M(2 - a_{i,pos(i)}) \le \epsilon$,

which concludes the proof.

Lemma D.8. Assume Assumption D.6 holds with $\rho \leq \frac{\delta \min(1,\epsilon)}{64M \ln(\frac{8Mn}{\epsilon})}$. For any $\epsilon > 0$, there exists an attention layer with embedding size O(d) and one causal attention head that can approximate the MEAN operation defined above. Formally, for any considered sequence of vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$, denote the attention output as $\mathbf{o}_1, \mathbf{o}_2, \ldots, \mathbf{o}_n$. Then, we have $\|\mathbf{o}_i - \mathbf{u}_i\|_{\infty} \leq \epsilon$ for all $i \in [n]$. Moreover, the ℓ_{∞} norm of attention parameters is bounded by $O(\operatorname{poly}(M, 1/\delta, \log(n), \log(1/\epsilon)))$.

Proof. The purpose of the attention head is to focus only on the token that satisfies the condition $k_j \cdot q_i \approx 0$. The key, query, and value components are as follows:

• Ouerv: $\lambda \mathbf{q}_i \in \mathbb{R}^d$

• Key: $\lambda \mathbf{k}_i \in \mathbb{R}^d$

• Value: $v_i \in \mathbb{R}^d$

where λ is a constant which will be defined later. The attention vector \boldsymbol{x}_i pays attention to the vector \boldsymbol{x}_j according to the formula $a_{i,j} = \exp(-\lambda(\boldsymbol{k}_i \cdot \boldsymbol{q}_j))$. We can set $\lambda = \frac{2\ln(\frac{8Mn}{\epsilon})}{\delta}$ which is bounded by $O(poly(\frac{nM}{\epsilon\delta}))$. We only need to consider the case of $\epsilon < 1$ and $M > \epsilon$. Note that the error comes from two parts, the little attention paid to the tokens not satisfying $\boldsymbol{k}_i \cdot \boldsymbol{q}_j = 0$ and the little difference of attention paid to the tokens satisfying $\boldsymbol{k}_i \cdot \boldsymbol{q}_j = 0$. For the vectors $\boldsymbol{v}_j \ \boldsymbol{k}_i \boldsymbol{q}_j \leq -\delta$, similar to the proof of the previous Lemma D.7, we have $a_{i,j} \leq \frac{\exp(\boldsymbol{k}_i \cdot \boldsymbol{q}_j)}{\exp(-\rho)} \leq \exp(-\lambda(\delta-\rho))$. Therefore, the first part of the error

$$\epsilon_1 \le 2Mn \cdot \exp\left(-\lambda(\delta - \rho)\right) \le 2Mn \cdot \exp\left(-\lambda\delta/2\right) \le \frac{\epsilon}{4}.$$

For the vectors $v_j |k_i q_j| \le \rho$, we expect to pay uniform attention to all the vectors, but the attention may not be uniform exactly. We denote $k = |\mathcal{S}_i|$ The error can be bounded as

$$\begin{split} \epsilon_2 \leq & 2Mk \max\left(\frac{1}{k} - \frac{\exp(-\rho\lambda)}{k \exp(\rho\lambda) + n \exp(-\lambda(\delta - \rho))}, \frac{\exp(\rho\lambda)}{k \exp(-\rho\lambda)} - \frac{1}{k}\right) \\ \leq & 2M\left(\exp(2\rho\lambda) - \exp(-2\rho\lambda)\frac{1}{1 + \frac{\epsilon}{8M}}\right) \\ \leq & 2M\left(\exp(2\rho\lambda) - \exp(-2\rho\lambda)(1 - \frac{\epsilon}{8M})\right) \\ \leq & 2M(\exp(4\rho\lambda) - 1) + \frac{\epsilon}{4} \\ \leq & 2M(\exp(\frac{\epsilon}{8M}) - 1) + \frac{\epsilon}{4} \\ \leq & \frac{3\epsilon}{4} \end{split}$$

Then, we can obtain:

$$\|\boldsymbol{o}_i - \boldsymbol{u}_i\|_{\infty} \le \epsilon_1 + \epsilon_2 \le \epsilon$$

Therefore, our construction is correct.

Finally, it is worth noting that the residual connections in all Attention/MLP layers can be replaced by concatenation with the same expressive power. Consider an MLP or an attention layer denoted as f, and let $[\boldsymbol{x}_1, \boldsymbol{x}_2]$ be any two vectors where $\boldsymbol{x}_2 = f(\boldsymbol{x}_1)$. We can construct another MLP or attention layer denoted as g such that $g([\boldsymbol{x}_1, 0]) + [\boldsymbol{x}_1, 0] = [\boldsymbol{x}_1, \boldsymbol{x}_2]$. Therefore, in the constructions presented in Appendices E to G, we utilize the concatenation operation to implement residual connections and aggregation of the attention heads' output. However, it is important to note that this modification can be easily replaced by the standard operation if desired. Moreover, for simplicity and clarity, in the proofs, we omit the unnecessary embeddings of the concatenation operation and only retain the embeddings that are utilized in subsequent layers.

E Arithmetic Formula

In this section, we prove that the autoregressive Transformer can evaluate arithmetic expressions when equipped with CoT, whereas the it cannot solve this task without CoT.

E.1 Proof of Theorem 3.3

For ease of reading, we restate Theorem 3.3 below:

Theorem E.1. For any prime p and integer n > 0, there exists an autoregressive Transformer defined in Section 2 with hidden size $d = O(\operatorname{poly}(p))$ (independent of n), depth L = 5, and 5 heads in each layer that can generate the CoT solution defined in Appendix C for all inputs in Arithmetic(n,p). Moreover, all parameter values in the Transformer are bounded by $O(\operatorname{poly}(n))$.

We first give a proof sketch below. The intuition behind our construction is that when the CoT output proceeds to a certain position, the Transformer can read the context related to this position and

determine whether it should copy a token or perform a calculation. Remarkably, the context only contains a *fixed* number of tokens (as discussed in Appendix C). Based on the key observation, we can construct our five-layer transformer. The first layer counts the number of equal signs (=) in the previous tokens and copies the position index of the last equal sign. The second and third layers determine whether to perform a calculation by examining the context related to the current token, which contains five tokens. The fourth layer and the fifth layers generate a sequence of tokens using the outcomes of the previous layer.

Proof. We construct each layer as follows.

Token Embeddings. Assume that we have a sequence of tokens s_1, \ldots, s_t and we want to generate the next token s_{t+1} . We can embed the token s_i using the format $\boldsymbol{x}_i^{(0)} = (\boldsymbol{e}_i, i, 1) \in \mathbb{R}^{\#\text{token}+2}$, where \boldsymbol{e}_i is a one-hot vector that represents the i-th token in the vocabulary, the $i \in \mathbb{N}_+$ is the positional embedding, and the constant embedding 1 is used as a bias term.

Layer 1. The first layer of the autoregressive Transformer uses two attention heads to perform the following tasks:

- 1. Count the number of equal signs in the previous tokens, denoted as n_i^{\pm} .
- 2. Copy the position index of the last equal sign, denoted as $p_i^{=}$.

Based on Lemma D.8, we can use the first attention head to perform a MEAN operation that counts the percentage of equal signs in the preceding sentences (i.e., $n_i^=/i$). This can be achieved by setting $\mathcal{S}_i = [i]$ and $v_j = \mathbb{I}[s_j = \text{`e'}]$ in Lemma D.8. Similarly, based on Lemma D.7, we can use the second attention head to perform a COPY operation that copies the position index of the last equal sign (i.e., $p_i^=$). This can be achieved by setting $\mathcal{S}_i = \{j \leq i : s_j = \text{`e'}\}$, $r_j = j$ and, $v_j = j$ in Lemma D.7. Using the residual connection, the output of the attention layer has the form $(e_i, i, 1, n_i^=/i, p_i^=)$. We can use an MLP to multiply $n_i^=/i$ and i to obtain $n_i^=$ according to Lemma D.1 and simultaneous compute the distance between the last equal sign and the next position, denoted as $d_i^= = i - p_i^= + 1$. The final output of the first layer has the form $\boldsymbol{x}_i^{(1)} = (e_i, i, n_i^=, d_i^=, 1)$.

Layer 2. The second layer of the transformer just does the preparation work for the next layer. It just uses its MLP to calculate $(d_i^=)^2$ and $(n_i^=)^2$, which can be simply done by Lemma D.1. Therefore, the attention layer of the second layer does nothing but maintain the input by the residual connection, and the output of the second layer is $\boldsymbol{x}_i^{(2)} = (\boldsymbol{e}_i, i, n_i^=, d_i^=, (n_i^=)^2, (d_i^=)^2, 1)$.

Layer 3. The intuition behind the third layer of the autoregressive Transformer is that it can determine whether it should perform a calculation at the current token or not by extracting five previous tokens related to this position. To do this, we need five attention heads to perform the following tasks:

- 1. Copy the embedding e_j located at position j such that $n_j^==n_i^=-1$ and $d_j^==d_i^=+k$ for $k \in \{1,2,3,4,5\}$.
- 2. Check if the copied expression can be evaluated according to the rule given in Appendix C. If it can be evaluated, compute the result and determine how much sentence length will be reduced after this calculation; otherwise, keep the token e_j with $n_j^= = n_i^= -1$ and $d_j^= = d_i^= +1$.

We can utilize the multi-head attention to perform the COPY operation five times in parallel. For each k, we construct the matrices K and Q of the COPY operation such that

$$\begin{split} \boldsymbol{K}\boldsymbol{x}_{i}^{(2)} = & [(n_{i}^{=})^{2} - 2n_{i}^{=} + 1, \quad 1, \quad n_{i}^{=} - 1, \quad (d_{i}^{=})^{2} - 2kd_{i}^{=} + k^{2}, \quad 1, \quad d_{i}^{=} - k]^{\top}, \\ \boldsymbol{Q}\boldsymbol{x}_{j}^{(2)} = & [\quad 1, \quad (n_{j}^{=})^{2}, \quad -2n_{j}^{=}, \quad 1, \quad (d_{j}^{=})^{2}, \quad -2d_{j}^{=}]^{\top}. \\ & \boldsymbol{K}\boldsymbol{x}_{i}^{(2)} \cdot \boldsymbol{Q}\boldsymbol{x}_{j}^{(2)} = (n_{i}^{=} - n_{j}^{=} - 1)^{2} + (d_{i}^{=} - d_{j}^{=} + k)^{2}. \end{split}$$

Therefore, $Kx_i^{(2)} \cdot Qx_j^{(2)} = 0$ only when $n_j^= = n_i^= -1$ and $d_j^= = d_i^= + k$, and $Kx_i^{(2)} \cdot Qx_j^{(2)} \ge 1$ otherwise. Therefore, Lemma D.7 guarantees that we can copy the desired token as Assumption D.6 is satisfied (we do not use r_i in Assumption D.6). The output of the attention layer can be written as

$$(e_i, e_{j_1}, e_{j_2}, e_{j_3}, e_{j_4}, e_{j_5}, i, n_i^=, d_i^=, (n_i^=)^2, (d_i^=)^2, 1),$$

where e_{j_k} is the embedding we copied by the k-th attention heads.

We can then use an MLP to perform the second task. As all embeddings e_i are one-hot vectors, whether the expression can be calculated or not forms a look-up table. Therefore, it can be implemented by a two-layer MLP with hidden dimension $O(\operatorname{poly}(p))$ acorrding to Lemma D.5. Similarly, how much sentence length will be reduced after this calculation can also be implemented. The final output of the third layer is represented by $\mathbf{x}_i^{(3)} = (e_i^{\text{outcome}}, e_{j_1}, \tan g_i, d_i^{=}, n_i^{=}, \operatorname{num}_i)$. Here, $\tan g_i$ is a Boolean value recording whether the copied expression can be calculated, e_i^{outcome} is the one-hot embedding of the outcome when the expression can be calculated, and $\tan g_i$ records the length of the expression that will be decreased.

Layer 4. The fourth layer of the autoregressive transformer utilizes two attention heads to perform the following tasks:

- 1. Check whether there is an index $j \leq i$ such that $n_j^{=} = n_i^{=}$ and tag_j in $\boldsymbol{x}_j^{(3)}$ is 1. Denote the result as tag_i' .
- 2. If the answer is yes $(tag'_i = 1)$, copy the embedding num_j located at position j with $tag_j = 1$ and $n_i^{=} = n_i^{=}$. Denote the result as $num'_i = num_j$. num'_i is undefined if $tag'_i = 0$.
- 3. Filter the outcome. Namely, if $tag_i = 1$, then maintain e_i^{outcome} and set $e_{j_1} = 0$; if $tag_i = 0$, then maintain e_{j_1} and set $e_i^{\text{outcome}} = 0$.

Similar to the construction of the third layer, we can construct the matrices \boldsymbol{K} and \boldsymbol{Q} of the MEAN operation and the COPY operation such that $\boldsymbol{K}\boldsymbol{x}_i^{(3)} = [(n_i^{=})^2, 1, n_i^{=}]^{\top}$ and $\boldsymbol{Q}\boldsymbol{x}_i^{(3)} = [1, (n_i^{=})^2, -2n_i^{=}]^{\top}$. We have $\boldsymbol{K}\boldsymbol{x}_i^{(3)} \cdot \boldsymbol{Q}\boldsymbol{x}_j^{(3)} = (n_i^{=} - n_j^{=})^2$. Therefore, $\boldsymbol{K}\boldsymbol{x}_i^{(3)} \cdot \boldsymbol{Q}\boldsymbol{x}_j^{(3)} = 0$ only when $n_j^{=} = n_i^{=}$, and $\boldsymbol{K}\boldsymbol{x}_i^{(3)} \cdot \boldsymbol{Q}\boldsymbol{x}_j^{(3)} \geq 1$ otherwise. The condition of $tag_j = 1$ in the second task can be achieved via the r_j term defined in the COPY operation. Moreover, the first task can be converted to the task of averaging all tag_j such that $n_j^{=} = n_i^{=}$. The output of the attention layer has the form

$$(e_i^{\text{outcome}}, e_{j_1}, d_i^{=}, n_i^{=}, \tan_i, \tan_i'/d_i^{=}, \text{num}_i'),$$

where $tag'_i/d_i^{=}$ is implemented by the MEAN operation.

We next use an MLP to perform the third task, which can be done according to Lemma D.4. We can simultaneously obtain tag_i' by multiplying $tag_i'/d_i^=$ with $d_i^=$. The final output of the fourth layer is represented by

$$\boldsymbol{x}_i^{(4)} = [\tilde{e}_i^{\text{outcome}}, \tilde{e}_{j_1}, \tan g_i, d_i^=, n_i^=, \text{num}_i, \tan g_i', \text{num}_i', (d_i^= + \text{num}_i')^2],$$

where $\tilde{e}_i^{ ext{outcome}}, \tilde{e}_{j_1}$ are the embeddings from $e_i^{ ext{outcome}}, e_{j_1}$ after filtering.

Layer 5. The final layer of the autoregressive Transformer uses one attention head to copy the corresponding token for generating the output when $tag_i' = 1$. Similar to previous layers, we can copy the embedding e_j located at position j such that $n_j^= = n_i^= -1$ and $d_j^= = d_i^= + num_i'$. The output of the attention layer is

$$(\tilde{e}_i^{\text{outcome}}, \tilde{e}_i, e_i, \tan_i, d_i^{=}, n_i^{=}, \text{num}_i, \tan_i', \text{num}_i'),$$

Then, we pass the embeddings through the MLP to filter and obtain the output. If $tag_i'=1$, then maintain e_j and set $\tilde{e}_{j_1}=0$, $\tilde{e}_i^{\text{outcome}}=0$, and if $tag_i=0$ then maintain \tilde{e}_{j_1} and $\tilde{e}_i^{\text{outcome}}$ and set $e_j=0$. Moreover, we sum up the three embeddings to get our final embedding. So the output of the MLP is $[\tilde{e}_{j_1}+e_j+\tilde{e}_i^{\text{outcome}}]$ and only one of them is a one-hot vector and others are zero vectors.

Finally, we pass it through a softmax layer to get the next token s_{i+1} .

Note that, we can tolerate O(1) (at most 0.5) error of the output of the final layer and the ℓ_{∞} norm embedding of the inner layer is bounded by O(poly(n)). So according to the previous lemmas in Appendices D.1 and D.2, the weight norm of the transformer constructed in this proof is bounded by O(poly(n)).

E.2 Proof of Theorem 3.1

We now prove that evaluating arithmetic expressions without CoT is extremely difficult for boundeddepth autoregressive Transformer. We will make the widely-believed assumption that $TC^0 \neq NC^1$ (see Appendix B.2 for definitions of these complexity classes). We further need to notion of *uniformity*: informally, this condition says that there exists an efficient algorithm to construct the circuits. For a rigorous definition, we refer readers to Arora & Barak [2].

Theorem E.2. Assume $TC^0 \neq NC^1$. For any prime number p, any integer L, and any polynomial Q, there exists a problem size n such that no log-precision autoregressive Transformer defined in Section 2 with depth L and hidden dimension $d \leq Q(n)$ can solve the problem Arithmetic(n, p).

Proof. Our proof is based on leveraging the NC^1 -completeness of a classic problem: Boolean Formula Evaluation. According to the Buss reduction [11], calculating whether a Boolean formula is true or false is complete for uniform NC^1 . Based on this theorem, it suffices to prove that the Boolean Formula Evaluation problem can be *reduced* to evaluating the arithmetic expression. This will yield the conclusion by using the result that bounded-depth log-precision Transformers with polynomial size are in TC^0 [36] as well as the assumption that $TC^0 \neq$ uniform NC^1 .

Formally, let $\Sigma = \{0, 1, \wedge, \vee, \neg, (,)\}$ be the alphabet. A Boolean formula is a string defined on alphabet Σ using the following recursive way:

- 0 and 1 are Boolean formulae;
- If φ is a Boolean formula, then $\neg \varphi$ is a Boolean formula;
- If φ_1, φ_2 are two Boolean formulae, then both $(\varphi_1 \wedge \varphi_2)$ and $(\varphi_1 \vee \varphi_2)$ are Boolean formulae.

The Boolean Formula Evaluation problem is to compute whether a Boolean formula is true (1) or false (0). We now show that we can translate this problem into the problem of evaluating arithmetic expressions. Given a Boolean formula s, the translation function f generates the corresponding arithmetic expression f(s) that has the same result as s under evaluation. The translation is recursively defined as follows:

- f(0) = 0 and f(1) = 1;
- For any Boolean formula φ , $f(\neg \varphi) = (1 \varphi)$;
- For any Boolean formulae $\varphi_1, \varphi_2, f((\varphi_1 \wedge \varphi_2)) = f(\varphi_1) \times f(\varphi_2);$
- For any Boolean formulae $\varphi_1, \varphi_2, f((\varphi_1 \vee \varphi_2)) = (1 (1 f(\varphi_1)) \times (1 f(\varphi_2))).$

It is easy to see that for any Boolean formula s, the length of f(s) is upper bounded by O(|s|). Moreover, the translation function can be efficiently implemented using a parallel algorithm within TC^0 complexity (TC^0 is required to perform bracket matching). Also note that the above construction does not depend on the modulus p. Therefore, by reduction we obtain that the problem of evaluating arithmetic expressions is NC^1 -hard. \square

F System of Linear Equations

In this section, we will prove that the autoregressive Transformer equipped with CoT can solve a system of linear equations, whereas the autoregressive Transformer without CoT cannot solve it.

F.1 Proof of Theorem 3.4

For ease of reading, we restate Theorem 3.3 below:

Theorem F.1. For any prime p and integer m > 0, there exists an autoregressive Transformer defined in Section 2 with hidden size $d = O(\operatorname{poly}(p))$ (independent of m), depth L = 5, and 5 heads in each layer that can generate the CoT solution defined in Appendix C for all inputs in Equation(m, p). Moreover, all parameter values in the Transformer are bounded by $O(\operatorname{poly}(m))$.

Proof. The proof technique is similar to that of Theorem 3.3. We recommend readers to read the proof Theorem 3.3 first as we will omit redundant details in the subsequent proof.

Token Embeddings. Assume that we have a sequence of tokens s_1, s_2, \ldots, s_t and we want to generate the next token s_{t+1} . We can embed the token s_i using the format $\mathbf{v}_i^0 = (\mathbf{e}_i, \mathbf{l}_i, i, i^2, 1)$:

1. The vector e_i represents the *i*-th token in the vocabulary using a one-hot encoding. However, since the number of variable tokens is m (which is unbounded), we consider representing

them using a unified (single) encoding and distinguishing them via the term l_i . This means that if s_i and s_j are two different variables, we have $e_i = e_j$ and $l_i \neq l_j$.

- 2. $l_i \in \mathbb{R}^3$ is a vector used to distinguish between different variables. Its first element, denoted as k_i , represents the index of a variable. If the token s_i is not a variable, then $l_i = (0,0,0)$ and $k_i = 0$. If it is the variable x_{k_i} ($k_i \in [m]$), then $l_i = (k_i, m^2 \sin(\frac{2k_i \pi}{m}), m^2 \cos(\frac{2k_i \pi}{m}))$.
- 3. i and i^2 are the position embeddings and represent the position of the token in the sequence.
- 4. The constant embedding 1 is used as a bias term.

Layer 1. The first layer of the autoregressive Transformer uses five attention heads to perform the following tasks:

- 1. Count the number of ';' (i.e., equations) in previous tokens, denoted as n_i^{eq} .
- 2. Count the number of \Longrightarrow in previous tokens, denoted as n_i^{cot} .
- 3. Determine the number of variables by copying k_j such that $r_j = 5k_jm^3 + j$ is the largest. Denote the result as n_i^{var} .
- 4. Get the largest position $j \le i$ such that s_j is either the token ';' or the token \Longrightarrow . Denote the result as $p_i^{\rm eq}$.
- 5. COPY the embedding e_{i-1} of the i-1-th token.

According to previous lemmas in Appendices D.1 and D.2, the first two attention heads of the autoregressive Transformer perform the MEAN operation to obtain the fraction of ';' and \Longrightarrow tokens in the previous tokens. The last three attention heads perform the COPY operation to copy the embedding k_j with the largest $r_j = k_j m^3 + j$, the position embedding j satisfying s_j is either ';' or \Longrightarrow , and the embedding e_{i-1} of the (i-1)-th token. The output of the attention layer is given by $(e_i, l_i, i, 1, n_i^{\rm eq}/i, n_i^{\rm cot}/i, n_i^{\rm var}, p_i^{\rm eq}, e_{i-1})$. We then use the MLP to calculate $n_i^{\rm eq}$ and $n_i^{\rm cot}$. Therefore, the output of the first layer is

$$(e_i, l_i, i, i^2, 1, n_i^{eq}, n_i^{cot}, n_i^{var}, p_i^{eq}, e_{i-1}).$$

Layer 2. As described in Appendix C, each CoT step corresponds to eliminating one variable and at the current position we are eliminating variable $x_{n_i^{\rm cot}}$. By the uniqueness of the solution, there must exist an equation with a nonzero coefficient for variable $x_{n_i^{\rm cot}}$. In the second Transformerlayer, we can determine which equation satisfies this condition. We also utilize the additional attention heads to perform some auxiliary calculations that will be used in subsequent layers. Precisely, the second layer utilizes four attention heads to perform the following three tasks:

- 1. COPY the embedding e_{j-1} and k_j at position j such that s_j is a variable with nonzero coefficient, $n_i^{\text{eq}} = n_j^{\text{eq}}$, and k_j is the smallest, which we denote as e'.
- 2. COPY the embedding $n_j^{\rm eq}$ of the nearest \Longrightarrow token and compute $d_i^{\rm eq}=n_i^{\rm eq}-n_j^{\rm eq}$, which corresponds to the index the current equation in the current CoT step.
- 3. COPY the embedding e_{i-k} of the (i-2)-th token and (i-3)-th token.

Using the same technique as in Appendix E.1, we can construct these attention heads to perform the tasks according to Lemma D.7. Then we pass the embedding through an MLP and compute a Boolean tag (denoted as tag_i), which is 1 only when $s_i = \text{`='}$, e' represents a number, and $k_j = n_i^{\text{cot}}$. We also use multiplication to compute some auxiliary quantities. The output of the MLP is

$$(e_i, l_i, i, i^2, 1, n_i^{\text{eq}}, (n_i^{\text{eq}})^2, n_i^{\text{cot}}, (n_i^{\text{cot}})^2, n_i^{\text{var}}, p^{\text{eq}}, d_i^{\text{eq}}, \text{tag}_i, e_{i-1}, e_{i-2}, e_{i-3}).$$

Layer 3. The third layer of the autoregressive Transformer uses one attention head to perform the following tasks:

- 1. COPY the embedding n_j^{eq} of token s_j satisfying that $\tan g_j = 1$, $n_j^{\text{cot}} = n_i^{\text{cot}} 1$, and has the smallest position embedding j, which we denote as n_i^{eq} .
- 2. Determine whether the output of the next token is a number. Denote the result as flag_i.
- 3. Determine the output of the next token if the next token is not a number. We denote its embedding as e_i^{next} .

4. Determine the variable index k'_i of the next token if the next token is variable.

We can perform COPY operation to complete the first task. Whether the output of the next token is a number can be purely determined by the previous token. Whether the output of the next token is a variable can also be purely determined by the previous token. When the next token is neither a variable nor a number (i.e., the symbols '+', '=', ';', or '==', we can determine the token by checking three tokens before it. When outputting a variable, we can also determine its index by checking three tokens before it. The output of this layer has the form

$$(e_i, l_i, i, i^2, 1, n_i^{\text{eq}}, (n_i^{\text{eq}})^2, n_i^{\text{cot}}, (n_i^{\text{cot}})^2, n_i^{\text{var}}, n_i^{\text{eq}}, \text{flag}_i, e_i^{\text{next}}, k_i', e_{i-1}).$$

Layer 4. The fourth layer of the autoregressive Transformer uses one attention head to perform the following tasks:

- 1. COPY the 3-dimensional embedding l_j for any j such that s_j is the variable $x_{k'_i}$. Denote the embedding as l'_i .
- 2. Do the preparation work for the next layer to perform the COPY operation.

The output of this layer is

$$(n_i^{\text{eq}}, (n_i^{\text{eq}} - n^{\text{var}})^2, n_i^{\text{eq'}}, (n_i^{\text{eq'}})^2, n_i^{\text{cot}}, (n_i^{\text{cot}})^2, k_i', (k_i')^2, n_i^{\text{var}}, e_i^{\text{next}}, l_i', l_i, e_{i-1}, 1).$$

Layer 5. The fifth layer of the autoregressive Transformer utilizes four attention heads to perform the following tasks:

- 1. COPY four coefficients that will be needed to calculate the next coefficient.
- 2. Filter the embedding to get the output.

We only need to copy the embedding in e_{j-1} for position j satisfying the following conditions:

- 1. $n_i^{\text{cot}} = n_i^{\text{cot}} + 1$
- 2. $n_i^{\text{cot}} = k_j \text{ or } k_i' = k_j$
- 3. $n_i^{\text{eq}} n_i^{\text{var}} = n_i^{\text{eq}} \text{ or } n_i^{\text{eq}} = n_i^{\text{eq}}$

It is easy to see that there are four positions j that satisfies the above conditions. We can use the four coefficients to calculate the number embedding of this token using an MLP (based on Lemma D.5), meanwhile using the MLP to filter useless embeddings and get the final output $(e_i^{\text{out}}, l_i^{\text{out}})$.

Finally, we pass it through a softmax layer to get the next token s_{i+1} .

Note that, we can tolerate O(1) (at most 0.5) error of the output of the fifth layer and the ℓ_{∞} norm embedding of the inner layer is bounded by O(poly(m)). So according to the previous lemma, the weight norm of the Transformer constructed in this proof is bounded by O(poly(m)).

F.2 Proof of Theorem 3.2

We will now prove that solving a system of linear equations without CoT is extremely difficult for bounded-depth autoregressive Transformer.

Theorem F.2. Assume $TC^0 \neq NC^1$. For any prime number p, any integer L, and any polynomial Q, there exists a problem size m such that no log-precision autoregressive Transformer defined in Section 2 with depth L and hidden dimension $d \leq Q(m)$ can solve the problem Equation(m, p).

Proof. Our proof is based on leveraging the NC^1 -completeness of a classic problem: Unsolvable Automaton Membership Testing. According to Barrington's theorem [3, 4], given a fixed unsolvable automaton, judging whether the automaton accepts an input is complete in NC^1 . Below, we will prove that solving the system of linear equations is NC^1 -hard by demonstrating that the Unsolvable Automaton Membership Testing problem is NC^0 reducible to the problem of solving a system of linear equations. This will yield the conclusion since bounded-depth log-precision Transformers with polynomial size are in TC^0 [36].

Let $D = (\mathcal{Q}, \Sigma, \delta, \mathcal{F}, q_0)$ be any automaton, where \mathcal{Q} is a set of states, Σ is a set of symbols (alphabet), $\delta : \mathcal{Q} \times \Sigma \to \mathcal{Q}$ is the transition function, $F \subset \mathcal{F}$ is a set of accept states, and q_0 is the initial state.

For any input string $\omega_1\omega_2\cdots\omega_n$, whether D accepts the string can be reduced into solving a system of linear equations defined as follows. The system of linear equations has $(n+1)|\mathcal{Q}|+1$ variables, which we denote as x^* and $x_{i,q}$ ($i\in\{0,\cdots,n\}, q\in\mathcal{Q}$). The equations are defined as follows:

$$\begin{cases} x^* = \sum_{q \in \mathcal{F}} x_{n,q} \\ x_{0,q_0} = 1 \\ x_{0,q} = 0 & \text{for } q \in \mathcal{Q} \backslash \{q_0\} \\ x_{i,q} = \sum_{\delta(r,\omega_i) = q} x_{i-1,r} & \text{for } 0 < i \leq n, q \in \mathcal{Q} \end{cases}$$

It is easy to see that $x_{i,q} = 1$ iff the automaton arrives at state q when taking the substring $\omega_1 \omega_2 \cdots \omega_i$ as input. Therefore, $x^* = 1$ iff the automaton accepts the input string. Note that the above solution does not depend on the modulus p, and the solution of these equations always exists and is unique.

Furthermore, the coefficient of each equation only depends on at most one input symbol. This implies that these equations can be efficiently constructed using a highly parallelizable algorithm within a complexity of NC^0 . Therefore, by reduction we obtain that the problem of judging whether there exists a solution such that $x^* = 1$ is NC^1 -hard.

Now consider solving linear equations using a Transformer Without CoT. While the output of the Transformer contains multiple tokens, we can arrange the order of variables such that the Transformer has to output the value of x^* first. The computation complexity of outputting the first token is bounded by TC^0 according to [36]. Therefore, it cannot judge whether there exists a solution satisfying $x^* = 0$.

G Dynamic Programming

G.1 Examples

Longest Increasing Subsequence (LIS). The LIS problem aims to compute the length of the longest increasing subsequence given an input sequence $s \in \mathbb{N}^n$. Formally, \tilde{s} is a subsequence of s if there exists indices $1 \le i_1 \le i_2 \le \cdots \le i_{|\tilde{s}|} \le n$ such that $\tilde{s}_k = s_{i_k}$ holds for all $k \in [|\tilde{s}|]$. A sequence \tilde{s} is called increasing if $\tilde{s}_1 < \tilde{s}_2 < \cdots < s_{|\tilde{s}|}$. The LIS problem aims to find an increasing subsequence of s with maximal length. A standard DP solution is to compute the length of the longest increasing subsequence that ends at each position i, which we denote as dp(i). It is easy to write the transition function as follows:

$$dp(i) = 1 + \max_{j < i, s_j < s_k} dp(j). \tag{10}$$

The final answer will be $\max_{i \in [n]} dp(i)$.

However, the above DP transition function does not match the form of (5), since dp(i) may depend on (an unbounded number of) all previous dp(j) (j < i). Nevertheless, this issue can be easily addressed using a different DP formulation. Let dp(j,k) be the longest increasing subsequence that ends at position j and the second last position is no more than k (k < j). In this case, it is easy to write the transition function as follows:

unction as follows:
$$dp(j,k) = \begin{cases} 1 & \text{if } k = 0\\ \max(dp(j,k-1), dp(k,k-1) \cdot \mathbb{I}[s_j > s_k] + 1) & \text{if } k > 0 \end{cases}$$
 (11)

The final answer will be $\max_{i \in [n]} dp(i, i - 1)$. This DP formulation fits our framework (5).

Edit Distance (ED). The ED problem aims to find the minimum operation cost that is required to convert a sequence $u \in \Sigma^{n_1}$ to another sequence $v \in \Sigma^{n_2}$. There are three types of operations: inserting a letter into any position, deleting a letter from any position, and replacing a letter at any position by a new one. The costs of insert, delete, and replace are a, b, and c, respectively. These operations are sequentially executed and the total operation cost is the summation of all costs of individual operations.

A standard DP solution is to compute the minimum operation cost to convert the substring $u_1u_2\cdots u_j$ to the substring $v_1v_2\cdots v_k$, which we denote as dp(j,k). It is easy to write the transition function as follows:

$$\mathsf{dp}(j,k) = \begin{cases} ak & \text{if } j = 0 \\ bj & \text{if } k = 0 \\ \min(\mathsf{dp}(j,k-1) + a, \mathsf{dp}(j-1,k) + b, \mathsf{dp}(j-1,k-1) + c\mathbb{I}[s_j^{(1)} \neq s_k^{(2)}]) & \text{otherwise} \end{cases}$$

The final answer will be $dp(n_1, n_2)$. This DP formulation fits our framework (5).

CFG Membership Testing. A context-free grammar (CFG) is a 4-tuple $G = (V, \Sigma, R, S)$, where:

- V is a finite set of non-terminal symbols.
- Σ is a finite set of terminal symbols, disjoint from V.
- R is a finite set of production rules, where each rule has the form $A \to \beta$, with $A \in V$ and $\beta \in (V \cup \Sigma)^*$.
- S is the start symbol, with $S \in V$.

The non-terminal symbols in V represent syntactic categories or parts of speech, while the terminal symbols in Σ represent the actual words or tokens in the language. The production rules in R specify how the non-terminal symbols can be replaced by sequences of terminal and non-terminal symbols.

Chomsky Normal Form (CNF) [49] is a formal representation of context-free grammar introduced by linguist Noam Chomsky. It has only three types of production rules: $A \to BC$, where non-terminal A can be replaced by a combination of non-terminals B and C, $A \to a$, where non-terminal A can be replaced by a terminal a, and $S \to \epsilon$, if ϵ is in L(G). Any context-free grammar can be transformed into a CNF grammar expressing the same language. Therefore, we only need to consider the CFG in Chomsky Normal Form. Moreover, for the rule $R[i]: s_1 \to s_2$, we denote $s_1 = \operatorname{left}(R[i])$, $s_2 = \operatorname{right}(R[i])$.

CFG Membership Testing problem is a fundamental problem, which is defined as follows: given CFG G, judge whether a string can be generated from G. The CYK algorithm [47] has a classic algorithm of $\mathcal{O}(N^3)$ complexity to solve the CFG Membership Testing problem. We can use our framework to rewrite the algorithm. Given a string \mathbf{v} , $n = |\mathbf{v}|$. The state space $\mathcal{S} = \{(i, j, k, l) : 1 \le i \le k \le j \le n, l \in [|R|]\}$. dp(i, j, k, l) means whether $\mathbf{v}[i:j]$ can be generated by the nonterminal left(R[l]) with first use the rule R[l'], l' < l to process left(R[l]) and string generated from left(R[l])[0] are at most k - i + 1.

$$\mathsf{dp}(i,j,k,l) = \left\{ \begin{array}{l} \mathbb{I}[\boldsymbol{v}[i] = \mathrm{right}(R[l])], \ i = j = k \\ \max(\mathsf{dp}(i,k,k,l_1) \cdot \mathsf{dp}(k,j,l_2), \mathsf{dp}(i,j,k-1,l), \mathsf{dp}(i,j,l')), \text{ otherwise }, \end{array} \right.$$

where l' is the largest number such that l' < l and left(R[l]) = left(R[l']). And the aggregation function is $dp(1, n, n, l^*)$, where $left(R[l^*]) = S$ and l^* is unique according to CNF.

It can be easily verified that the state spaces of the three problems mentioned above are at most polynomial size, satisfying the assumption stated in Assumption 4.2. Additionally, the MLP with the Rectified Linear Unit (ReLU) activation function can implement the functions

- 1. $\max(a, b), a, b \in \mathbb{R}$
- 2. $\mathbb{I}(a \neq b), a, b \in \mathbb{Z}$
- 3. $\mathbb{I}(a < b), a, b \in \mathbb{Z}$
- 4. $a \times b$ where $a \in \mathbb{R}b \in \{0, 1\}$

This implies that the MLP with ReLU activation can approximate all the functions specified in Assumptions 4.3 and 4.5 and ??. According to Lemma D.2, these functions can be efficiently approximated by a perceptron of constant size with Gaussian Error Linear Units (GeLU) activation. Therefore, all three problems can be solved by a transformer with CoT.

G.2 Proof of Theorem 4.7

In this subsection, we will give proof of the Theorem 4.7.

Theorem G.1. Consider any DP problem that satisfies Assumptions 4.2, 4.3 and 4.5 and ??. For any integer $n \in \mathbb{N}$ and $\epsilon > 0$, there exists an autoregressive Transformer with constant depth L, hidden dimension d and attention heads H (independent of n or ϵ), such that the answer generated by the Transformer can be arbitrary close to the ground truth for all input sequences s of length no more than n, with error uniformly bounded by ϵ . Moreover, all parameter values are bounded by $O(\operatorname{poly}(n, 1/\epsilon))$.

Proof. Input Format. Assume that we have a sequence of tokens s_1, \dots, s_t and we want to generate the next token s_{t+1} . We can embed the token s_k using the format

$$[e_k^{\text{type}}, e_k^{\text{input}}, e_k^{\text{state}}, e_k^{\text{dp}}, e_k^{\text{answer}}, e_k^{\text{aux}}, k, 1],$$

 $[e_k^{\rm type},e_k^{\rm input},e_k^{\rm state},e_k^{\rm dp},e_k^{\rm answer},e_k^{\rm aux},k,1],$ where $e_k^{\rm type}$ indicates the type of the token s_k and $e_k^{\rm input},e_k^{\rm state},e_k^{\rm dp},e_k^{\rm answer},e_k^{\rm aux}$ represent the embeddings of the input, states, values in the DP array, answers, and some special signs respectively. Moreover, we use a one-hot vector $e_k^{\rm aux}$ to embed the auxiliary signs such as the separators. The position embedding k indicates the index of the token within the sequence.

Layer 1. The first block of the autoregressive transformer containing several layers uses N attention heads and the MLP to perform the following tasks:

- Copy the position embedding of the N separating signs $p_k^{\text{sep1}}, \cdots, p_k^{\text{sepN}}$.
- Use the MLP to calculate the problem scale $\mathbf{N} = (p_k^{\text{sep1}}, p_k^{\text{sep2}} p_k^{\text{sep1}}, \cdots, p_k^{\text{sepN}} p_k^{\text{sep(N-1)}}).$
- Use the MLP to obtain the next state i_k^{Next} .

In the first layer, the attention layer copies the position embedding of the special signs. This can be simply done by the lemma. According to the assumption, we can use an MLP to convert the current state i_k to the next state i_k^{Next} . It is a key observation that we can use l transformer layers to implement a *l*-layer MLP. We just let the attention layers do nothing but maintain the input using the residual connection. Then we can simply stack l two-layer perceptrons and use them to implement the l-layer MLP. Because the state transition may need a multiple-layer perceptron. We can use the rest layers of the first block to implement a multilayer perceptron. Therefore, the output of this block is

$$(e_k^{ ext{type}}, e_k^{ ext{input}}, e_k^{ ext{state}}, e_k^{ ext{Next state}}, e_k^{ ext{dp}}, e_k^{ ext{answer}}, e_k^{ ext{aux}}, \mathbf{N}_k, k, 1).$$

Layer 2. The second layer of the autoregressive transformer utilizes the MLP to perform the following

- Calculate $h(i_k^{\text{Next}})$ and $g(i_k^{\text{Next}})$.
- Judge if the current state is the final state and set the tag embedding t^{state}
- Judge if the current state is the final need to be aggregated for the final answer and set the tag embedding t^{answer} .

In the second block, the attention layer does nothing but maintains the output by the residual connection. And similar to the first block, we stack several two-layer perceptrons to implement a multilayer perceptron. According to the assumption, we can use an MLP to complete the three tasks. Denoting tag = $[t^{\text{state}}, t^{\text{answer}}]$, therefore, the output of this block is

$$(\boldsymbol{e}_k^{\text{type}},\boldsymbol{e}_k^{\text{input}},\boldsymbol{e}_k^{\text{state}},\boldsymbol{e}_k^{\text{Next state}},\boldsymbol{e}^{i_1},\cdots,\boldsymbol{e}^{i_K},\text{indx}_k^1,\cdots,\text{indx}_k^J,\boldsymbol{e}_k^{\text{dp}},\boldsymbol{e}_k^{\text{answer}},M,\text{tag}_k,k,1)$$

Layer 3. The third block of the autoregressive transformer containing only one transformer layer uses one (for the operation \max and \min) or two attention heads (for the operation \sum) and the MLP to perform the following tasks:

- Calculate the square of the indices and the states to prepare for the COPY operation.
- Aggregate the information of the dp array by now.

According to the previous lemmas, the first task can be simply done by the MLP. And for the second task, we use one attention head to simply copy the embedding with $t_{answer} = 1$ and the largest or smallest value in the dp array, which can implement the min, max operation. For the \sum operation, we can utilize two attention heads. One attention head can be used to compute the mean, while the other attention head can be used to calculate the fraction of elements in the sequence and then obtain the number. We denote the maximum, the minimum, or the summation as e_k^{agg} . Therefore, the output of this layer is

$$(e_k^{ ext{type}}, e_k^{ ext{input}}, e_k^{ ext{state}}, (e_k^{ ext{state}})^2, e_k^{ ext{Next state}}, e_k^{i_1}, (e_k^{i_1})^2, \cdots, e_k^{i_K}, (e_k^{i_K})^2, \\ ext{indx}_1, (ext{indx}_1)^2, \cdots, ext{indx}_J, (ext{indx}_J)^2, e_k^{dp}, e_k^{ ext{answer}}, ext{tag}_k, e_k^{ ext{agg}}, k, 1).$$

Layer 4. The fourth block of the autoregressive transformer utilizes K + J heads to perform the following tasks:

- Copy the embeddings $e_{dp_1}, \dots, e_{dp_K}$ of the values in dp array according to the states.
- Copy the embeddings $e_{\mathsf{input}_1}, \cdots, e_{\mathsf{input}_J}$ of the input sequence according to the indices.
- · Calculate the output.

We can use similar tricks when we prove the autoregressive transformer can calculate the arithmetic formulas in Appendix E.1 to copy the K+J embeddings. According to the assumptions, we can use the MLP to calculate the embedding of the $\operatorname{dp}(i_N)$ and the final answer, and we can set the embedding e_{type} . Therefore the output of this layer is

$$(oldsymbol{e}_k^{ ext{type}}, oldsymbol{e}_k^{ ext{input}}, oldsymbol{e}_k^{ ext{Next state}}, oldsymbol{e}_k^{ ext{Next dp}}, oldsymbol{e}_k^{ ext{answer}}, oldsymbol{e}_k^{ ext{aux}})$$

Then we add the new position embedding to the output of the transformer and add it to the sequence to generate the next embedding. \Box

G.3 Proof of the Theorem 4.8

Theorem G.2. Assume $TC^0 \neq P$. There exists a context-free language such that for any depth L and any polynomial Q, there exists a sequence length $n \in \mathbb{N}$ where no log-precision autoregressive transformer with depth L and hidden dimension $d \leq Q(n)$ can generate the correct answer for the CFG Membership Testing problem for all input strings of length n.

Proof. According to the previous work [28], the CFG Membership Testing problem is P-complete. With the assumption that $NC^1 \neq P$, the CFG Membership Testing problem is out of the capacity of the log-precision autoregressive transformer.

H Experimental Details

In this section, we present the experimental details.

H.1 Datasets

We set the number field p=11 in the math experiments. In the LIS experiment, we set the number of different input tokens to 150; in the ED experiment, we set the number of different input tokens to 26. The vocabulary is constructed by including all symbols. For all tasks and settings (direct v.s. CoT), the size of the training and testing dataset is 1M and 0.1M respectively. The constructions of different datasets are introduced below.

Arithmetic Expression. All arithmetic expression problems are generated according to Algorithm 1. In Algorithm 1, we first create a number that serves as the answer to the problem. We then decompose the number using sampled operators sequentially, serving as the problem, until the maximum number of operators is met. The CoT procedure is precisely defined by reversing this problem generation process. For example, a sample in the direct dataset looks like

$$1 + 5 \times (1 - 2) = 7$$

while the corresponding sample in the CoT data looks like

$$1+5 \times (1-2) = 1+5 \times 10 = 1+6=7$$

Linear Equation. All linear equation problems are generated according to algorithm 2. In Algorithm 2, we consider the linear systems that only have a unique solution. Given a sampled linear system that satisfies this condition, we "translate" it to a sequence by concatenating all the equations (separated by commas), which serves as the problem. The answer to the problem is also a sequence consisting of variables and the corresponding values. The CoT solution of each problem is the calculation process of the Gaussian elimination algorithm applied to each variable sequentially. For example, a sample in the direct dataset looks like

$$2x_1 + 3x_2 + 3x_3 = 8$$
, $1x_1 + 7x_2 + 0x_3 = 0$, $0x_1 + 2x_2 + 1x_3 = 1$, [SEP] $x_1 = 4$, $x_2 = 1$, $x_3 = 10$,

Algorithm 1: Arithmetic Expression Problem Generation

```
Input: Number of Operators n
   Input: Vocabulary of numbers V = \{0, 1...10\} / / number field p = 11
   Output: Arithmetic expression s
 1 Sample the first number t uniformly from V;
2 s = [];
3 Append t to s;
4 for i \leftarrow 1 to n do
       Sample p uniformly from \{0, 1, ..., len(s) - 1\}, satisfying s[p] is a number;
       Sample o uniformly from \{+, -, \times, \div\};
       Sample numbers t_1, t_2, satisfying the result of o(t_1, t_2) equals s[p];
7
       if s[p-1] = \div or (o \in \{+, -\} and s[p-1] \in \{-, \times\}) or (o \in \{+, -\} and
8
        s[p+1] \in \{\times, \div\}) then
          pop s[p];
insert [(], [t_1], [o], [t_2], [)] sequentially into s[p];
 9
10
       else
11
           pop s[p];
12
           insert [t_1], [o], [t_2] sequentially into s[p];
13
       end
14
15 end
```

while the corresponding sample in the CoT dataset looks like

```
2x_1 + 3x_2 + 3x_3 = 8, 1x_1 + 7x_2 + 0x_3 = 0, 0x_1 + 2x_2 + 1x_3 = 1, [SEP] x_1 + 7x_2 + 7x_3 = 4, 0x_2 + 4x_3 = 7, 2x_2 + 1x_3 = 1, [SEP] x_1 + 9x_3 = 6, x_2 + 6x_3 = 6, 4x_3 = 7, [SEP] x_1 = 4, x_2 = 1, x_3 = 10,
```

Algorithm 2: Linear Equation Data Generation

```
Input :Number of Variable n
Input :Vocabulary of numbers V = \{0, 1...10\} / / number field p = 11
Output:Linear Equation s
1 Sample b uniformly from V^{n \times 1};
2 do
3 | Sample A uniformly from V^{n \times n};
4 while A is not invertible;
5 s \leftarrow "A_{11}x_1 + ... + A_{1n}x_n = b_1, ..., A_{n1}x_1 + ... + A_{nn}x_n = b_n"
```

Longest Increasing Subsequence. All input sequences (i.e., problems) are generated according to Algorithm 3. To make the task challenging enough, we first concatenate several increasing subsequences of given length, and then randomly insert numbers into the whole sequence. The CoT solution of the problem is exactly the DP array, which is defined in Section 4.1. The inputs has 150 different tokens, ranging from 101 to 250 to avoid token overlap with dp array. For example, a sample in the direct dataset looks like

```
103 107 109 112 101 103 105 107 115 109 111 113 102 [SEP] 7
```

while the corresponding sample in the CoT dataset looks like

```
103 107 109 112 101 103 105 107 115 109 111 113 102

[SEP] 1 2 3 4 1 2 3 4 5 5 6 7 2

[SEP] 7
```

Algorithm 3: LIS Data Generation

```
Input : Sequence Length n
  Input : Vocabulary of numbers V = \{101, 101...250\}
  Output : Sequence s
1 Sample l uniformly from \{3, 4...n\};
2 Sample t uniformly from \{1, 2, 3\};
a = [];
4 push 0 to a;
5 if t=2 then
      Sample j uniformly from \{1, 2... | l/2| + 1\};
      push j to a;
s else if t=3 then
      Sample j uniformly from \{1, 2... | l/3| + 1\};
      Sample k uniformly from \{1, 2... | (l-j)/2 | + 1 \};
10
      push i to a:
11
      push j + k to a;
13 push l to a;
14 s \leftarrow \text{Sample } l \text{ numbers from } V;
15 for i \leftarrow 1 to t do
      Sort s[a[i-1]:a[i]];// This process makes sure the LIS of the generated
           sequence s is at least \lceil l/t \rceil.
17 end
18 r \leftarrow \text{Sample } n - l \text{ numbers from } V;
19 Randomly insert r into s;
```

Edit Distance. All input sequences (i.e., problems) are generated according to Algorithm 4. In Algorithm 4, we generate the first string randomly. For the generation of the second string, we use two methods. In the first method, we generate the second string randomly, corresponding to a large edit distance. In the second method, we copy the first string with random corruption, corresponding to a small edit distance. The two strings are concatenated by "|", and the concatenation is used as the model input. For the calculation of edit distance, we assign different costs to different operators. The costs for the ADD and DELETE operators are set to 2, while the Substitute operator is assigned a cost of 3. The CoT procedure is also the DP array, defined in Section 4.1. For example, a sample in the direct dataset looks like

while the corresponding sample in the CoT dataset looks like

Algorithm 4: ED Data Generation

```
Input: Length of the First String n
   Input :Alphabet V = \{a, b...z\}
   Output : Sequence s_1, s_2
1 Sample t uniformly from \{3, 4...10\};
2 T \leftarrow \text{Sample } t \text{ letters from } V;
3 s_1 \leftarrow \text{Sample } n \text{ letters uniformly from } T;
4 Sample p uniformly from [0, 1];
5 if p < 0.4 then
       Sample l uniformly from \{n-3, n-2, ..., n+2\};
       s_2 \leftarrow \text{Sample } l \text{ letters uniformly from } T;
7
8 else
9
       do
10
            s_2 \leftarrow s_1;
           for i \leftarrow 1 to n do
11
                Sample p uniformly from \{0, 1...len(s_2) - 1\};
12
                Sample l uniformly from T;
13
                Randomly conduct one of the followings: pop s_2[p], substitute s_2[p] with l, insert l
14
                 into s_2[p];
15
       while len(s_2) not in [n-3, n+2];
16
17 end
```

H.2 Model training

We use the minGPT implementation⁴ for all the experiments, where the detailed Transformer layer are listed below.

$$\boldsymbol{X}^{(0)} = \text{LayerNorm}\left(\left[\boldsymbol{v}_1 + \boldsymbol{p}_1, \cdots, \boldsymbol{v}_n + \boldsymbol{p}_n\right]^{\top}\right)$$
(13)

$$\operatorname{Attn}^{(l)}(\boldsymbol{X}) = \sum_{h=1}^{H} \left(\operatorname{softmax} \left(\boldsymbol{X} \boldsymbol{W}_{Q}^{(l,h)} (\boldsymbol{X} \boldsymbol{W}_{K}^{(l,h)})^{\top} / \sqrt{d} + \boldsymbol{M} \right) \right) \boldsymbol{X} \boldsymbol{W}_{V}^{(l,h)} \boldsymbol{W}_{Q}^{(l,h)}$$
(14)

$$FFN^{(l)}(\boldsymbol{X}) = \sigma(\boldsymbol{X}\boldsymbol{W}_{1}^{(l)})\boldsymbol{W}_{2}^{(l)}$$
(15)

$$\boldsymbol{Y}^{(l-1)} = \boldsymbol{X}^{(l-1)} + \operatorname{Attn}^{(l)}(\operatorname{LayerNorm}(\boldsymbol{X}^{(l-1)}))$$
(16)

$$\boldsymbol{X}^{(l)} = \boldsymbol{Y}^{(l-1)} + \text{FFN}^{(l)}(\text{LayerNorm}(\boldsymbol{Y}^{(l-1)}))$$
(17)

We use sinusoidal positional embedding and use Xavier initialization for all the parameters. The activation function is chosen to be GeLU. The dimension of the embedding is set to 256, and the number of heads is set to 4. The hidden size in the FFN layer is set to 1024.

We use the same hyperparameter configuration for all experiments, i.e., the performance comparison between the models trained on the direct and CoT datasets of Arithmetic, Equation, LIS, and ED tasks, and the additional length extrapolation experiments (which we use relative positional encodings [42] instead of absolute positional encodings). In detail, we use AdamW optimizer with β_1 , β_2 = 0.9, 0.999. The learning rate is set to 1e-4, and the weight decay is set to 0.01. We set the batch size to 512 during training with a linear learning rate decay scheduler. We use learning rate warm-up, and the warm-up stage is set to 5 epochs. The total number of training epochs is set to 100.

⁴https://github.com/karpathy/minGPT