# On the Empirical Complexity of Reasoning and Planning in LLMs

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### Abstract

001 Large Language Models (LLMs) work surprisingly well for some complex reasoning 003 problems via chain-of-thought (CoT) or treeof-thought (ToT), but the underlying reasons remain unclear. We seek to understand the performance of these methods by conducting experimental case studies and linking the out-007 800 comes to sample and computational complexity in machine learning. We found that if problems can be decomposed into a sequence of reason-011 ing steps and learning to predict the next step has a low sample and computational complexity, explicitly outlining the reasoning chain with all necessary information for predicting the next step may improve performance. Conversely, for problems where predicting the next step is computationally hard, adopting ToT may yield better reasoning outcomes than attempting to formulate a short reasoning chain. 019

### 1 Introduction

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Reasoning and planning tasks are often challenging due to their inherently multi-step processes. Recently, large language models (LLMs) showed surprising results on reasoning problems when they were asked to explain their reasoning step-by-step through a chain of thought (CoT) (Wei et al., 2022) before providing their answers. This was followed by improvements through the use of search algorithms in the tree-of-thought (ToT) (Yao et al., 2023; Xie et al., 2023).

Despite these advancements, the conditions for the effectiveness of chain-of-thought and tree-ofthought methods remain unclear. For example, CoT has been very successful in solving grade school math problems, but in the Game of 24, where four numbers need to be manipulated with arithmetic operations to obtain the number 24, CoT provides a solution with a short reasoning chain and fails badly, whereas ToT works reasonably well (Yao et al., 2023) (see Fig 1 for CoT and ToT representation of the Game of 24).

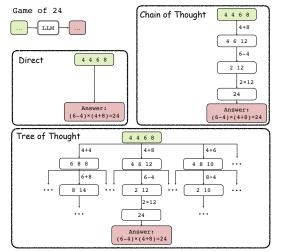


Figure 1: An illustration of LLM reasoning methods on the Game of 24. Give four poker cards, the player combines the cards using basic arithmetic operations,  $(+, -, \times, \div)$ , to reach the target number of 24.

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We investigate reasoning and planning problems in the context of natural language processing. A reasoning problem entails deducing the answer to a question from provided evidence and applicable reasoning rules. It often requires applying various rules multiple times to connect different pieces of evidence. Planning, a subset of reasoning, requires an action sequence to achieve a desired goal state from a current state. This involves considering available actions and transition functions, which estimate the resultant state from a current state and action. Planning often requires reasoning over a long time horizon, making it computationally harder to solve.

In this paper, we investigate when and why CoT and ToT are effective in reasoning and planning problems from the viewpoint of sample complexity, computational complexity of learning, and computational complexity of reasoning. Sample complexity measures how much data is required for learning. If a learning problem is less complex, as measured by the number of parameters or description length, it correspondingly requires less training data (Shalev-Shwartz and Ben-David, 2014). This motivates us to analyse the sample complexity of decomposing a problem into multiple steps. Furthermore, learning may become computationally intractable if the values of hidden variables are not observed during learning (Aloise et al., 2009; Blum and Rivest, 1988), motivating us to consider the presence of hidden variables during learning of chain-of-thought. Finally, for reasoning and planning problems that are computationally hard to solve, e.g. NP-hard problems, it is unlikely that a small predictor producing a short chain of thought that can solve the problem that exists in the worst case. This motivates the use of more complex thought structures, e.g., a search tree.

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We empirically study these issues through four case studies on grade school mathematics (Cobbe et al., 2021), a simple dynamic programming problem (Dziri et al., 2023), air travel planning (Zhao et al., 2023), and Game of 24 (Yao et al., 2023). Common grade school maths problems and the dynamic programming problem we consider have computationally efficient reasoning components. Air travel planning has two different efficient solutions that we compare. Finally, the Game of 24 appears to be computationally difficult.

We study the problems under different settings, including using pre-trained models, fine-tuning, and in-context learning. Our main findings are consistent over the different settings and can be summarized as follows:

- *CoT and ToT can enhance LLM reasoning by lowering the sample complexity through decomposing a problem.* In all four cases, decomposition by a chain or tree structure reduces sample complexity and improves performance. In air travel planning, the decomposition with smaller sample complexity performs better.
- Explicitly annotating all necessary information in predicting the next step can improve CoT performance. In the dynamic programming problem, we show that explicitly demonstrating the relevant variables helps to improve chainof-thought reasoning further.
- When finding a short chain solution is computationally hard, a tree structure may be helpful. For tasks like Game of 24, finding a short-chain solution is likely computationally hard, and the tree of thought works substantially better.

These findings suggest a few guiding principles for using LLM to solve reasoning and planning tasks in practice: 1) if simple decomposed problem representations can be found, consider using CoT or ToT, 2) explicitly annotate information required for next-step prediction in the prompts, and 3) use the chain of thought to solve problems in which finding a short chain solution is computationally efficient, otherwise, consider using the tree of thought.

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### 2 Related Works

LLMs have shown significant progress in tackling reasoning and planning problems. Initial studies (Wei et al., 2022; Wang et al., 2022; Kojima et al., 2022; Chen et al., 2022; Gao et al., 2023) unveiled various prompting techniques that enable LLMs to demonstrate reasoning processes step by step, thereby substantially boosting their reasoning abilities. This approach has been swiftly adapted to address everyday planning issues (Huang et al., 2022a,b; Ahn et al., 2022; Song et al., 2023; Wang et al., 2023; Singh et al., 2023). Subsequent research has integrated LLMs with diverse search algorithms, further enhancing their capability to solve complex reasoning and planning challenges (Zhang et al., 2023; Yao et al., 2023; Zhao et al., 2023; Xie et al., 2023; Ding et al., 2023; Feng et al., 2023; Hao et al., 2023; Liu et al., 2023). Nonetheless, a systematic exploration of the conditions under which these methodologies excel or falter is lacking. Our work delves into the empirical principles guiding LLM behaviour across different reasoning frameworks, offering insights into selecting appropriate reasoning strategies for varied task types. While similar efforts (Zhao et al., 2023) have discussed different methods' sample complexity for solving planning problems, they overlook computational implications. One recent study (Dziri et al., 2023) discussed the Chain-of-thought's limitation of compositional reasoning, but they lack a systematic discussion on how to decide the right structure for assembling the reasoning steps. Our research systematically discusses LLM's capability from the sample complexity and the computational complexity of learning and reasoning.

### **3** Preliminaries

### 3.1 Sample and Computational Complexity

We are interested in learning predictors, which take an input, e.g., a sequence of words, and produce a prediction, e.g. a label that may be used directly or as a component of a larger reasoning process. The predictors often have parameters that need to be learned, and for simplicity, we assume that the parameters are discretized with a finite discretization.

Instead of the number of parameters, we use a more 167 general notion of description length as a measure of 168 the complexity of a predictor, where the description 169 length is the number of bits required to describe 170 the learnable part of the predictor. Predictors with a small description length can be shown to require 172 less training data, i.e. a small sample complexity 173 (Shalev-Shwartz and Ben-David, 2014), in order to 174 achieve low generalization error. 175

Computational complexity is relevant in two ways in this paper: 1) in the amount of computation required for learning, e.g. finding the correct parameters in the predictor given the training data, and 2) in the amount of computation required for reasoning, e.g. finding the solution given a problem after learning.

### 3.2 LLM reasoning methods

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Many LLM reasoning methods have been proposed for performing reasoning using LLMs; we mainly study three representatives and their variants in this paper, namely **Direct**, Chain-of-thought (**CoT**), and Tree-of-thought (**ToT**).

**Direct** The Direct approach utilizes LLMs to solve reasoning tasks by prompting the model to provide immediate answers. This method may have a low sample complexity if the neural network architecture closely aligns with the reasoning algorithm (Xu et al., 2020), meaning a small predictor can effectively represent the algorithm. However, challenges arise when unobserved variables make learning computationally intractable (Aloise et al., 2009; Blum and Rivest, 1988), though overparameterization might ease learning difficulties (Allen-Zhu et al., 2019). Analyzing the alignment between the predictor and algorithm is complex, so we explore a tabular representation for simplicity. In problems with N variables, each taking K values, direct answers require learning a table of size  $K^N$ , which exponentially increases with more variables. Empirical observations in case studies assess whether the transformer architecture can learn the problem or if it resembles table-filling behaviour.

**CoT** The Chain-of-thought (Wei et al., 2022) 209 method engages LLMs in generating reasoning 210 steps before reaching a conclusion, either by demon-211 strating these steps in the prompt or by prompting 212 213 the model "Let's think step by step" (Kojima et al., 2022) at the end of the prompt. CoT often outper-214 forms the Direct approach in reasoning tasks by 215 decomposing problems into actionable components. 216 The LLM extracts or generates actions based on 217

language descriptions or world knowledge, applies these actions through a *prediction function* (i.e., *transition function* in planning) to get the next observations, and grounds variable values as needed. With A possible actions, each depending on  $a_i$ variables, the description length for these actions is proportional to  $\sum_{i=1}^{A} K^{a_i}$ . We also need a *policy* function predicting action to select based on observations with its description length of  $K^M$  if it depends on M variables. If the policy depends only on whether the variables have been observed rather than their values, then a binary table of size  $2^M$  is sufficient. We use the description length of transition functions and policies as indicators of the sample complexity for decomposed problems. 218

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ToT A tree-of-thought method combines LLMs with a search algorithm, structuring reasoning steps into a tree and selecting promising next steps by self-evaluation. It shows significant improvement in hard problems (Yao et al., 2023). Unlike CoT, ToT may not use a policy but relies on an evaluation function for decision-making and a goal recognizer for termination. The complexity of transition functions and the evaluation process in ToT is analyzed similarly to CoT. The computational complexity of solving (versus learning) a reasoning or planning problem becomes a key factor in choosing between CoT and ToT, especially since some problems, e.g. NP-complete problems, have verifiable solutions in polynomial time but are unlikely to have an efficient policy to find solutions. ToT, with its search algorithm, presents a viable solution approach for such hard problems.

We seek to understand the complexity of the problems in the case studies using simple representations. However, LLM learning uses the transformer architecture and is difficult to analyse. Furthermore, the effects of pre-training, which we do not control, are present throughout. Instead, we empirically observe whether the analysis reflects the practical behaviour of the LLMs and whether the insights from analysis are useful in practice, i.e. when analysis suggests that a particular method is preferred, whether it is indeed preferred empirically.

### 4 Case Studies<sup>1</sup>

### 4.1 Grade School Maths

GSM8K (Cobbe et al., 2021) consists of grade school math problems described in natural language. It is a real-world problem that LLMs solve very well

<sup>&</sup>lt;sup>1</sup>See Appendix A and E for experimental details and complete prompts.

with CoT (Achiam et al., 2023). We investigated a subset of 50 randomly selected problems and discovered that 49 of them can be solved with a chain-style algorithm where, at each step, an equation can be selected such that the values of all variables except one in the equation be known, allowing the value of the remaining variable to be inferred. The remaining problem that cannot be solved this way can be solved using simultaneous equations with two variables, but we ignore this type of problem in the remainder of this study.

### 4.1.1 Analysis

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**Direct** Consider a problem with *N* variables each can take *K* values. A tabular representation would require a table of size  $K^N$  and description length of  $O(K^N \log K)$  for each question type, assuming each answer also takes *K* possible values. In the GSM8K dataset, the variable values are usually limited to no more than 6 digits and the average number of variables per question is 3.93. Fig. 2a shows that both GPT-3.5 and GPT-4 do not achieve very high accuracy using Direct.

**CoT** For chain-of-thought (CoT), assuming A dif-289 290 ferent actions whose transition functions require  $a_i$ variables, the total description length of these oper-291 ations would be  $O(\sum_{i=1}^{A} K^{a_i} \log K)$ . In the dataset, 292 the average number of variables in a reasoning step is 2.19, so each step is relatively simple. From our analysis, the number of equations that need to be learned as world knowledge appears to be relatively 296 small (see Appendix B.1), and the average number of reasoning steps in the dataset is 3.17. To decide the next equation, we can select an equation where the values of all except one variable are known. There exists a linear time forward chaining algo-301 rithm, which we describe in the Appendix B.2, to 302 do that; this translates to a relatively small policy that needs to be learned. These components of the decomposed problems look relatively simple 305 and suggest that decomposition with CoT may be reasonable for this problem. However, the LLM 307 still needs to learn to extract the equations from the question, to learn those that do not appear in the question as world knowledge, and to ground the values of the variables from the previous observations. The LLMs, particularly GPT-4, do remarkably well 313 on GSM8K (see Fig. 2a), indicating that extraction and grounding may not be major hurdles for LLMs, 314 which have been trained on large amounts of data. 315 Some errors are still present and are discussed in the Appendix B.3. 317

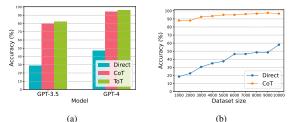


Figure 2: (a) Results of GPT-3.5 and GPT-4 on GSM8K Test set; (b) Fine-tuning results on Llama2-7b

**ToT** We run a beam search ToT, branching after each sentence on the choice of the next sentences suggested by the LLM. We prompt the same LLM to self-evaluate the quality of each proposed reasoning step. As discussed for CoT, there is a simple policy for deciding the next equation to solve, hence search may give limited improvement; this agrees with our experiments as shown in Fig. 2a. 318

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### 4.1.2 Fine-tuning Experiments

The GPT experiments suggest that LLMs have difficulties learning to solve GSM type questions directly. To check that, we do fine-tuning experiments with a simplified math word problem. We construct one template word problem with seven variables:

In a zoo, there are  $v_1$  giraffes. The number of penguins is  $v_2$  times the number of giraffes, and there are  $v_3$  times as many monkeys as giraffes. The zoo also has zebras, which are  $1/v_4$ , the number of penguins, and lions, which are  $1/v_5$ , the number of monkeys. If penguins, monkeys, lions, and zebras together make up  $v_6$ % of the zoo's total animal population, and elephants constitute  $v_7$ % of the total, find out how many elephants are there in the zoo.

Colored font indicates a variable, the problem is essentially solving one equation: elephant =  $(v_1v_2 + v_1v_3 + v_1v_3/v_5 + v_1v_2/v_4)v_7/v_6$ .

We randomly generate 10k configurations of the variables and perform supervised fine-tuning with Direct and CoT with varying amounts of data from 1k to 10k. The results are shown in Fig. 2b. Note that each CoT example provides substantially more information than each Direct example, but CoT is substantially better even when Direct is provided with 10 times more training examples (Direct at 10k vs CoT at 1k). This suggests that the transformer in the LLM is behaving more like a tabular predictor and is not able to learn to decompose the problem internally without being trained explicitly to do so.

### 4.2 Dynamic Programming

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We study another problem, the Maximum Weighted Independent Set problem (MWIS) (Kleinberg and Tardos, 2005): Given a sequence of integers, find a subsequence with maximum sum such that no two elements in the subsequence are adjacent in the original sequence. The problem can be solved in linear time using dynamic programming (see Appendix C.1). MWIS was studied in (Dziri et al., 2023), showing that LLMs trained on short sequences generalize poorly to longer sequences. In this paper, we focus on the amount of annotation provided in learning where only the answer is provided in Direct, whereas different levels of explicitness in annotation can be provided in CoT.

### 4.2.1 Analysis

**Direct** Consider a sequence with *N* integers; each may take *K* values. A tabular representation would have  $K^N$  entries, where each entry needs *N* bits to indicate the presence of the *N* number in the subsequence, giving a description length of  $O(NK^N)$ . **CoT** Using CoT (see Appendix E.2 for examples), we can see each reasoning step as applying a function to known variables and derive some intermediate results. The function may take up to 3 variables with a constant number of unique functions. We also need a table of size O(N) to indicate which function to use in the next step. The description length of CoT would be  $O(K^3 \log K + N)$  which appears manageable.

### 4.2.2 In-context Learning

In this section, we will compare prompting LLMs to answer the MWIS problem directly with prompting them to answer using CoT. We will also study two versions of CoT demonstrations and demonstrate that a more explicit demonstration can improve performance substantially.

Consider the following line from the CoT demonstration (see E.3 for the entire demonstration): Implicit prompt (from (Dziri et al., 2023)): ... Since dp[0] != input[0] + dp[2] (6 != -4 + 5)We can make it more explicit as follows: Explicit prompt: ... Since dp[0]=6, input[0]=-4, dp[2]=5, input[0] + dp[2] = 1 != 6 = dp[0]

Both prompts demonstrate steps to use DP to solve the MWIS problem, but in the Implicit prompt, when autoregressively generating the token "!=", the values of dp[0], input[0], dp[2], and input[0]+dp[2] are not explicitly stated in the immediate context and need to be inferred from all

#### previous observations.

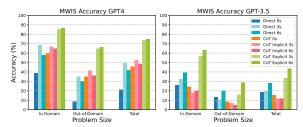


Figure 3: In-context learning results on MWIS. 3-shot prompts have one example each for sizes 4, 5, and 6, while 6-shot prompts have two examples for these sizes. "In-domain" refers to test examples of sizes 4, 5, and 6, and "Out-of-Domain" refers to test examples ranging from size 6 to 10.

As shown in Fig. 3, making the demonstrations explicit provides more than 20% improvement in many cases compared to the implicit demonstrations from (Dziri et al., 2023). This is consistent with the learning problem becoming computationally easier if the relevant variables are made explicit during learning. The sample complexity may also be smaller: the explicit demonstrations is decomposing the single reasoning steps into multiple simpler steps, effectively creating a small chain-of-thought. In contrast to the making the single step a small CoT, we can view deciding between "!=" and "==" in the implicit demonstration as a function of all the previously observed variables. The tabular representation of such a function would have a large description length which suggests that it would require a larger sample complexity to learn.

We observe that prompting LLM to directly give an answer yields performance comparable to the implicit CoT method in Fig. 3. This suggests that while we prompt the LLM to "directly" give an answer, the underlying transformer model is not necessarily learning it by populating a table of size  $K^N$  as it is unlikely to encounter a very large number of examples of the MWIS problem during pre-training. This suggest that the transformer used in the LLM may align well with the reasoning algorithm used here. We explore this further in fine-tuning experiments.

### 4.2.3 Fine-tuning Experiments

We perform fine-tuning experiments to study both in- and out-of-domain performance.

To examine the generalizability of the fine-tuned model to OOD examples, we define two types of Domain: 1) *Problem size*: Fine-tune with problems of sizes 4, 5, and 6. Test with problems of size ranging from 4 to 10. All numbers in the input array are uniformly sampled from [-100, 100] 2) *Number range*: Fine-tune and test with problems 409

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of sizes 4, 5, and 6. For fine-tuning data, numbers in the input array are uniformly sampled from [-100, 100], while for OOD test examples, numbers are uniformly sampled from [-1000, 1000].

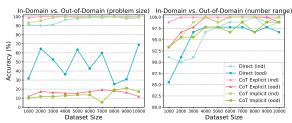


Figure 4: Results of fine-tuning Llama2-7B-chat on MWIS problem.

**Results** For in-domain test examples, we observe that CoT Explicit performs better with the same number of training examples compared with CoT Implicit and Direct. Interestingly, with more finetuning data, Direct can achieve performance similar to CoT Explicit. This differs from the math word problem in 4.1.2 where Direct is not comparable with CoT even with ten times more fine-tuning data. Training the transformer to directly approximate the result of this dynamic programming algorithm seems easier than training it to compute the result of a multivariate equation in 4.1.2. But it is unclear whether the difficulty in word math problem is due to computational complexity in learning or poor alignment of transformer with solving that equation; we discuss more about this in Appendix D.

As shown in (Dziri et al., 2023), CoT is terrible at generalizing to reasoning length longer than training data, worse than Direct, possibly because LLMs learn by doing pattern matching rather than in a compositional manner (Dziri et al., 2023; Kharitonov and Chaabouni, 2020). However, all methods exhibit fairly good generalization to different ranges of numbers. In this case, pattern matching may be less of an issue as the structure of the solution remains the same.

# 4.3 Air Travel Planning

Consider the problem of planning for an air trip: 479 given the starting city and destination, provide 480 the flight route using the direct flights out of each 481 city. For example, if the problem is: What is the 482 flight route from Singapore to New Orleans? One 483 valid answer might be: Singapore-San Francisco-484 485 Houston-New Orleans. It is a typical graph search problem: there is an implicit graph where nodes are 486 cities on the earth, and edges are direct flights out 487 of each city. Given a pair of nodes, we aim to find 488 a valid path connecting two graph nodes. To solve 489

this problem, we can either use LLM to predict the flight route directly or use the LLM's knowledge of the flight graph between cities to conduct a graph search. This problem has been studied in (Zhao et al., 2023) using prompting. In this paper, we go further and linearize the graph search algorithm into a CoT, allowing us to study fine-tuning and learning of the graph search algorithm. 490

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# 4.3.1 Analysis

Assume there are N cities in the domain, and we randomly select two cities as the current and target cities. We first repeat the description length analysis from (Zhao et al., 2023), then extend it to a linearized ToT.

**Direct & CoT** Generating the path directly is essentially the same as CoT as we generate the next city on the path autoregressively. A concise representation of this approach is a table: the row and column of this table are the current city and goal city, and the table entry records the next city to fly to in order to get to the goal. This table has  $N^2$ entries in total, and each entry takes log *N* bits to describe. Thus, the description length of this table is  $O(N^2 \log N)$  bits.

**ToT** Another method is to use ToT reasoning, in which the LLM acts as the graph, i.e., predicts the direct flight from the current city, together with a hand-coded breadth-first search (BFS) algorithm to find the valid route. Assuming that the total number of edges grows proportionally to the number of cities, describing a sparse graph with N nodes takes approximately  $O(N \log N)$  bits, with  $\log N$  bits to describe each city in the adjacency list. The graph describes the transition functions; thus, ToT can be described using  $O(N \log N)$  bits if the other components are hand-coded. We can linearize the BFS algorithm into a CoT which is entirely generated by the LLM. Other than providing the adjacent cities to each city, the components include being maintaining a first-in-first-out queue, checking whether a city has been visited and recognizing the goal city. For a sparse graph as described, the runtime of BFS is O(N), which translates to the existence of relatively small predictors for all the functions.

# 4.3.2 Experiments

Since Direct and CoT are essentially the same, we compare CoT with ToT experimentally. For ToT, the LLM is used only in the expansion step of BFS, when it is queried to generate the neighbour of a city. In addition, we linearize the ToT process into a CoT by generating all the intermediate steps in the BFS computation in **ToT-linear**.

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We use the Kaggle World Cities<sup>2</sup> database data and sample 212 cities with more than 1 million populations. We divide the cities into a large city group (with a population of more than 5 million) and a mid-sized city group (with a population between 1 million and 5 million). We sampled 58 large cities and 154 mid-sized cities. We use the Virtual Radar Server<sup>3</sup> to get the real-time (Jan 13, 2024) flight data as the ground truth. We evaluate the settings of travelling between large cities and mid-sized cities.

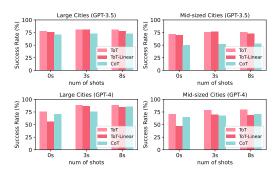


Figure 5: Results of GPT-3.5 and GPT-4 in air travel planning.

In-context learning The result for in-context learning is shown in Fig. 5. For GPT-3.5, ToT outperforms CoT slightly in large cities and substantially in mid-sized cities. This is consistent with the analysis where the description length of CoT and ToT are  $O(N^2 \log N)$  and  $O(N \log N)$  respectively: the gap between CoT and ToT would be larger when N is larger. Surprisingly, ToT-linear is comparable to ToT, even for zero-shot, where the steps in the BFS algorithm are briefly described in the prompt without any examples of its execution, indicating that there is some pre-training of the BFS algorithm in GPT-3.5. GPT-4 generally does better than GPT-3.5 for ToT and CoT, possibly because it has been trained with more data. Interestingly, GPT-4 does not do so well for ToT-linear, particularly for zero-shot, indicating that its pre-training for the BFS algorithm is possibly poorer than GPT-3.5.

**Fine-tuning Experiments** In-context learning depends substantially on the pre-training, which we do not control. Fine-tuning allows us to better control the amount of training data used in the experiments. The results of our fine-tuning experiments are in Fig. 6. Each ToT-linear example is longer than a CoT example; hence, we plot the results based on the number of edges observed in training. The

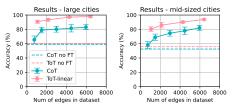


Figure 6: Results of fine-tuning Llama2-7b using different dataset sizes. The *CoT no FT* and *ToT no FT* means using the pre-trained Llama2-7b with CoT and ToT.

results are consistent with the complexity analysis, with ToT-linear performing better than CoT.

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### 4.4 Game of 24

Unlike the above-mentioned problems that can be solved in polynomial time, many puzzle tasks are much harder and unlikely to be efficiently solvable. We use the Game of 24 shown in the introduction: given four numbers, the player must use basic arithmetic operations  $(+, -, \times, \div)$  and all four numbers to reach 24. These types of puzzle games are often designed to be hard to solve (Kendall et al., 2008), although we are not aware of results on the computational complexity of the Game of 24<sup>4</sup>. The results in (Yao et al., 2023), obtained with in-context learning, show that CoT fails while ToT does substantially better. We extend the results by showing that CoT fails in fine-tuning as well, suggesting that the failure is likely due to the mismatch between the computational structure of CoT and the problem. We also consider the decomposition of the actions for in-context learning and show that the decomposition of complex actions into a sequence of simpler actions within a ToT can lead to substantial improvement in performance.

### 4.4.1 Analysis

We provide a general form of Game of 24 for analysis. Assume *N* numbers are given, and each number can take *K* different values. The goal is to use those numbers with arithmetic operations  $(+, -, \times, \div)$  to reach *T*. For the standard Game of 24, N = 4, T = 24.

**Direct** Represented as a table, there are  $K^N$  inputs. A solution is an expression consisting of the *N* numbers together with N - 1 operations and corresponding parentheses. Assuming log *K* bits to represent numbers, this can be represented using  $O(N \log K)$  bits, giving a total table size of

<sup>2</sup>https://www.kaggle.com/datasets/max-mind/world -cities-database

<sup>&</sup>lt;sup>3</sup>https://github.com/vradarserver/standing-data

<sup>&</sup>lt;sup>4</sup>A modified version with N rather than four numbers, arbitrary target number instead of 24, and only addition and multiplication with zero allowed is the same as subset-sum, an NP-complete problem. This suggests that similar puzzles are computationally difficult to solve.

 $O(NK^N \log K)$  bits. 615 **CoT** For CoT, the N - 1 operations are produced 616 in a step-by-step manner. For each step, there are 617 N(N-1)/2 ways to select two numbers and 6 dis-618 tinct operations (both ordering for - and  $\div$ , while + 619 and \* are symmetric), giving possible 3N(N-1)actions. Each operation can be represented with 621 a table with  $K^2$  entries using  $O(K^2 \log K)$  bits, although pretraining likely has learned these oper-623 ations for small K. This gives a total description 624 length of  $O(N^2K^2\log K)$  if each action is learned 625 using its own table. If we decompose the selection of two numbers and the arithmetic operation into two steps, then the total description length is  $O(N^2 + K^2 \log K)$ , and we consider this decomposition in our experiments. Like other computationally 630 difficult problems, there is no simple known policy 631 for selecting the next action. A simple tabular policy would have  $O(K^N)$  entries, and each described using  $O(\log N)$  bits.

**ToT** ToT uses the same actions as CoT but does not need a policy. Instead, we have a goal recognizer and an evaluation function that decides which nodes to expand. Verifying whether a solution is correct can be done in O(N) time, hence a goal recognizer with a small representation exists. Difficult computational problems typically do not have a simple evaluation function; a tabular evaluation function would have  $O(K^N)$  entries. However, a ToT may use a larger computation budget to search a larger part of the search tree when the evaluation function is weaker, compared to CoT, where the next action is selected with a fixed learned policy.

#### 4.4.2 Experiments

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As in (Yao et al., 2023), we use the hard games indexed 901-1000 from 4nums.com for testing. In our experiments, we consider the output as correct if the expression evaluates to 24 and uses all the input numbers once. To show that it is unlikely that a small chain solution can be easily learned, we finetuned Llama-7b-chat with 1200 solution trajectories of Game of 24. Both CoT and Direct failed in all test cases, showing that moderate amounts of data are unlikely sufficient for learning in these settings. For in-context learning, the success rate of the 100 games is reported in Fig. 7.

For ToT, we use a beam search with a beam width of 5 and the same action and self-evaluation prompts as (Yao et al., 2023). We also constructed a more decomposed version of ToT, ToT-Decomp, where we decompose the action into two steps: the

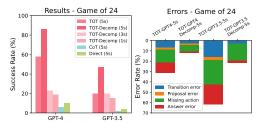


Figure 7: Results of Game of 24. 5s, 3s and 1s means 5, 3, and 1 examples in the prompt for few-shot in-context learning.

selection of two numbers and the arithmetic operation (see Appendix E.5.1 for examples). Also, ToT-Decomp uses a small CoT that provides the steps for constructing the final equation from the sequence of actions and states in the solution, whereas ToT directly generates the final equation from the action-state sequence.

The results are consistent with those from (Yao et al., 2023), with ToT clearly outperforming CoT and Direct. We also find that ToT-Decomp substantially outperforms ToT, demonstrating the advantages of decomposition even within the components of ToT. We perform error analysis as shown in Fig. 7, where we categorize the errors into four types: 1) transition error, where the next state (remaining numbers) is generated incorrectly; 2) proposal error, where the LLM does not generate the correct numbers in the action expression; 3) missing actions, where there are valid actions but not proposed by the LLM; and 4) answer error, where the search is correct but the final expression is incorrect. The results show a substantial reduction in each type of error in ToT-Decomp compared to ToT.

### 5 Conclusion

This paper introduces a detailed empirical study to understand the effectiveness of chain-of-thought (CoT) and tree-of-thought (ToT) reasoning in planning and reasoning tasks from sample and computational complexity in machine learning. We view the CoT and the ToT as decomposition methods for the underlying problem and study the complexity of the component predictors in the decomposed problems. Our study finds that when the solution can be decomposed as a chain of reasoning steps where predicting the next step is not difficult, explicitly demonstrating the reasoning chain during learning can be helpful. Leaving out important variables for deciding the next reasoning step instead of making all relevant variables explicit in the demonstrations can also make learning more difficult. Finally, when algorithmic analysis indicates that predicting the next reasoning step in a CoT is computationally hard, a ToT structure can be helpful.

**Limitations** The suggested methodology from 709 this paper is to analyse the chain-of-thought as 710 a decomposition of the problem and to analyse 711 the complexity of its components. If learning the 712 components has low sample complexity and the 713 computational complexity of predicting the next 714 reasoning step is low, then learning to solve the 715 problem using a chain-of-thought would be rea-716 sonable. On the other hand, if the computational 717 complexity of predicting the next reasoning step is 718 high, it may be reasonable to consider learning the components and using a tree-of-thought to solve 720 the problem. This oversimplifies various aspects of the problem. Even though the components have 722 low sample complexity, it may be difficult to learn 723 them in practice as the computational complexity of learning may be high, although this may be allevi-725 ated by overparameterization of the predictors used to learn the components. Another issue is out-of-727 domain generalization. As shown in the MWIS case study, generalization in-domain does not mean that the method will generalize out-of-domain, which may be further exacerbated by overparameterization. Further limitations may apply when doing 732 in-context learning where very few examples are 733 used. Performance may depend heavily on the pretrained LLM used in this setting. Nonetheless, our 735 case studies suggest that the proposed methodology may still be useful in the in-context learning setting. 737 We would suggest using the guidelines proposed in this paper in a similar way that the Occam Razor 739 principle in the philosophy of science is used. Oc-740 cam's Razor suggests that simple explanations for 741 a scientific phenomenon be preferred until shown 742 743 otherwise by observations. The suggestions we proposed may not work all the time but should 744 similarly be preferred until empirical observations 745 suggest otherwise.

Ethics Statement This paper studies reasoning 747 and planning in LLMs from a general perspective. 748 While we do not focus on ethics issues, reasoning 749 and planning techniques can potentially be useful in ensuring that AI agents behave ethically through 751 the use of appropriate reward or goal functions that may possibly be learned from data. They may 753 also be used in harmful ways in planning more 755 sophisticated attacks against others. Research on both the use of reasoning and planning for ensuring ethical AI agent behaviour and in mitigating the use of reasoning and planning in performing harmful attacks should be encouraged. 759

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# **A** Experimental Details

All prompting experiments are done with gpt-3.5turbo-1106 and gpt-4-1106-preview. All finetuning experiments are done with Llama2-7B-chat (Touvron et al., 2023) with LoRA r = 64,  $\alpha = 16$ (Hu et al., 2021) applied to query and value matrices, and uses *batch\_size* = 1 and gradient accumulation steps= 32. The template word problem is fine-tuned for 10 epochs with a learning rate of 1e - 3. MWIS and Game of 24 are fine-tuned for 5 epochs with a learning rate of 3e - 4. Travel planning is fine-tuned for 300 gradient optimization steps with a learning rate of 3e - 4. The finetuning data is wrapped in the template "<*s*> [INST] {*[prompt]*] [/INST] {*[completion]*] </s>" and the loss is calculated on completion tokens.

# B GSM8K

B.1 Common Rules in GSM8K

We analyzed 50 problems from the GSM8K training set and identified a set of rules. The first five are general rules that can be inferred from the questions and are applicable to multiple problems. The last four are question-specific rules, involving commonsense knowledge that are not mentioned in the questions.

- 1. Amount A = Amount B \* multiplier
- 948 2. Amount A = Amount B + difference
  - 3. Total = N\_unit \* Amount per unit
    - 4. Total = Sum of components
      - 5. Current Amount = Initial Amount Amount Given + Amount Received
      - 6. Question-specific (implicit): One hour = 60 Minutes
      - 7. Question-specific (implicit): one sandwich has two slices of bread
      - 8. Question-specific (implicit): face has two eyes
        - 9. Question-specific (implicit): 1 quarter = 25 cent; 1 dime = 10 cent; 1 nickel = 5 cent

### **B.2** An Efficient Algorithm for GSM8K

Based on our analysis of the GSM8K problems in 4.1.1, we give a formulation of the GSM8K problems, and show that there exists an algorithm that has runtime linear to the total input length.

### **Problem Formulation**

**Input**: A set of *N* variables  $\{V_1, ..., V_N\}$ , where the values of some variables are known (from natural language input), while some are unknown (to be inferred); A set of *M* equations  $\{R_1, ..., R_M\}$ , where all equations have exactly one variable on LHS; A target variable  $V_t$  whose value we want to know.

**Output**: The value of  $V_t$ .

The solvability of the problem ensures that for all variables, if the value is not given in the natural language question, will appear on the LHS of some equation.

### **An Efficient Algorithm :**

Inspired by (Dowling and Gallier, 1984), we design an algorithm whose runtime is linear to the size of the problem (total length of all equations).

We maintain a list numvars [M] which stores the number of unsolved variables on RHS for each equation; a list lhslist[M] which stores which variable is on LHS of an equation; a list equationlist[N] which stores the index of the equations where the corresponding variable appears on RHS. We say an equation  $R_i$  is ready to be processed if numvars[i] = 0. We maintain a queue that will contain the equations that are ready to be processed, and it is initialized to contain the equations that are ready to process given the known variables from natural language input.

Then we loop over the queue. Let equation1 be the current head of the queue and let nextvar=lhslist[equation1] be the variable on the LHS of of equation1. Pop the head of the queue, and iterate over equationlist[nextvar], for every equation2 in it, reduce numvars[equation2] by 1, and if numvars[equation2] becomes 0, add equation2 to the queue.

Loop until the queue is empty, we would have solved the values of all N variables. Refer to Algorithm 1 for a more concise representation of the algorithm.

**Complexity of the Algorithm** numvars and lhslist can be initialized in O(L), where *L* is the total length of all equations. When processing an equation, the decrement of numvars corresponds to the "*deletion*" of occurrences of the variable in an equation, each variable in the equation is looked only once, thus processing all equations also runs in O(L). Overall, the runtime of the algorithm is O(L), i.e. linear to the total length of the equations. If we assume each variable appears only once on the

Algorithm	1	Forward	Chaining	Algorithm	for
GSM8K Pro	obl	ems			

#### **Require:**

N variables  $\{V_1, \ldots, V_N\}$ , with known and unknown values.

*M* equations  $\{R_1, \ldots, R_M\}$ , each with one variable on LHS.

Target variable  $V_t$  to find the value of.

### **Ensure:**

Value of  $V_t$ .

- 1: numvars $[1...M] \leftarrow$  Number of unsolved variables on RHS of each  $R_i$ .
- 2:  $lhslist[1...M] \leftarrow Variable on LHS of each R_i$ .
- 3: equationlist  $[1...N] \leftarrow$  Indices of  $R_i$  where  $V_i$  appears on RHS.
- 4: Initialize queue readyQueue with indices of *R<sub>i</sub>* where numvars[*i*] = 0.
- 5: while readyQueue is not empty do
- 6:  $i \leftarrow \text{Dequeue from readyQueue.}$
- 7:  $V_i \leftarrow \text{lhslist}[i]$ .

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8: for each k in equation list [i] do
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9: numvars[k] \leftarrow numvars[k] - 1.
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- 10: **if** numvars[k] = 0 **then**
- 11: Enqueue *k* into readyQueue.
- 12: **end if**
- 13: **end for**
- 14: end while

```
15: return Value of V_t.
```

LHS of equations, and each equation has a number1017of variables up to a constant C (as we have seen1018in 4.1.1, this is often true for GSM8K problems),1019the runtime of the algorithm would be O(N), i.e.1020linear to the number of variables in the problem.1021

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### B.3 GSM8K Errors

We observe three types of errors from GPT, namely grounding error, calculation error, and missing rule. We provide an example for each type.

#### Listing 1: Grounding Error

Ouestion: Annie was given a pack of crayons. The pack contained 21 crayons. She already had a box of 36 crayons in her locker. Her friend Bobby gave her half the amount she already had in her locker. She decided to give her sister Mary 1/3 of her total amount of crayons. How many crayons does she give to Mary? GPT-3.5 response: "Annie originally had 21 crayons in the pack and 36 crayons in her locker. So she had a total of 21 + 36 = 57 crayons. Bobby gave her half the amount she already had, so he gave her 57 / 2 = 28.5 crayons, but since you can't have half a crayon, let's round down to 28. So she now has 57 + 28 = 85 crayons. So 1/3 of her total amount of crayons is 85 / 3 = 28.33 crayons, but since you can't have a fraction of a crayon, let' s round down to 28 crayons. So she gives Mary 28 crayons. So the answer is 28.'

In Listing 1, the problem involves using the rule "Amount A = Amount B \* multiplier", which should be grounded as "Amount from Bobby = Amount in Locker \* 1/2", not "Amount from Bobby = Amount Annie have in total \* 1/2".

#### Listing 2: Calculation Error

Question: To get free delivery, Alice needs to spend a minimum of \$35.00 online at her favorite grocery store. In her cart she has 1.5 pounds of chicken at \$6.00 per pound, 1 pack of lettuce for \$3.00, cherry tomatoes for \$2.50, 4 sweet potatoes at \$0 .75 each, 2 heads of broccoli for \$2.00 each and a pound of Brussel sprouts for \$2.50. How much more does she need to spend in order to get free delivery? GPT-3.5 response: "Alice's total so far is: (1.5 \* 6) + 3 + 2.50 + (4 \* 0.75) + (2 \* 2) + 2.50 = 9 + 3 + 2.50 + 3 + 4 + 2 + 2.50 = 26.00To get free delivery, she needs to spend at least \$35.00. So she needs to spend 35 - 26= 9.00 more to get free delivery.

So the answer is 9.00."

#### In Listing 2, the calculation is wrong.

#### Listing 3: Missing Rule

Question:
A Ferris wheel can accommodate 70 people in 20 minutes. If
the Ferris wheel is open from 1:00 pm until 7:00 pm, how many
people will get to ride?

GPT-3.5 response:

"The Ferris wheel can accommodate 70 people in 20 minutes. There are 6 periods of 20 minutes from 1:00 pm to 7:00 pm.

```
So in total, the Ferris wheel can accommodate 70 * 6 = 420
people.
So 420 people will get to ride the Ferris wheel from 1:00 pm
until 7:00 pm.
So the answer is 420."
```

In Listing 3, one commonsense knowledge (one hour has 60 minutes) not mentioned in the question is not properly used in the solution.

### C Dynamic Programming

### C.1 Algorithm for MWIS

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An algorithm that solves the Maximum Weighted Independent Set problem and runs in time O(N)where N is the number of numbers in the input is shown in Algorithm 2.

### D Inductive bias of Transformers

From the math word problem and dynamic programming fine-tuning experiments, we see that for some tasks (maximum weighted independent set), the transformer can learn to directly answer the problem efficiently, while for some other tasks (word problem), the direct answer is hard to learn.

We conduct two more experiments to study what might affect the performance of learning to direct answer other than sample complexity: 1) learn the max function, where the input is a list of integers, and the expected output is the maximum value in the input list. This requires only looping over the sequence once, and storing one intermediate value; 2) another dynamic programming problem called rain water<sup>5</sup> that requires looping over the array three times and storing two one-dimensional arrays for memorization. These two problems are similar to MWIS as they all require looping over the input sequence and maintaining some internal variables during the iteration. We use them to study whether the difference between learning to directly answer the template word problem and MWIS is related to the inductive bias of transformers. To eliminate the confounding part, the difficulty of language in the template word problem described in 4.1.2, we perform a modified version of the problem, where we remove all natural language in the prompt. The input would look like "1, 6, 4, 3, 2, 14, 8", and the expected output for this example would be "8".

From the results in Table 1, we see that the modified word problem has a similar performance as the original version described in 4.1.2 and Fig. 2b, which suggests that natural language is not the

<sup>5</sup>https://leetcode.com/problems/trapping-rainwater/ Algorithm 2 Dynamic Programming Algorithm for the Maximum Weighted Independent Set problem

Require: An array arr of integers

**Ensure:** A sequence of decisions maximizing a certain criterion based on *arr* 

- 1:  $N \leftarrow \text{length of } arr$
- 2: Initialize dp[0...N-1] with zeros
- 3:  $dp[N-1] \leftarrow \max(arr[N-1], 0)$
- 4:  $dp[N-2] \leftarrow \max(arr[N-1], arr[N-2], 0)$
- 5: for  $i \leftarrow N 3$  downto 0 do
- 6:  $dp[i] \leftarrow \max(dp[i+1], arr[i] + dp[i+2], 0)$
- 7: end for
- 8: Initialize *result* as an empty list
- 9:  $can\_access\_next\_item \leftarrow true$
- 10: for  $i \leftarrow 0$  to N 3 do
- 11: **if** dp[i] = arr[i] + dp[i + 2] and can\_access\_next\_item **then**
- 12: Append 1 to *result*
- 13:  $can\_access\_next\_item \leftarrow false$
- 14: **else**
- 15: Append 2 to *result*
- 16:  $can\_access\_next\_item \leftarrow true$
- 17: **end if**
- 18: end for
- 19: if dp[N-2] = arr[N-2] and  $can_access\_next\_item$  then
- 20: Append 1 to *result*
- 21: **else**
- 22: Append 2 to *result*
- 23: end if
- 24: if dp[N-1] = arr[N-1] and  $can_access\_next\_item$  then
- 25: Append 1 to *result*
- 26: else
- 27: Append 2 to *result*
- 28: end if
- 29: **return** *result*

Task	Accuracy (%)
MWP	58.00
MWIS $(n \in [4, 5, 6])$	98.89
MWIS ( $n = 200$ )	0.01
$\max(n = 30)$	99.50
rain water $(n = 10)$	89.00

Table 1: Fine-tuning results of different problems. MWP stands for the modified word problem where the input contains only 7 numbers. All tasks are fine-tuned with 10k direct answer examples and evaluated on in-domain examples.

bottleneck of the template word problem. From 1129 the table, we also see that MWIS, max, and rain 1130 water perform significantly better than MWP. This 1131 suggests that it might be easy for transformers to 1132 learn this loop type of problem when the problem 1133 size is small. However, when the problem size 1134 of MWIS is large (n = 200), the model fails to 1135 generalize to unseen test examples. This aligns 1136 with previous findings (Weiss et al., 2021; Zhou 1137 et al., 2024) that suggest that it would consume one 1138 transformer layer to approximate one iteration in 1139 an algorithm. And with a problem size of 200, it 1140 can be hard for transformers to approximate the 1141 algorithm in a generalizable way, thus some other 1142 patterns in the training set may be exploited, leading 1143 to poor generalization. 1144

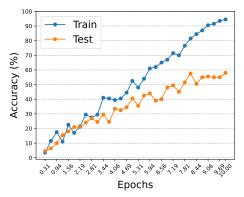


Figure 8: Results of fine-tuning word problem.

From Fig. 8 we can see that for the template 1145 word problem, the transformer can fit the training 1146 set reasonably well, while the test set performance 1147 peaks at 58.0%. This suggests that by learning 1148 to answer directly, the transformer is behaving 1149 similarly to learning by filling a table, instead of 1150 learning the underlying rational function, which 1151 supports our description length analysis. 1152

### E Prompts

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### E.1 GSM8K Prompts

#### Listing 4: GSM8K Direct prompt

direct\_8s = """Please answer a math word problem given the following exapmles. Respond only the answer, in the format " The answer is ###." Example: Question: There are 15 trees in the grove. Grove workers will plant trees in the grove today. After they are done, there will be 21 trees. How many trees did the grove workers plant today? The answer is 6. Question: If there are 3 cars in the parking lot and 2 more cars arrive, how many cars are in the parking lot? The answer is 5.

Question: Leah had 32 chocolates and her sister had 10 more chocolates than her. If they ate 35, how many pieces do they have left in total? The answer is 39.

Question: Jason had 20 lollipops. He gave Denny some lollipops. Now Jason has 12 lollipops. How many lollipops did Jason give to Denny? The answer is 8.

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Question: Shawn has five toys. For Christmas, he got two toys each from his mom and dad. How many toys does he have now? The answer is 9.

Question: There were nine computers in the server room. Five more computers were installed each day, from monday to thursday. How many computers are now in the server room? The answer is 29.

Question: Michael had 58 golf balls. On tuesday, he lost 23 golf balls. On wednesday, he lost 2 more. How many golf balls did he have at the end of wednesday? The answer is 33.

Question: Olivia has \$23. She bought five bagels for \$3 each. How much money does she have left? The answer is 8.

Question: {question} The answer is

#### Listing 5: GSM8K CoT and ToT prompt

cot\_8s = """Please answer a math word problem given the following example. Respond with reasoning steps, and end with the answer, in the format "So the answer is ###. Example: Let's think step by step. Question: There are 15 trees in the grove. Grove workers will plant trees in the grove today. After they are done, there will be 21 trees. How many trees did the grove workers plant todav? Solution: There are 15 trees originally. And there were 21 trees after some more were planted. So 21 - 15 = 6 trees were planted. So the answer is 6. Let's think step by step. Question: If there are 3 cars in the parking lot and 2 more cars arrive, how many cars are in the parking lot? Solution: There are originally 3 cars And 2 more cars arrive So there are 3 + 2 = 5 cars now. So the answer is 5. Let's think step by step. Question: Leah had 32 chocolates and her sister had 10 more chocolates than her. If they ate 35, how many pieces do they have left in total? Solution: Originally, Leah had 32 chocolates. And her sister had 10 more chocolates than her So her sister had 42 chocolates So in total they had 32 + 42 = 74 chocolates Then they ate 35 chocolates. Therefore they had 74 - 35 = 39 chocolates left. So the answer is 39. Let's think step by step. Question: Jason had 20 lollipops. He gave Denny some lollipops Now Jason has 12 lollipops. How many lollipops did Jason give to Denny? Solution: Jason started with 20 lollipops. Then he had 12 after giving some to Denny. So he gave Denny 20 · 12 = 8 lollipops. So the answer is 8. Let's think step by step. Ouestion: Shawn has five toys. For Christmas, he got two toys each from his mom and dad. How many toys does he have now? Solution: Shawn started with 5 toys. And he got 2 toys each from his mom and dad So he got 2 + 2 = 4 toys. Therefore, he has 5 + 4 = 9 toys now So the answer is 9. Let's think step by step.

Question: There were nine computers in the server room. Five more computers were installed each day, from monday to thursday. How many computers are now in the server room?

Solution: There were originally 9 computers. And 5 more computers were added from onday to thursday. There are 4 days between monday and thursday. So 5 \* 4 = 20 computers were added in total. So there are 9 + 20 = 29 computers now. So the answer is 29. Let's think step by step. Question: Michael had 58 golf balls. On tuesday, he lost 23 golf balls. On wednesday, he lost 2 more. How many golf balls did he have at the end of wednesday? Solution: Michael started with 58 golf balls. And he lost 23 golf balls on tuesday. So after losing 23 on tuesday, he had 58 -23 = 35. And then he lost 2 more golf balls on wednesday. So after losing 2 more on wednesday, he had 35 - 2 = 33 golf balls So the answer is 33. Let's think step by step. Question: Olivia has \$23. She bought five bagels for \$3 each. How much money does she have left? Solution: Olivia had 23 dollars. And she bought 5 bagels. And each bagel costs 3 dollars. So she spent 5 \* 3 = 15 dollars. So she has 23 - 15 = 8 dollars left. So the answer is 8. Let's think step by step. Question: {question} Solution:

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#### Listing 6: GSM8K ToT self-evaluation prompts

evaluate\_prompt = ''' Q: Julie climbed 15 steps up the giant slide. She climbed down 6 steps to talk to her friend, Maria. Then she climbed up 8 steps to get to the top. How many steps does the slide have? Julie climbed 15 steps up. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A) Then she climbed down 6 steps. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A) Then she climbed up 8 steps. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A) So she climbed 15 + 8 = 23 steps. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (B), because she also climbed down 6 steps, so she climbed 23 - 6 = 17 steps. So the slide has 23 steps. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A), but the value of steps of slides is incorrect. So the answer is 23. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A), but the value of steps of slides is incorrect. 0: Suzanne read the first 15 pages of her book on Monday. She

read 16 more pages than that on Tuesday. Then there were 18 pages left. How many pages are in Suzanne's book altogether?

Suzanne read 15 pages on Monday.

# Is the above step of reasoning: # (A) Correct (B) Incorrect # The above step of reasoning is (A) Then she read 16 more pages on Tuesday. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A) So she read 15 + 16 = 31 pages in total. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (B), because she read 16 more pages than that on Tuesday, so she read 15 + 31 = 46 pages in total. Then there were 18 pages left. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A), but the value of total read pages of monday and tuesday is incorrect. So the book had 31 + 18 = 49 pages. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A), but the value of total read pages of monday and tuesday is incorrect. So the book had 46 + 18 = 64 pages. So the answer is 49. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A), but the value of total read pages of monday and tuesday is incorrect. Q: Allison brought some CDs online. Each CD cost \$7. There was an additional charge of \$4 per order for shipping costs. The total bill came to \$60. How many CDs did Allison buy? Each CD cost 7 dollars. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A) And there was an additional charge of 4 dollars. # Is the above step of reasoning: # (A) Correct

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# (B) Incorrect # The above step of reasoning is (A) So the total cost of each CD is 7 + 4 = 11 dollars. # Is the above step of reasoning: # (A) Correct # (B) Incorrect

# The above step of reasoning is (B), because each CD cose 7 dollars. So 60 / 11 = 5.45.

# Is the above step of reasoning: # (A) Correct

# (B) Incorrect

# The above step of reasoning is (B), because it cost 4

dollars for shipping costs. So the cost of CDs is 60 - 4 = 56dollars. So Allison bought 56 / 7 = 8 CDs.

So the answer is 5

# Is the above step of reasoning:

# (A) Correct

(B) Incorrect

# The above step of reasoning is (A), but the value of number of CDs is incorrect.

0: Luis and Cameron shared some stickers is the ratio 5:2. Luis received 15 more stickers than Cameron. How many stickers were there altogether?

Let's say there were x stickers. # Is the above step of reasoning: # (A) Correct

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# (B) Incorrect # The above step of reasoning is (A) Then Luis got 5x/7 and Cameron got 2x/7. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A) Luis got 15 more than Cameron, so 5x/7 - 2x/7 = 15. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A) So 3x/7 = 15. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A) So x = 105. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (B), because 3x/7 = 15. So x = 15 \* 7 / 3 = 35. So there were 35 stickers. So the answer is 105. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A), but the value of number of stickers is incorrect. Q: Alexa has 92 cents in her pocket. She wants to buy 3 pencils at the school supply store. Each pencil costs 8 cents. How much money will Alexa have left?

A٠ Alexa has 92 cents. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A) And 3 pencils for 8 cents each will be  $3 \times 8 = 24$  cents. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A) So she has 92 - 24 = 68 cents left. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A) So the answer is 68. # Is the above step of reasoning: # (A) Correct # (B) Incorrect # The above step of reasoning is (A)

Q: {input}

A: {output}
# Is the above step of reasoning:
# (A) Correct
# (B) Incorrect
# The above step of reasoning is '''

# E.2 MWIS Prompts

#### Listing 7: Direct prompts

direct\_0s = """Given a sequence of integers, find a subsequence with the highest sum, such that no two numbers in the subsequence are adjacent in the original sequence.

To indicate the selected numbers, print an array with "1" for chosen numbers and "2" for unchosen ones. For instance, [1, 2, 2, 2, 2] implies selecting only the first number. If multiple solutions exist, select the lexicographically smallest.

#### {prompt}

direct\_3s = """Given a sequence of integers, find a subsequence with the highest sum, such that no two numbers in the subsequence are adjacent in the original sequence.

To indicate the selected numbers, print an array with "1" for chosen numbers and "2" for unchosen ones. For instance, [1, 2, 2, 2, 2] implies selecting only the first number. If multiple solutions exist, select the lexicographically smallest.

Let\'s solve input = [1, 1, -5, -1]. Answer: [1, 2, 2, 2]

Let\'s solve input = [3, 2, 1, -1, 2]. Answer: [1, 2, 1, 2, 1]

Let\'s solve input = [0, 4, -2, 3, -3, -1]. Answer: [2, 1, 2, 1, 2, 2]

{prompt}

direct\_6s = """Given a sequence of integers, find a subsequence with the highest sum, such that no two numbers in the subsequence are adjacent in the original sequence.

To indicate the selected numbers, print an array with "1" for chosen numbers and "2" for unchosen ones. For instance, [1, 2, 2, 2, 2] implies selecting only the first number. If multiple solutions exist, select the lexicographically smallest.

Let\'s solve input = [1, 1, -5, -1]. Answer: [1, 2, 2, 2]

Let\'s solve input = [3, 2, 1, -1, 2]. Answer: [1, 2, 1, 2, 1]

Let\'s solve input = [0, 4, -2, 3, -3, -1]. Answer: [2, 1, 2, 1, 2, 2]

Let\'s solve input = [-3, -4, 4, -1] Answer: [2, 2, 1, 2]

Let\'s solve input = [3, 4, -3, -1, -4] Answer: [2, 1, 2, 2, 2]

Let\'s solve input = [-4, 5, 0, 2, 3, -4] Answer: [2, 1, 2, 2, 1, 2]

{prompt}

### Listing 8: CoT Implicit prompts

cot\_implicit\_3s = """Given a sequence of integers, find a subsequence with the highest sum, such that no two numbers in the subsequence are adjacent in the original sequence.

To indicate the selected numbers, print an array with "1" for chosen numbers and "2" for unchosen ones. For instance, [1, 2, 2, 2, 2] implies selecting only the first number. If multiple solutions exist, select the lexicographically smallest.

We will solve any task instance by using dynamic programming. We define dp[i] as the maximum sum of a subsequence that does not include adjacent elements, when considering only the elements of the input from the i-th position onwards.

Let\'s solve input = [1, 1, -5, -1].

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Since dp[4] != input[4] (0 != -3) or can use next item == dp[3] = max(input[3], 0) = max(-1, 0) = 0dp[2] = max(input[2], input[3], 0) = max(-5, -1, 0) = 0 dp[1] = max(dp[2], input[1] + dp[3], 0) = max(0, 1 + 0, 0) = 1 dp[0] = max(dp[1], input[0] + dp[2], 0) = max(1, 1 + 0, 0) = 1Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output" Let can\_use\_next\_item = True. Since dp[0] == input[0] + dp[2] (1 == 1 + 0) and can\_use\_next\_item == True, we store output[0] = 1. We update can\_use\_next\_item = False. Since dp[1] != input[1] + dp[3] (1 != 1 + 0) or can\_use\_next\_item == False, we store output[1] = 2. We update can\_use\_next\_item = True. Since dp[2] != input[2] (0 != -5) or can\_use\_next\_item == False, we store output[2] = 2. We update can\_use\_next\_item = True Since dp[3] != input[3] (0 != -1) or can\_use\_next\_item = False, we store output[3] = 2. Reconstructing all together, output=[1, 2, 2, 2]. Let\'s solve input = [3, 2, 1, -1, 2]. dp[4] = max(input[4], 0) = max(2, 0) = 2 dp[3] = max(input[3], input[4], 0) = max(-1, 2, 0) = 2 dp[2] = max(dp[3], input[2] + dp[4], 0) = max(2, 1 + 2, 0) = 3 dp[1] = max(dp[2], input[1] + dp[3], 0) = max(3, 2 + 2, 0) = 4 dp[0] = max(dp[1], input[0] + dp[2], 0) = max(4, 3 + 3, 0) = 6Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output". Let can\_use\_next\_item = True. Since dp[0] == input[0] + dp[2] (6 == 3 + 3) and can\_use\_next\_item == True, we store output[0] = 1. We update can\_use\_next\_item = False. Since dp[1] != input[1] + dp[3] (4 != 2 + 2) or can\_use\_next\_item == False, we store output[1] = 2. We update can\_use\_next\_item = True. Since dp[2] == input[2] + dp[4] (3 == 1 + 2) and can\_use\_next\_item == True, we store output[2] = 1. We update can use next item = False Since dp[3] != input[3] (2 != -1) or can\_use\_next\_item == False, we store output[3] = 2. We update can\_use\_next\_item = True. Since dp[4] == input[4] (2 == 2) and can\_use\_next\_item == True, we store output[4] = 1. Reconstructing all together, output=[1, 2, 1, 2, 1]. Let\'s solve input = [0, 4, -2, 3, -3, -1]. dp[5] = max(input[5], 0) = max(-1, 0) = 0 dp[4] = max(input[4], input[5], 0) = max(-3, -1, 0) = 0 dp[3] = max(dp[4], input[3] + dp[5], 0) = max(0, 3 + 0, 0) = 3 dp[2] = max(dp[3], input[2] + dp[4], 0) = max(3, -2 + 0, 0) = dp[1] = max(dp[2], input[1] + dp[3], 0) = max(3, 4 + 3, 0) = 7 dp[0] = max(dp[1], input[0] + dp[2], 0) = max(7, 0 + 3, 0) = 7 Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output". let can use next item = True Since dp[0] != input[0] + dp[2] (7 != 0 + 3) or can\_use\_next\_item == False, we store output[0] = 2. We update can\_use\_next\_item = True. Since dp[1] == input[1] + dp[3] (7 == 4 + 3) and can\_use\_next\_item == True, we store output[1] = 1. We update can\_use\_next\_item = False. Since dp[2] != input[2] + dp[4] (3 != -2 + 0) or can\_use\_next\_item == False, we store output[2] = 2. We update can\_use\_next\_item = True. Since dp[3] == input[3] + dp[5] (3 == 3 + 0) and can\_use\_next\_item == True, we store output[3] = 1. We update can\_use\_next\_item = False.

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False, we store output[4] = 2. We update can\_use\_next\_item = True. Since dp[5] != input[5] (0 != -1) or can\_use\_next\_item == False, we store output[5] = 2. Reconstructing all together, output=[2, 1, 2, 1, 2, 2]. {prompt}

cot\_implicit\_6s = """Given a sequence of integers, find a subsequence with the highest sum, such that no two numbers in the subsequence are adjacent in the original sequence.

To indicate the selected numbers, print an array with "1" for chosen numbers and "2" for unchosen ones. For instance, [1, 2, 2, 2, 2] implies selecting only the first number. If multiple solutions exist, select the lexicographically smallest.

We will solve any task instance by using dynamic programming. We define dp[i] as the maximum sum of a subsequence that does not include adjacent elements, when considering only the elements of the input from the i-th position onwards.

Let\'s solve input = [1, 1, -5, -1].

dp[3] = max(input[3], 0) = max(-1, 0) = 0 dp[2] = max(input[2], input[3], 0) = max(-5, -1, 0) = 0 dp[1] = max(dp[2], input[2], 0) = max(0, 1, 0) = 0dp[0] = max(dp[2], input[1] + dp[3], 0) = max(0, 1 + 0, 0) = 1dp[0] = max(dp[1], input[0] + dp[2], 0) = max(1, 1 + 0, 0) = 1

Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output".

Let can\_use\_next\_item = True. Since dp[0] == input[0] + dp[2] (1 == 1 + 0) and can\_use\_next\_item == True, we store output[0] = 1. We update can\_use\_next\_item = False. Since dp[1] != input[1] + dp[3] (1 != 1 + 0) or can\_use\_next\_item == False, we store output[1] = 2. We update can\_use\_next\_item = True. Since dp[2] != input[2] (0 != -5) or can\_use\_next\_item == False, we store output[2] = 2. We update can\_use\_next\_item = True Since dp[3] != input[3] (0 != -1) or can\_use\_next\_item == False, we store output[3] = 2.

Reconstructing all together, output=[1, 2, 2, 2].

Let\'s solve input = [3, 2, 1, -1, 2].

dp[4] = max(input[4], 0) = max(2, 0) = 2 dp[3] = max(input[3], input[4], 0) = max(-1, 2, 0) = 2  $dp[2] = max(dp[3], input[2] + dp[4], 0) = max(2, 1 + 2, 0) = 3 \\ dp[1] = max(dp[2], input[1] + dp[3], 0) = max(3, 2 + 2, 0) = 4$ dp[0] = max(dp[1], input[0] + dp[2], 0) = max(4, 3 + 3, 0) = 6

Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output".

Let can\_use\_next\_item = True. Since dp[0] == input[0] + dp[2] (6 == 3 + 3) and can\_use\_next\_item == True, we store output[0] = 1. We update can\_use\_next\_item = False. Since dp[1] != input[1] + dp[3] (4 != 2 + 2) or can\_use\_next\_item == False, we store output[1] = 2. We update can\_use\_next\_item = True. Since dp[2] == input[2] + dp[4] (3 == 1 + 2) andcan\_use\_next\_item == True, we store output[2] = 1. We update can\_use\_next\_item = False. Since dp[3] != input[3] (2 != -1) or can\_use\_next\_item == False, we store output[3] = 2. We update can\_use\_next\_item = True. Since dp[4] == input[4] (2 == 2) and can\_use\_next\_item == True, we store output[4] = 1.

Reconstructing all together, output=[1, 2, 1, 2, 1].

Let\'s solve input = [0, 4, -2, 3, -3, -1]. dp[5] = max(input[5], 0) = max(-1, 0) = 0 dp[4] = max(input[4], input[5], 0) = max(-3, -1, 0) = 0 dp[3] = max(dp[4], input[3] + dp[5], 0) = max(0, 3 + 0, 0) = 3dp[2] = max(dp[3], input[2] + dp[4], 0) = max(3, -2 + 0, 0) =dp[1] = max(dp[2], input[1] + dp[3], 0) = max(3, 4 + 3, 0) = 7 dp[0] = max(dp[1], input[0] + dp[2], 0) = max(7, 0 + 3, 0) = 7Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output". Let can\_use\_next\_item = True. Since dp[0] != input[0] + dp[2] (7 != 0 + 3) or can\_use\_next\_item == False, we store output[0] = 2. We update can\_use\_next\_item = True. Since dp[1] == input[1] + dp[3] (7 == 4 + 3) and can\_use\_next\_item == True, we store output[1] = 1. We update can\_use\_next\_item = False. Since dp[2] != input[2] + dp[4] (3 != -2 + 0) or can\_use\_next\_item == False, we store output[2] = 2. We update can\_use\_next\_item = True. Since dp[3] == input[3] + dp[5] (3 == 3 + 0) and can\_use\_next\_item == True, we store output[3] = 1. We update can\_use\_next\_item = False. Since dp[4] != input[4] (0 != -3) or can\_use\_next\_item == False, we store output[4] = 2. We update can\_use\_next\_item = True. Since dp[5] != input[5] (0 != -1) or can\_use\_next\_item == False, we store output[5] = 2. Reconstructing all together, output=[2, 1, 2, 1, 2, 2]. Let\'s solve input = [-3, -4, 4, -1]. dp[3] = max(input[3], 0) = max(-1, 0) = 0 dp[2] = max(input[2], input[3], 0) = max(4, -1, 0) = 4 dp[1] = max(dp[2], input[1] + dp[3], 0) = max(4, -4 + 0, 0) =dp[0] = max(dp[1], input[0] + dp[2], 0) = max(4, -3 + 4, 0) =Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output". Let can use next item = True. Since dp[0] != input[0] + dp[2] (4 != -3 + 4) or can\_use\_next\_item == False, we store output[0] = 2. We update can\_use\_next\_item = True. Since dp[1] != input[1] + dp[3] (4 != -4 + 0) or can\_use\_next\_item == False, we store output[1] = 2. We update can\_use\_next\_item = True. Since dp[2] == input[2] (4 == 4) and can\_use\_next\_item == True, we store output[2] = 1. We update can\_use\_next\_item = False. Since dp[3] != input[3] (0 != -1) or can\_use\_next\_item == False, we store output[3] = 2. Reconstructing all together, output=[2, 2, 1, 2]. Let\'s solve input = [3, 4, -3, -1, -4]. dp[4] = max(input[4], 0) = max(-4, 0) = 0dp[3] = max(input[3], input[4], 0) = max(-1, -4, 0) = 0 dp[2] = max(dp[3], input[2] + dp[4], 0) = max(0, -3 + 0, 0) =0 dp[1] = max(dp[2], input[1] + dp[3], 0) = max(0, 4 + 0, 0) = 4 dp[0] = max(dp[1], input[0] + dp[2], 0) = max(4, 3 + 0, 0) = 4Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output". Let can\_use\_next\_item = True. Since dp[0] != input[0] + dp[2] (4 != 3 + 0) or can\_use\_next\_item == False, we store output[0] = 2. We update can\_use\_next\_item = True. Since dp[1] == input[1] + dp[3] (4 == 4 + 0) and can\_use\_next\_item == True, we store output[1] = 1. We update

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

can use next item = False.

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can\_use\_next\_item = True. Since dp[3] != input[3] + dp[5] (3 != 2 + 0) or can\_use\_next\_item == False, we store output[3] = 2. We update can\_use\_next\_item = True. Since dp[4] == input[4] (3 == 3) and can\_use\_next\_item == True,

we store output[4] = 1. We update can\_use\_next\_item == False. Since dp[5] != input[5] (0 != -4) or can\_use\_next\_item == False, we store output[5] = 2.

Reconstructing all together, output=[2, 1, 2, 2, 1, 2].

{prompt}

#### Listing 9: CoT Explicit prompts

cot\_explicit\_3s = """Given a sequence of integers, find a subsequence with the highest sum, such that no two numbers in the subsequence are adjacent in the original sequence.

To indicate the selected numbers, print an array with "1" for chosen numbers and "2" for unchosen ones. For instance, [1, 2, 2, 2, 2] implies selecting only the first number. If multiple solutions exist, select the lexicographically smallest.

We will solve any task instance by using dynamic programming. We define dp[i] as the maximum sum of a subsequence that does not include adjacent elements, when considering only the elements of the input from the i-th position onwards.

Let\'s solve input = [1, 1, -5, -1].

There are 4 numbers in the input sequence, so we will use a list of size 4 to store the dynamic programming values. We initialize all values to 0. dp[3] = max(input[3], 0) = max(-1, 0) = 0 dp[2] = max(input[2], input[3], 0) = max(-5, -1, 0) = 0 dp[1] = max(dp[2], input[1] + dp[3], 0) = max(0, 1 + 0, 0) = max(0, 1, 0) = 1 dp[0] = max(dp[1], input[0] + dp[2], 0) = max(1, 1 + 0, 0) = max(1, 1, 0) = 1 Finally, we reconstruct the lexicographically smallest

subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named " output".

Let can\_use\_next\_item = True. Since dp[0]=1, input[0]=1, dp[2]=0, input[0] + dp[2] = 1 == 1 = dp[0] and can\_use\_next\_item == True, we store output[0] = 1. We update can\_use\_next\_item = False. Since can\_use\_next\_item == False, we store output[1] = 2. We update can\_use\_next\_item = True. Since dp[2] = 0, input[2] = -5, dp[2] != input[2], we store output[2] = 2. We update can\_use\_next\_item = True. Since dp[3] = 0, input[3] = -1, dp[3] != input[3], we store output[3] = 2. Reconstructing all together, output=[1, 2, 2, 2]. Let\'s solve input = [3, 2, 1, -1, 2]. There are 5 numbers in the input sequence, so we will use a list of size 5 to store the dynamic programming values. We initialize all values to 0. dp[4] = max(input[4], 0) = max(2, 0) = 2 dp[3] = max(input[3], input[4], 0) = max(-1, 2, 0) = 2 dp[2] = max(dp[3], input[2] + dp[4], 0) = max(2, 1 + 2, 0) = max(2, 3, 0) = 3dp[1] = max(dp[2], input[1] + dp[3], 0) = max(3, 2 + 2, 0) = max(3, 4, 0) = 4dp[0] = max(dp[1], input[0] + dp[2], 0) = max(4, 3 + 3, 0) = max(4, 6, 0) = 6Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output". Let can\_use\_next\_item = True. Since dp[0]=6, input[0]=3, dp[2]=3, input[0] + dp[2] = 6 == 6 = dp[0] and can\_use\_next\_item == True, we store output[0] = 1. We update can\_use\_next\_item = False. Since can\_use\_next\_item == False, we store output[1] = 2. We update can\_use\_next\_item = True. Since dp[2]=3, input[2]=1, dp[4]=2, input[2] + dp[4] = 3 == 3 = dp[2] and can\_use\_next\_item == True, we store output[2] = 1. We update can\_use\_next\_item = False. Since can\_use\_next\_item == False, we store output[3] = 2. We update can\_use\_next\_item = True. Since dp[4] = 2, input[4] = 2, dp[4] == input[4] and can\_use\_next\_item == True, we store output[4] = 1. Reconstructing all together, output=[1, 2, 1, 2, 1]. Let\'s solve input = [0, 4, -2, 3, -3, -1]. There are 6 numbers in the input sequence, so we will use a list of size 6 to store the dynamic programming values. We initialize all values to 0. dp[5] = max(input[5], 0) = max(-1, 0) = 0 dp[4] = max(input[4], input[5], 0) = max(-3, -1, 0) = 0 dp[3] = max(dp[4], input[3] + dp[5], 0) = max(0, 3 + 0, 0) =max(0, 3, 0) = 3dp[2] = max(dp[3], input[2] + dp[4], 0) = max(3, -2 + 0, 0) = max(3, -2, 0) = 3dp[1] = max(dp[2], input[1] + dp[3], 0) = max(3, 4 + 3, 0) =max(3, 7, 0) = 7dp[0] = max(dp[1], input[0] + dp[2], 0) = max(7, 0 + 3, 0) = max(7, 3, 0) = 7Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output". Let can use next item = True. Since dp[0]=7, input[0]=0, dp[2]=3, input[0] + dp[2] = 3 != 7 = dp[0], we store output[0] = 2. We update can\_use\_next\_item = True. Since dp[1]=7, input[1]=4, dp[3]=3, input[1] + dp[3] = 7 == 7 = dp[1] and can\_use\_next\_item == True, we store output[1] = 1. We update can\_use\_next\_item = False. Since can\_use\_next\_item == False, we store output[2] = 2. We update can\_use\_next\_item = True. Since dp[3]=3, input[3]=3, dp[5]=0, input[3] + dp[5] = 3 == 3 = dp[3] and can\_use\_next\_item == True, we store output[3] = 1. We update can\_use\_next\_item = False.

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Since can\_use\_next\_item == False, we store output[4] = 2. We

cot\_explicit\_6s = """Given a sequence of integers, find a subsequence with the highest sum, such that no two numbers in the subsequence are adjacent in the original sequence. To indicate the selected numbers, print an array with "1" for chosen numbers and "2" for unchosen ones. For instance, [1, 2, 2, 2, 2] implies selecting only the first number. If multiple solutions exist, select the lexicographically smallest. We will solve any task instance by using dynamic programming. We define dp[i] as the maximum sum of a subsequence that does not include adjacent elements, when considering only the elements of the input from the i-th position onwards. Let\'s solve input = [1, 1, -5, -1]. There are 4 numbers in the input sequence, so we will use a list of size 4 to store the dynamic programming values. We initialize all values to 0. dp[3] = max(input[3], 0) = max(-1, 0) = 0 dp[2] = max(input[2], input[3], 0) = max(-5, -1, 0) = 0 dp[1] = max(dp[2], input[1] + dp[3], 0) = max(0, 1 + 0, 0) = max(0, 1, 0) = 1dp[0] = max(dp[1], input[0] + dp[2], 0) = max(1, 1 + 0, 0) = max(1, 1, 0) = 1Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output". Let can\_use\_next\_item = True. Since dp[0]=1, input[0]=1, dp[2]=0, input[0] + dp[2] = 1 == 1 = dp[0] and can\_use\_next\_item == True, we store output[0] = 1. We update can\_use\_next\_item = False. Since can\_use\_next\_item == False, we store output[1] = 2. We update can\_use\_next\_item = True. Since dp[2] = 0, input[2] = -5, dp[2] != input[2], we store output[2] = 2. We update can\_use\_next\_item = True. Since dp[3] = 0, input[3] = -1, dp[3] != input[3], we store output[3] = 2.Reconstructing all together, output=[1, 2, 2, 2].

update can use next item = True.

output[5] = 2.

{prompt}

Since dp[5] = 0, input[5] = -1, dp[5] != input[5], we store

Reconstructing all together, output=[2, 1, 2, 1, 2, 2].

Let\'s solve input = [3, 2, 1, -1, 2].

There are 5 numbers in the input sequence, so we will use a list of size 5 to store the dynamic programming values. We initialize all values to 0. dp[4] = max(input[4], 0) = max(2, 0) = 2 dp[3] = max(input[3], input[4], 0) = max(-1, 2, 0) = 2 dp[2] = max(dp[3], input[2] + dp[4], 0) = max(2, 1 + 2, 0) = max(2, 3, 0) = 3dp[1] = max(dp[2], input[1] + dp[3], 0) = max(3, 2 + 2, 0) =

 $\max(3, 4, 0) = 4$  $dp[0] = \max(dp[1], input[0] + dp[2], 0) = \max(4, 3 + 3, 0) = \max(4, 6, 0) = 6$ 

Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named " output".

Let can\_use\_next\_item = True. Since dp[0]=6, input[0]=3, dp[2]=3, input[0] + dp[2] = 6 == 6 = dp[0] and can\_use\_next\_item == True, we store output[0] = 1. We update can\_use\_next\_item = False.

Since can\_use\_next\_item == False, we store output[1] = 2. We update can\_use\_next\_item = True.

Since dp[2]=3, input[2]=1, dp[4]=2, input[2] + dp[4] = 3 == 3 = dp[2] and can\_use\_next\_item == True, we store output[2] = 1. We update can\_use\_next\_item = False.

Since can\_use\_next\_item == False, we store output[3] = 2. We update can\_use\_next\_item = True.

Since dp[4] = 2, input[4] = 2, dp[4] == input[4] and dp[4] = max(input[4], 0) = max(-4, 0) = 0dp[3] = max(input[3], input[4], 0) = max(-1, -4, 0) = 0can use next item == True, we store output[4] = 1. dp[2] = max(dp[3], input[2] + dp[4], 0) = max(0, -3 + 0, 0) =Reconstructing all together, output=[1, 2, 1, 2, 1]. max(0, -3, 0) = 0dp[1] = max(dp[2], input[1] + dp[3], 0) = max(0, 4 + 0, 0) =Let\'s solve input = [0, 4, -2, 3, -3, -1]. There are 6 numbers in the input sequence, so we will use a list of size 6 to store the dynamic programming values. We initialize all values to 0. dp[5] = max(input[5], 0) = max(-1, 0) = 0dp[4] = max(input[4], input[5], 0) = max(-3, -1, 0) = 0 dp[3] = max(dp[4], input[3] + dp[5], 0) = max(0, 3 + 0, 0) = max(0, 3, 0) = 3dp[2] = max(dp[3], input[2] + dp[4], 0) = max(3, -2 + 0, 0) =max(3, -2, 0) = 3dp[1] = max(dp[2], input[1] + dp[3], 0) = max(3, 4 + 3, 0) = max(3, 7, 0) = 7dp[0] = max(dp[1], input[0] + dp[2], 0) = max(7, 0 + 3, 0) =max(7, 3, 0) = 7Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output". Let can\_use\_next\_item = True. Since dp[0]=7, input[0]=0, dp[2]=3, input[0] + dp[2] = 3 != 7 = dp[0], we store output[0] = 2. We update can\_use\_next\_item = True. Since dp[1]=7, input[1]=4, dp[3]=3, input[1] + dp[3] = 7 == 7 = dp[1] and can\_use\_next\_item == True, we store output[1] = 1. We update can\_use\_next\_item = False. Since can\_use\_next\_item == False, we store output[2] = 2. We update can\_use\_next\_item = True. Since dp[3]=3, input[3]=3, dp[5]=0, input[3] + dp[5] = 3 == 3 = dp[3] and can\_use\_next\_item == True, we store output[3] = 1. We update can\_use\_next\_item = False. Since can\_use\_next\_item == False, we store output[4] = 2. We update can\_use\_next\_item = True. Since dp[5] = 0, input[5] = -1, dp[5] != input[5], we store output[5] = 2.Reconstructing all together, output=[2, 1, 2, 1, 2, 2]. Let\'s solve input = [-3, -4, 4, -1]. There are 4 numbers in the input sequence, so we will use a list of size 4 to store the dynamic programming values. We initialize all values to 0. dp[3] = max(input[3], 0) = max(-1, 0) = 0 dp[2] = max(input[2], input[3], 0) = max(4, -1, 0) = 4 dp[1] = max(dp[2], input[1] + dp[3], 0) = max(4, -4 + 0, 0) =max(4, -4, 0) = 4dp[0] = max(dp[1], input[0] + dp[2], 0) = max(4, -3 + 4, 0) =max(4, 1, 0) = 4Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output". Let can\_use\_next\_item = True. Since dp[0]=4, input[0]=-3, dp[2]=4, input[0] + dp[2] = 1 != 4 = dp[0], we store output[0] = 2. We update can\_use\_next\_item = True. Since dp[1]=4, input[1]=-4, dp[3]=0, input[1] + dp[3] = -4 != 4 = dp[1], we store output[1] = 2. We update can\_use\_next\_item = True. Since dp[2] = 4, input[2] = 4, dp[2] == input[2] and can\_use\_next\_item == True, we store output[2] = 1. We update can\_use\_next\_item = False. Since can\_use\_next\_item == False, we store output[3] = 2. Reconstructing all together, output=[2, 2, 1, 2]. Let\'s solve input = [3, 4, -3, -1, -4].

There are 5 numbers in the input sequence, so we will use a

list of size 5 to store the dynamic programming values. We

initialize all values to 0.

max(0, 4, 0) = 4dp[0] = max(dp[1], input[0] + dp[2], 0) = max(4, 3 + 0, 0) = max(4, 3, 0) = 4Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output". Let can\_use\_next\_item = True. Since dp[0]=4, input[0]=3, dp[2]=0, input[0] + dp[2] = 3 != 4 = dp[0], we store output[0] = 2. We update can\_use\_next\_item = True. Since dp[1]=4, input[1]=4, dp[3]=0, input[1] + dp[3] = 4 == 4 = dp[1] and can\_use\_next\_item == True, we store output[1] = 1. We update can\_use\_next\_item = False. Since can\_use\_next\_item == False, we store output[2] = 2. We update can\_use\_next\_item = True. Since dp[3] = 0, input[3] = -1, dp[3] != input[3], we store output[3] = 2. We update can\_use\_next\_item = True. Since dp[4] = 0, input[4] = -4, dp[4] != input[4], we store output[4] = 2.Reconstructing all together, output=[2, 1, 2, 2, 2]. Let\'s solve input = [-4, 5, 0, 2, 3, -4]. There are 6 numbers in the input sequence, so we will use a list of size 6 to store the dynamic programming values. We initialize all values to 0. dp[5] = max(input[5], 0) = max(-4, 0) = 0 dp[4] = max(input[4], input[5], 0) = max(3, -4, 0) = 3 dp[3] = max(dp[4], input[3] + dp[5], 0) = max(3, 2 + 0, 0) = max(3, 2, 0) = 3dp[2] = max(dp[3], input[2] + dp[4], 0) = max(3, 0 + 3, 0) = max(3, 3, 0) = 3dp[1] = max(dp[2], input[1] + dp[3], 0) = max(3, 5 + 3, 0) =max(3, 8, 0) = 8dp[0] = max(dp[1], input[0] + dp[2], 0) = max(8, -4 + 3, 0) =max(8, -1, 0) = 8Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output". Let can\_use\_next\_item = True. Since dp[0]=8, input[0]=-4, dp[2]=3, input[0] + dp[2] = -1 != 8 = dp[0], we store output[0] = 2. We update can\_use\_next\_item = True. Since dp[1]=8, input[1]=5, dp[3]=3, input[1] + dp[3] = 8 == 8 = dp[1] and can\_use\_next\_item == True, we store output[1] = 1. We update can\_use\_next\_item = False. Since can\_use\_next\_item == False, we store output[2] = 2. We update can\_use\_next\_item = True. Since dp[3]=3, input[3]=2, dp[5]=0, input[3] + dp[5] = 2 != 3 = dp[3], we store output[3] = 2. We update can\_use\_next\_item = True. Since dp[4] = 3, input[4] = 3, dp[4] == input[4] and can\_use\_next\_item == True, we store output[4] = 1. We update can\_use\_next\_item = False. Since can\_use\_next\_item == False, we store output[5] = 2.

Reconstructing all together, output=[2, 1, 2, 2, 1, 2].

{prompt}

#### **Comparison between CoT Implicit and E.3** CoT Explicit

#### Listing 10: Compare CoT Implicit with CoT Explicit

Given a sequence of integers, find a subsequence with the highest sum, such that no two numbers in the subsequence are adjacent in the original sequence.

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To indicate the selected numbers, print an array with "1" for chosen numbers and "2" for unchosen ones. For instance, [1, 2, 2, 2, 2] implies selecting only the first number. If multiple solutions exist, select the lexicographically smallest.

We will solve any task instance by using dynamic programming. We define dp[i] as the maximum sum of a subsequence that does not include adjacent elements, when considering only the elements of the input from the i-th position onwards.

Let's solve input = [-45, 40, 77, -93, 25, -73].

#### ###

Explicit: There are 6 numbers in the input sequence, so we will use a list of size 6 to store the dynamic programming values. We initialize all values to 0. dp[5] = max(input[5], 0) = max(-73, 0) = 0 dp[4] = max(input[4], input[5], 0) = max(25, -73, 0) = 25 Implicit: dp[3] = max(dp[4], input[3] + dp[5], 0) = max(25, -93 + 0, 0) = 25 Explicit: dp[3] = max(dp[4], input[3] + dp[5], 0) = max(25,  $-93 + 0, 0) = \max(25, -93, 0) = 25$ Implicit: dp[2] = max(dp[3], input[2] + dp[4], 0) = max(25, 77 + 25, 0) = 102Explicit: dp[2] = max(dp[3], input[2] + dp[4], 0) = max(25, 77 + 25, 0) = max(25, 102, 0) = 102Implicit: dp[1] = max(dp[2], input[1] + dp[3], 0) = max(102, 40 + 25, 0) = 102 Explicit: dp[1] = max(dp[2], input[1] + dp[3], 0) = max(102, 40 + 25, 0) = max(102, 65, 0) = 102 Implicit: dp[0] = max(dp[1], input[0] + dp[2], 0) = max(102, -45 + 102, 0) = 102 Explicit: dp[0] = max(dp[1], input[0] + dp[2], 0) = max(102, -45 + 102, 0) = max(102, 57, 0) = 102Finally, we reconstruct the lexicographically smallest subsequence that fulfills the task objective by selecting numbers as follows. We store the result on a list named output" Let can\_use\_next\_item = True. Implicit: Since dp[0] != input[0] + dp[2] (102 != -45 + 102)
or can\_use\_next\_item == False, we store output[0] = 2. We update can\_use\_next\_item = True. . Explicit: Since dp[0]=102, input[0]=-45, dp[2]=102, input[0] + dp[2] = 57 != 102 = dp[0], we store output[0] = 2. We update can\_use\_next\_item = True. Implicit: Since dp[1] != input[1] + dp[3] (102 != 40 + 25) or can\_use\_next\_item == False, we store output[1] = 2. We update can\_use\_next\_item = True. Explicit: Since dp[1]=102, input[1]=40, dp[3]=25, input[1] + dp[3] = 65 != 102 = dp[1], we store output[1] = 2. We update can\_use\_next\_item = True. Implicit: Since dp[2] == input[2] + dp[4] (102 == 77 + 25) and can\_use\_next\_item == True, we store output[2] = 1. We update can\_use\_next\_item = False. Explicit: Since dp[2]=102, input[2]=77, dp[4]=25, input[2] + dp[4] = 102 == 102 = dp[2] and can\_use\_next\_item == True, we store output[2] = 1. We update can\_use\_next\_item = False.
Implicit: Since dp[3] != input[3] + dp[5] (25 != -93 + 0) or can\_use\_next\_item == False, we store output[3] = 2. We update can\_use\_next\_item = True. Explicit: Since can\_use\_next\_item == False, we store output[3] = 2. We update can\_use\_next\_item = True. Implicit: Since dp[4] == input[4] (25 == 25) and can\_use\_next\_item == True, we store output[4] = 1. We update can\_use\_next\_item = False. Explicit: Since dp[4] = 25, input[4] = 25, dp[4] == input[4] and can\_use\_next\_item == True, we store output[4] = 1. We update can\_use\_next\_item = False. Implicit: Since dp[5] != input[5] (0 != -73) o can\_use\_next\_item == False, we store output[5] = 2. Explicit: Since can\_use\_next\_item == False, we store output[5] = 2.

Reconstructing all together, output=[2, 2, 1, 2, 1, 2].

#### **E.4** Travel planning prompts

Listing 11: CoT prompts

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prompt\_cot\_zero\_shot = """

The user will ask for a flight route between two cities. You need to generate a response with the route. Your response should be in the format "[city 1]-[city 2]-[city 3]-...-[city n]". If there is no solution, reply "Answer: None. Question: {input} Answer:

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prompt\_cot\_1s = """ The user will ask for a flight route between two cities. You need to generate a response with the route. Your response should be in the format "Answer: [city 1]-[city 2]-[city 3]-...-[city n]". If there is no solution, reply "Answer: None.

Ouestion: What is the flight route from Dublin to Sydney? Answer: Dublin-London-Sydney. Question: {input} Answer:

prompt\_cot\_3s = """

The user will ask for a flight route between two cities. You need to generate a response with the route. Your response should be in the format "[city 1]-[city 2]-[city 3]-...-[city n]". If there is no solution, reply "Answer: None. Question: What is the flight route from Dublin to Sydney? Answer: Dublin-London-Sydney. Question: What is the flight route from New York to Amsterdam? Answer: New York-London-Amsterdam. Question: What is the flight route from Toronto to Sydney? Answer: Toronto-San Francisco-Sydney. Question: {input} Answer: prompt\_cot\_8s = """ The user will ask for a flight route between two cities. You need to generate a response with the route. Your response should be in the format "[city 1]-[city 2]-[city 3]-...-[city n]". If there is no solution, reply "Answer: None. " Question: What is the flight route from Dublin to Sydney? Answer: Dublin-London-Svdnev. Question: What is the flight route from New York to Amsterdam? Answer: New York-London-Amsterdam. Question: What is the flight route from Toronto to Sydney? Answer: Toronto-San Francisco-Sydney. Question: What is the flight route from Astana to Rome? Answer: Astana-Moscow-Rome.

Question: What is the flight route from Visakhapatnam to Odense?

Answer: Visakhapatnam-Hyderabad-Copenhagen-Odense. Question: What is the flight route from Shanghai to Nanjing? Answer: Shanghai-Nanjing.

Question: What is the flight route from Singapore to Taipei? Answer: Singapore-Taipei.

Question: What is the flight route from Sydney to Istanbul? Answer: Sydney-Singapore-Istanbul. Question: {input} Answer: """

### Listing 12: ToT prompts

prompt\_tot\_propose\_zero\_shot = '''List a few possible cities to fly to from the current city via one direct flight. If the goal city can be reached via one direct flight from the current city, just answer the goal city. Format of your response is "Answer: [city 1], [city 2], [city 3], ... [city n ٦.

Question: {input}

prompt\_tot\_propose\_1s = '''List the a few possible cities to fly to from the current city via one direct flight. If the goal city can be reached via one direct flight from the current city, just answer the goal city. Format of your response is "Answer: [city 1], [city 2], [city 3], ... [city n י ר Question: You want to go to Sydney and you are at Dublin. Propose a few possible cities with direct flights to go to for the next step. Answer: London, Paris, Frankfurt, Amsterdam, Zurich. Question: {input}

prompt\_tot\_propose\_3s = '''List the a few possible cities to fly to from the current city via one direct flight. If the goal city can be reached via one direct flight from the current city, just answer the goal city. Format of your response is "Answer: [city 1], [city 2], [city 3], ... [city n Ouestion: You want to go to Sydney and you are at Dublin. Propose a few possible cities with direct flights to go to for the next step. Answer: London, Paris, Mombai. Question: You want to go to Nanjing and you are at Shanghai. Propose a few possible cities with direct flights to go to for the next step. Answer: Nanjing. Question: You want to go to Amsterdam and you are at New York. Propose a few possible cities with direct flights to go to for the next step. Answer: London, Paris, Frankfurt, Amsterdam. Question: {input} prompt\_tot\_propose\_8s = '''List the a few possible cities to fly to from the current city via one direct flight. If the goal city can be reached via one direct flight from the current city, just answer the goal city. Format of your response is "Answer: [city 1], [city 2], [city 3], ... [city n יי ר Question: You want to go to Sydney and you are at Dublin. Propose a few possible cities with direct flights to go to for the next step. Answer: London, Paris, Mombai. Question: You want to go to Amsterdam and you are at New York. Propose a few possible cities with direct flights to go to for the next step. Answer: London, Paris, Frankfurt. Question: You want to go to Sydney and you are at Toronto. Propose a few possible cities with direct flights to go to for the next step. Answer: San Francisco, Los Angeles, Vancouver. Question: You want to go to Nanjing and you are at Shanghai. Propose a few possible cities with direct flights to go to for the next step. Answer: Nanjing. Question: You want to go to Rome and you are at Astana. Propose a few possible cities with direct flights to go to for the next step. Answer: Moscow, Rome, Istanbul. Question: You want to go to Odense and you are at Visakhapatnam. Propose a few possible cities with direct flights to go to for the next step. Answer: Hyderabad, Copenhagen, Odense, Question: You want to go to Taipei and you are at Singapore. Propose a few possible cities with direct flights to go to for the next step. Answer: Taipei. Question: You want to go to Istanbul and you are at Sydney. Propose a few possible cities with direct flights to go to for the next step. Answer: Singapore, Dubai, Abu Dhabi. Question: {input} Listing 13: ToT Linear prompts

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prompt\_tot\_linear\_zero\_shot = """The user will ask for a flight route between two cities. You need to generate a response with the route.

- You are simulating bfs process to find the route between two cities. In the beginning, you have a queue ['start city'] and an empty explored list []. You need to proceed with the following steps:
- 1. Take the first city in the queue as the current city. If the city is in the explored list, skip it. Otherwise, put the city into the explored list.

2. Propose the possible cities with direct flights to go to for the next step. Do not propose the explored cities and cities in the queue.

3. Put the cities into the queue.

Repeat steps 1-3 until the goal city is included in the queue. Respond with reasoning steps, and end with the answer, in the format "Answer: [city 1]-[city 2]-[city 3]-...-[city n]" Question: {input}

Let's think step by step.

prompt\_tot\_linear\_cot\_1s = """The user will ask for a flight route between two cities. You need to generate a response with the route.

You are simulating bfs process to find the route between two cities. In the beginning, you have a queue ['start city'], and you need to proceed the following steps:

format "Answer: [city 1]-[city 2]-[city 3]-...-[city n]" Question: What is the flight route from Guatemala City to Guangzhou? The queue is [Guatemala City]. Take the first path, Guatemala City, from the queue. The current city is Guatemala City, which is not in the explored list. Thus, put the current city into the explored list. The explored list is [Guatemala City] The current city is Guatemala City and the goal is Guangzhou. For the next step, the promising cities to go to are [New York, Los Angeles, Mexico City]. Puting those cities into the queue. The queue is [Guatemala City-New York, Guatemala City-Los Angeles, Guatemala City-Mexico City]. Take the first path, Guatemala City-New York, from the queue. The current city is New York, which is not in the explored list. Thus, put the current city into the explored list. The explored list is [Guatemala City, New York] The current city is New York and the goal is Guangzhou. For the next step, the promising cities to go to are [Helsinki, Guangzhou, Lahorel. The goal city is Guangzhou. Since Guangzhou is in the found, and the current selected path is Guatemala City-New York, the route is Guatemala City-New York-Guangzhou. Answer: Guatemala City-New York-Guangzhou Question: {input} Let's think step by step. prompt\_tot\_linear\_cot\_2s = """The user will ask for a flight route between two cities. You need to generate a response with the route. You are simulating bfs process to find the route between two cities. In the beginning, you have a queue ['start city'], and you need to proceed the following steps: 1. Take the first city in the queue as the current city. 2. Propose the possible cities with direct flights to go to for the next step. Do not propose the explored cities and

1. Take the first city in the queue as the current city.

cities in the queue.

3. Put the cities into the queue.

2. Propose the possible cities with direct flights to go to

Repeat steps 1-3 until the goal city is included in the queue.

Respond with reasoning steps, and end with the answer, in the

for the next step. Do not propose the explored cities and

cities in the queue. 3. Put the cities into the queue.

Repeat steps 1-3 until the goal city is included in the queue. Respond with reasoning steps, and end with the answer, in the format "Answer: [city 1]-[city 2]-[city 3]-...-[city n]' Question: What is the flight route from Guatemala City to Guangzhou?

The queue is [Guatemala City]. Take the first path, Guatemala City, from the queue.

The current city is Guatemala City, which is not in the explored list. Thus, put the current city into the explored list. The explored list is [Guatemala City]

The current city is Guatemala City and the goal is Guangzhou. For the next step, the promising cities to go to are [New York, Los Angeles, Mexico City].

Puting those cities into the queue. The queue is [Guatemala City-New York, Guatemala City-Los Angeles, Guatemala City-Mexico City].

Take the first path. Guatemala City-New York, from the queue. The current city is New York, which is not in the explored list. Thus, put the current city into the explored list. The explored list is [Guatemala City, New York]

The current city is New York and the goal is Guangzhou. For the next step, the promising cities to go to are [Helsinki, Guangzhou, Lahore].

The goal city is Guangzhou. Since Guangzhou is in the found, and the current selected path is Guatemala City-New York, the route is Guatemala City-New York-Guangzhou. Answer: Guatemala City-New York-Guangzhou

Question: What is the flight route from Tegucigalpa to Helsinki?

The queue is [Tegucigalpa]. Take the first path, Tegucigalpa, from the queue.

The current city is Tegucigalpa, which is not in the explored list. Thus, put the current city into the explored list. The explored list is [Tegucigalpa]

The current city is Tegucigalpa and the goal is Helsinki. For the next step, the promising cities to go to are [Guatemala City, Miami].

Puting those cities into the queue. The queue is [Tegucigalpa-Guatemala City, Tegucigalpa-Miami].

Take the first path, Tegucigalpa-Guatemala City, from the

aueue. The current city is Guatemala City, which is not in the explored list. Thus, put the current city into the explored list. The explored list is [Tegucigalpa, Guatemala City] The current city is Guatemala City and the goal is Helsinki. For the next step, the promising cities to go to are [New York, Los Angeles, Mexico City]. Puting those cities into the queue. The queue is [Tegucigalpa-Miami, Tegucigalpa-Guatemala City-New York, Tegucigalpa-Guatemala City-Los Angeles, Tegucigalpa-Guatemala City-Mexico City]. Take the first path, Tegucigalpa-Miami, from the queue. The current city is Miami, which is not in the explored list. Thus, put the current city into the explored list. The explored list is [Tegucigalpa, Guatemala City, Miami] The current city is Miami and the goal is Helsinki. For the next step, the promising cities to go to are [Sao Paulo, Buenos Aires, Chicago]. Puting those cities into the queue. The queue is [Tegucigalpa-Guatemala City-New York, Tegucigalpa-Guatemala City-Los Angeles, Tegucigalpa-Guatemala City-Mexico City, Tegucigalpa-Miami-Sao Paulo, Tegucigalpa-Miami-Buenos Aires, Tegucigalpa-Miami-Chicago]. Take the first path, Tegucigalpa-Guatemala City-New York, from the queue. The current city is New York, which is not in the explored list. Thus, put the current city into the explored list. The explored list is [Tegucigalpa, Guatemala City, Miami, New York The current city is New York and the goal is Helsinki. For the next step, the promising cities to go to are [Helsinki, Guangzhou, Lahore]. The goal city is Helsinki. Since Helsinki is in the found, and the current selected path is Tegucigalpa-Guatemala City-New York, the route is Tegucigalpa-Guatemala City-New York-Helsinki. Answer: Tegucigalpa-Guatemala City-New York-Helsinki Question: {input} Let's think step by step.

#### E.5 Game of 24 prompts

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#### Listing 14: CoT prompts

cot\_prompt\_1s = '''Use numbers and basic arithmetic operations (+ -  $\star$  /) to obtain 24. Each step, you are only allowed to choose two of the remaining numbers to obtain a new number. Please strictly follow the format of the example. Do not include unnecessary information in your output. Do not include serial numbers that are not in the example. Input: 4 4 6 8 Steps: 4 + 8 = 12 (left: 4 6 12) 6 - 4 = 2 (left: 2 12) 2 \* 12 = 24 (left: 24) Answer: (6 - 4) \* (4 + 8) = 24Input: {input} cot\_prompt\_3s = '''Use numbers and basic arithmetic operations (+ - \* /) to obtain 24. Each step, you are only allowed to choose two of the remaining numbers to obtain a new number. Please strictly follow the format of the example. Do not include unnecessary information in your output. Do not include serial numbers that are not in the example. Input: 4 4 6 8 Steps: 4 + 8 = 12 (left: 4 6 12) 6 - 4 = 2 (left: 2 12)

2 \* 12 = 24 (left: 24) Answer: (6 - 4) \* (4 + 8) = 24 Input: 2 9 10 12 Steps: 12 \* 2 = 24 (left: 9 10 24) 10 - 9 = 1 (left: 1 24) 24 \* 1 = 24 (left: 24) Answer:  $(12 \times 2) \times (10 - 9) = 24$ Input: 4 9 10 13 Steps: 13 - 10 = 3 (left: 3 4 9) 9 - 3 = 6 (left: 4 6) 4 \* 6 = 24 (left: 24) Answer: 4 \* (9 - (13 - 10)) = 24 Input: {input}

cot\_prompt\_5s = '''Use numbers and basic arithmetic operations (+ - \* /) to obtain 24. Each step, you are only allowed to choose two of the remaining numbers to obtain a new number. Please strictly follow the format of the example. Do not include unnecessary information in your output. Do not include serial numbers that are not in the example. Input: 4 4 6 8 Steps: 4 + 8 = 12 (left: 4 6 12) 6 - 4 = 2 (left: 2 12) 2 \* 12 = 24 (left: 24) Answer: (6 - 4) \* (4 + 8) = 24Input: 2 9 10 12 Steps: 12 \* 2 = 24 (left: 9 10 24) 10 - 9 = 1 (left: 1 24) 24 \* 1 = 24 (left: 24) Answer: (12 \* 2) \* (10 - 9) = 24Input: 4 9 10 13 Steps: 13 - 10 = 3 (left: 3 4 9) 9 - 3 = 6 (left: 4 6) 4 \* 6 = 24 (left: 24) Answer: 4 \* (9 - (13 - 10)) = 24 Input: 1 4 8 8 Steps: 8 / 4 = 2 (left: 1 2 8) 1 + 2 = 3 (left: 3 8) 3 \* 8 = 24 (left: 24) Answer: (1 + 8 / 4) \* 8 = 24Input: 5 5 5 9 Steps: 5 + 5 = 10 (left: 5 9 10) 10 + 5 = 15 (left: 9 15) 15 + 9 = 24 (left: 24) Answer: ((5 + 5) + 5) + 9 = 24 Input: {input}

#### Listing 15: ToT prompts

propose\_prompt\_1s = '''Use numbers and basic arithmetic operations (+ - \* /) to propose possible next steps of operation. Each step, you are only allowed to choose two of the input numbers to obtain a new number. Do not include serial numbers that are not in the example. Do not include unnecessary information in your output. Input: 2 8 8 14 Possible next steps: 2 + 8 = 10 (left: 8 10 14) 8 / 2 = 4 (left: 4 8 14) 14 + 2 = 16 (left: 8 8 16) 2 \* 8 = 16 (left: 8 14 16) 8 - 2 = 6 (left: 6 8 14) 14 - 8 = 6 (left: 2 6 8) 14 / 2 = 7 (left: 7 8 8) 14 - 2 = 12 (left: 8 8 12) Input: {input} Possible next steps: propose\_prompt\_3s = '''Use numbers and basic arithmetic operations (+ - \* /) to propose possible next steps of operation. Each step, you are only allowed to choose two of the input numbers to obtain a new number. Do not include serial numbers that are not in the example. Do not include unnecessary information in your output. Input: 2 8 8 14 Possible next steps: 2 + 8 = 10 (left: 8 10 14) 8 / 2 = 4 (left: 4 8 14) 14 + 2 = 16 (left: 8 8 16) 2 \* 8 = 16 (left: 8 14 16) 8 - 2 = 6 (left: 6 8 14) 14 - 8 = 6 (left: 2 6 8) 14 / 2 = 7 (left: 7 8 8) 14 - 2 = 12 (left: 8 8 12) Input: 1 2 7 10 Possible next steps: 1 + 2 = 3 (left: 3 7 10) 2 + 7 = 9 (left: 1 9 10) 7 + 10 = 17 (left: 1 2 17) 1 \* 2 = 2 (left: 2 7 10) 2 \* 7 = 14 (left: 1 14 10)

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7 * 10 = 70 (left: 1 2 70) 1 - 2 = -1 (left: -1 7 10) 2 - 7 = -5 (left: 1 -5 10) 7 - 10 = -3 (left: 1 2 -3) 1 / 2 = 0.5 (left: 0.5 7 10) 2 / 7 = 0.29 (left: 1 0.29 10) 7 / 10 = 0.7 (left: 1 2 0.7)
<pre>Input: 4 4 6 8 Possible next steps: 4 + 4 = 8 (left: 6 8 8) 4 + 6 = 10 (left: 8 10 8) 6 + 8 = 14 (left: 4 14 8)</pre>
4 * 4 = 16 (left: 6 8 16) 4 * 6 = 24 (left: 8 24 8) 6 * 8 = 48 (left: 4 48 8) 4 - 4 = 0 (left: 0 6 8) 4 - 6 = -2 (left: -2 8 8) 6 - 8 = -2 (left: 4 -2 8)
<pre>4 / 4 = 1 (left: 1 6 8) 4 / 6 = 0.67 (left: 8 0.67 8) 6 / 8 = 0.75 (left: 4 0.75 8) Input: {input} Possible next steps: '''</pre>
<pre>propose_prompt_5s = '''Use numbers and basic arithmetic operations (+ - * /) to propose possible next steps of operation. Each step, you are only allowed to choose two of the input numbers to obtain a new number. Do not include serial numbers that are not in the example. Do</pre>
not include unnecessary information in your output. Input: 2 8 8 14 Possible next steps: 2 + 8 = 10 (left: 8 10 14)
8 / 2 = 4 (left: 4 8 14) 14 + 2 = 16 (left: 8 8 16) 2 * 8 = 16 (left: 8 14 16) 8 - 2 = 6 (left: 6 8 14)
14 - 8 = 6 (left: 2 6 8) 14 / 2 = 7 (left: 7 8 8) 14 - 2 = 12 (left: 8 8 12) Input: 1 2 7 10
Possible next steps: 1 + 2 = 3 (left: 3 7 10) 2 + 7 = 9 (left: 1 9 10) 7 + 10 = 17 (left: 1 2 17)
1 * 2 = 2 (left: 2 7 10) 2 * 7 = 14 (left: 1 14 10) 7 * 10 = 70 (left: 1 2 70) 1 - 2 = -1 (left: -1 7 10)
2 - 7 = -5 (left: 1 - 5 10) 7 - 10 = -3 (left: 1 2 - 3) 1 / 2 = 0.5 (left: 0.5 7 10) 2 / 7 = 0.29 (left: 1 0.29 10)
7 / 10 = 0.7 (left: 1 2 0.7) Input: 4 4 6 8 Possible next steps: 4 + 4 = 8 (left: 6 8 8)
$\begin{array}{l} 4 + 6 = 10 \ (\text{left: 8 10 8}) \\ 6 + 8 = 14 \ (\text{left: 4 14 8}) \\ 4 * 4 = 16 \ (\text{left: 6 8 16}) \\ 4 * 6 = 24 \ (\text{left: 8 24 8}) \end{array}$
$ \begin{array}{l} 6 + 8 = 48 \ (\text{left: } 4 \ 48 \ 8) \\ 4 - 4 = 0 \ (\text{left: } 0 \ 6 \ 8) \\ 4 - 6 = -2 \ (\text{left: } -2 \ 8 \ 8) \\ 6 - 8 = -2 \ (\text{left: } 4 -2 \ 8) \end{array} $
4 / 4 = 1 (left: 1 6 8) 4 / 6 = 0.67 (left: 8 0.67 8) 6 / 8 = 0.75 (left: 4 0.75 8) Input: 3 4 5 6
Possible next steps: 3 + 4 = 7 (left: 5 6 7) 4 + 5 = 9 (left: 6 9 7) 4 + 6 = 10 (left: 5 10 7)
5 + 6 = 11 (left: 4 11 7) 3 * 4 = 12 (left: 5 6 12) 4 * 5 = 20 (left: 6 20 7) 4 * 6 = 24 (left: 5 24 7)
5 * 6 = 30 (left: 4 30 7) 3 - 4 = -1 (left: -1 5 6) 4 - 5 = -1 (left: 6 -1 7) 4 - 6 = -2 (left: 5 -2 7)
5 - 6 = -1 (left: 4 - 1 7) $3 / 4 = 0.75 (left: 0.75 5 6)$ $4 / 5 = 0.8 (left: 6 0.8 7)$ $4 / 6 = 0.67 (left: 5 0.67 7)$ $5 / 6 = 0.62 (left: 4 0.82 7)$
5 / 6 = 0.83 (left: 4 0.83 7)

Input: 2 4 6	2860
•	
Possible next steps:	2861
2 + 4 = 6 (left: 6 6)	2862
4 + 6 = 10 (left: 6 10)	2863
2 * 4 = 8 (left: 6 8)	2864
4 * 6 = 24 (left: 6 24)	2865
2 - 4 = -2 (left: -2 6)	2866
4 - 6 = -2 (left: 8 -2)	2867
2 / 4 = 0.5 (left: 0.5 6)	2868
4 / 6 = 0.67 (left: 8 0.67)	2869
Input: {input}	2870
Possible next steps:	2871
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## E.5.1 ToT Decomp prompts

### Listing 16: ToT Decomp prompts

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For example for example for example for example for example for example for each of the format of th	<pre>ample, (2) 8 8 (14 of the example. include serial nc clude unnecessary 1 2 7 10 all combinations 1 2 7 10 all combinations (7) 10 (7) 10 (7) 10 (7) 10 (7) 10 (7) 10 (7) 10 (7) 10 (10) 7 (10) 7 (10) { (input} all combinations</pre>	4) means select umbers that are information in of two numbers	using bracket.
For exa format Do not input: Select Output (7) (8) (7) 8 Input: Output	ample, (2) 8 8 (14 of the example. include serial nu clude unnecessary 7 8 9 all combinations : ) 9 (9) (9) (2.33 6	4) means select umbers that are information in	
Select Output (1) (2) 1 (2) 1 2 (7) (1) 2 (1) 2 1 (2) Input:	1 2 7 10 all combinations 7 10 (7) 10 (7) 10 (7) 10 7 (10) 7 (10) 7 (10) 7 (10) 8 (input) all combinations		
For exa format Do not not ind Input: Select Output (7) (8) (7) 8 Input: Output (2.33) Input:	<pre>ample, (2) 8 8 (14 of the example. include serial nu clude unnecessary 7 8 9 all combinations (9) 2.33 6 (6) 1 2 7 10 all combinations :</pre>	4) means select umbers that are information in of two numbers	using bracket.
() (2	,		

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1 (2) (7) 10 1 2 (7) (10) (1) 2 (7) 10 (1) 2 7 (10) 1 (2) 7 (10) Input: 0.66 8 9 Select all combinations of two numbers using bracket. Output: (0.66) (8) 9 0.66 (8) (9) (0.66) 8 (9) Input: 2 8 8 14 Select all combinations of two numbers using bracket. Output: (2) (8) 8 14 2 (8) (8) 14 2 8 (8) (14) (2) 8 (8) 14 (2) 8 8 (14) 2 (8) 8 (14) Input: {input} Select all combinations of two numbers using bracket. Output: propose\_prompt\_1s = '''Use the two numbers in the bracket and basic arithmetic operations to propose possible next steps. Then, remove the selected numbers by the new number. Use the format '(left: ...)' to present the remaining numbers. Do not include serial numbers that are not in the example. Do not include unnecessary information in your output. Input: (2) 8 8 (14) 2 + 14 = 16, replace 2 14 by 16 (left: 8 8 16) 2 \* 14 = 28, replace 2 14 by 28 (left: 8 8 28) 2 / 14 = 0.14, replace 2 14 by 0.14 (left: 8 8 0.14) 14 / 2 = 7, replace 2 14 by 7 (left: 8 8 7) 14 - 2 = 12, replace 2 14 by 12 (left: 8 8 12) 2 - 14 = -12, replace 2 14 by -12 (left: 8 8 -12) Input: {input} propose\_prompt\_3s = '''Use the two numbers in the bracket and basic arithmetic operations to propose possible next steps. Then, remove the selected numbers by the new number. Use the format '(left:  $\ldots$ )' to present the remaining numbers. Do not include serial numbers that are not in the example. Do not include unnecessary information in your output. Input: (2) 8 8 (14) 2 + 14 = 16, replace 2 14 by 16 (left: 8 8 16) 2 \* 14 = 28, replace 2 14 by 28 (left: 8 8 28) 2 / 14 = 0.14, replace 2 14 by 0.14 (left: 8 8 0.14) 14 / 2 = 7, replace 2 14 by 7 (left: 8 8 7) 14 - 2 = 12, replace 2 14 by 12 (left: 8 8 12) 2 - 14 = -12, replace 2 14 by -12 (left: 8 8 -12) Input: 1 (2) 7 (10) 2 + 7 = 9, replace 2 7 by 9 (left: 1 9 10) 2 \* 7 = 14, replace 2 7 by 14 (left: 1 14 10) 2 / 7 = 0.29, replace 2 7 by 0.29 (left: 1 0.29 10) 7 / 2 = 3.5, replace 2 7 by 3.5 (left: 1 3.5 10) 7 - 2 = 5, replace 2 7 by 5 (left: 1 5 10) 2 - 7 = -5, replace 2 7 by -5 (left: 1 -5 10) Input: (7) (8) 9 7 + 8 = 15, replace 7 8 by 15 (left: 15 9) 7 \* 8 = 56, replace 7 8 by 56 (left: 56 9) 7 / 8 = 0.88, replace 7 8 by 0.88 (left: 0.88 9) 8 / 7 = 1.14, replace 7 8 by 1.14 (left: 1.14 9) 8 - 7 = 1, replace 7 8 by 1 (left: 1 9) 7 - 8 = -1, replace 7 8 by -1 (left: -1 9) Input: {input} propose\_prompt\_5s = '''Use the two numbers in the bracket and basic arithmetic operations to propose possible next steps. Then, remove the selected numbers by the new number. Use the format '(left: ...)' to present the remaining numbers. Do not include serial numbers that are not in the example. Do not include unnecessary information in your output. Input: (2) 8 8 (14) 2 + 14 = 16, replace 2 14 by 16 (left: 8 8 16)

2 \* 14 = 28, replace 2 14 by 28 (left: 8 8 28) 2 / 14 = 0.14, replace 2 14 by 0.14 (left: 8 8 0.14) 14 / 2 = 7, replace 2 14 by 7 (left: 8 8 7) 14 - 2 = 12, replace 2 14 by 12 (left: 8 8 12) 2 - 14 = -12, replace 2 14 by -12 (left: 8 8 -12) Input: 1 (2) 7 (10) 2 + 7 = 9, replace 2 7 by 9 (left: 1 9 10) 2 \* 7 = 14, replace 2 7 by 14 (left: 1 14 10) 2 / 7 = 0.29, replace 2 7 by 0.29 (left: 1 0.29 10) 7 / 2 = 3.5, replace 2 7 by 3.5 (left: 1 3.5 10) 7 - 2 = 5, replace 2 7 by 5 (left: 1 5 10) 2 - 7 = -5, replace 2 7 by -5 (left: 1 -5 10) Input: (7) (8) 9 7 + 8 = 15, replace 7 8 by 15 (left: 15 9) 7 \* 8 = 56, replace 7 8 by 56 (left: 56 9) 7 / 8 = 0.88, replace 7 8 by 0.88 (left: 0.88 9) 8 / 7 = 1.14, replace 7 8 by 1.14 (left: 1.14 9) 8 - 7 = 1, replace 7 8 by 1 (left: 1 9) 7 - 8 = -1, replace 7 8 by -1 (left: -1 9) Input: (2.33) (6) 2.33 + 6 = 8.33, replace 2.33 6 by 8.33 (left: 8.33) 2.33 \* 6 = 14, replace 2.33 6 by 14 (left: 14) 2.33 / 6 = 0.39, replace 2.33 6 by 0.39 (left: 0.39) 6 / 2.33 = 2.57, replace 2.33 6 by 2.57 (left: 2.57) 6 - 2.33 = 3.67, replace 2.33 6 by 3.67 (left: 3.67) 2.33 - 6 = -3.67, replace 2.33 6 by -3.67 (left: -3.67) Input: 0.66 (8) (9) 8 + 9 = 17, replace 8 9 by 17 (left: 0.66 17) 8 \* 9 = 72, replace 8 9 by 72 (left: 0.66 72) 8 / 9 = 0.89, replace 8 9 by 0.89 (left: 0.66 0.89) 9 / 8 = 1.12, replace 8 9 by 1.12 (left: 0.66 1.12) 9 - 8 = 1, replace 8 9 by 1 (left: 0.66 1) 8 - 9 = -1, replace 8 9 by -1 (left: 0.66 -1) Input: {input} assembly\_prompt\_1s = '''Use the previous steps of equations to form a final equation that obtains 24. Use 'Answer: ' to present your final answer. Input: 4 4 6 8 Steps: 4 + 8 = 12 (left: 4 6 12) 6 - 4 = 2 (left: 2 12) 2 \* 12 = 24 (left: 24) Let's do it step by step: f1 = 4 + 8 = 12. In this step, 4 and 8 are from the input. f2 = 6 - 4 = 2. In this step, 6 and 4 are from the input. f3 = 2 \* 12 = 24. In this step, 2 is from f2, and 12 is from f1. Thus, we replace 2 by f2: f3 = 2 \* 12 = f2 \* 12 = 24Thus, we replace 12 by f1: f3 = 2 \* 12 = f2 \* f1 = 24Since f1 = 4 + 8, we replace f1 by 4 + 8: f3 = 2 \* 12 = f2 \* (4 + 8) = 24Since  $f_2 = 6 - 4$ , we replace  $f_2$  by 6 - 4:  $f_3 = 2 + 12 = (6 - 4)$ (4) \* (4 + 8) = 24Answer: (6 - 4) \* (4 + 8) = 24Input: {input}Let's do it step by step: f1 =assembly\_prompt\_3s = '''Use the previous steps of equations to form a final equation that obtains 24. Use 'Answer: to present your final answer. Input: 4 4 6 8 Steps: 4 + 8 = 12 (left: 4 6 12) 6 - 4 = 2 (left: 2 12) 2 \* 12 = 24 (left: 24) Let's do it step by step: f1 = 4 + 8 = 12. In this step, 4 and 8 are from the input. f2 = 6 - 4 = 2. In this step, 6 and 4 are from the input. f3 =  $2 \times 12 = 24$ . In this step, 2 is from f2, and 12 is from f1 Thus, we replace 2 by f2: f3 = 2 \* 12 = f2 \* 12 = 24Thus, we replace 12 by f1: f3 = 2 \* 12 = f2 \* f1 = 24Since f1 = 4 + 8, we replace f1 by 4 + 8: f3 = 2 \* 12 = f2 \* (4 + 8) = 24Since f2 = 6 - 4, we replace f2 by 6 - 4: f3 = 2 \* 12 = (6 -4) \* (4 + 8) = 24Answer: (6 - 4) \* (4 + 8) = 24Input: 2 9 10 12 Steps: 12 \* 2 = 24 (left: 9 10 24) 10 - 9 = 1 (left: 1 24)  $24 \times 1 = 24$  (left: 24) Let's do it step by step: f1 = 12  $\star$  2 = 24. In this step, 12 and 2 are from the input. f2 = 10 - 9 = 1. In this step, 10 and 9 are from the input. f3 = 24 + 1 = 24. In this step, 24 is from f1, and 1 is from f2. Thus, we replace 24 by f1: f3 = 24 \* 1 = f1 \* 1 = 24 Thus, we replace 1 by f2: f3 = 24 \* 1 = f1 \* f2 = 24 Since f1 = 12 \* 2, we replace f1 by 12 \* 2: f3 = 24 \* 1 = (12 \* 2) \* f2 = 24 Since  $f_2 = 10 - 9$ , we replace  $f_2$  by 10 - 9:  $f_3 = 24 + 1 = (12)$ \* 2) \* (10 - 9) = 24

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Answer: (12 \* 2) \* (10 - 9) = 24Input: 4 9 10 13 Steps: 13 - 10 = 3 (left: 3 4 9) 9 - 3 = 6 (left: 4 6) 4 \* 6 = 24 (left: 24) Let's do it step by step: f1 = 13 - 10 = 3. In this step, 13 and 10 are from the input. f2 = 9 - 3 = 6. In this step, 9 is from the input, and 3 is from f1. Thus, we replace 3 by f1: f2 = 9 - 3 = 9 - f1 = 6f3 = 4 + 6 = 24. In this step, 4 is from the input, and 6 is from f2. Thus, we replace 6 by f2: f3 = 4 \* 6 = 4 \* f2 = 24Since f2 = 9 - f1, we replace f2 by 9 - f1: f3 = 4 \* 6 = 4 \*(9 - f1) = 24 Since f1 = 13 - 10, we replace f1 by 13 - 10: f3 = 4 \* 6 = 4 \* (9 - (13 - 10)) = 24 Answer: 4 \* (9 - (13 - 10)) = 24 Input: {input}Let's do it step by step: f1 = ''' assembly\_prompt\_5s = '''Use the previous steps of equations to form a final equation that obtains 24. Use 'Answer: ' to present your final answer. Input: 4 4 6 8 Steps: 4 + 8 = 12 (left: 4 6 12) 6 - 4 = 2 (left: 2 12) 2 \* 12 = 24 (left: 24) Let's do it step by step: f1 = 4 + 8 = 12. In this step, 4 and 8 are from the input. f2 = 6 - 4 = 2. In this step, 6 and 4 are from the input. f3 = 2 \* 12 = 24. In this step, 2 is from f2, and 12 is from f1. Thus, we replace 2 by f2: f3 = 2 \* 12 = f2 \* 12 = 24Thus, we replace 12 by f1: f3 = 2 \* 12 = f2 \* f1 = 24Since f1 = 4 + 8, we replace f1 by 4 + 8: f3 = 2 + 12 = f2 + 12(4 + 8) = 24Since  $f_2 = 6 - 4$ , we replace  $f_2$  by 6 - 4:  $f_3 = 2 * 12 = (6 - 4)$ (4) \* (4 + 8) = 24Answer: (6 - 4) \* (4 + 8) = 24Input: 2 9 10 12 Steps: 12 \* 2 = 24 (left: 9 10 24) 10 - 9 = 1 (left: 1 24) 24 \* 1 = 24 (left: 24) Let's do it step by step: f1 = 12  $\star$  2 = 24. In this step, 12 and 2 are from the input. f2 = 10 - 9 = 1. In this step, 10 and 9 are from the input. f3 = 24 \* 1 = 24. In this step, 24 is from f1, and 1 is from f2. Thus, we replace 24 by f1: f3 = 24 \* 1 = f1 \* 1 = 24 Thus, we replace 1 by f2: f3 = 24 + 1 = f1 + f2 = 24Since f1 = 12 \* 2, we replace f1 by 12 \* 2: f3 = 24 \* 1 = (12 \* 2) \* f2 = 24 Since  $f_2 = 10 - 9$ , we replace  $f_2$  by 10 - 9:  $f_3 = 24 * 1 = (12 * 2) * (10 - 9) = 24$ Answer: (12 \* 2) \* (10 - 9) = 24 Input: 4 9 10 13 Steps: 13 - 10 = 3 (left: 3 4 9) 9 - 3 = 6 (left: 4 6) 4 \* 6 = 24 (left: 24) Let's do it step by step: f1 = 13 - 10 = 3. In this step, 13 and 10 are from the input. f2 = 9 - 3 = 6. In this step, 9 is from the input, and 3 is from f1. Thus, we replace 3 by f1: f2 = 9 - 3 = 9 - f1 = 6f3 = 4 \* 6 = 24. In this step, 4 is from the input, and 6 is from f2. Thus, we replace 6 by f2: f3 = 4 + 6 = 4 + f2 = 24Since f2 = 9 - f1, we replace f2 by 9 - f1: f3 = 4 \* 6 = 4 \* (9 - f1) = 24Since f1 = 13 - 10, we replace f1 by 13 - 10: f3 = 4 \* 6 = 4 \* (9 - (13 - 10)) = 24Answer: 4 \* (9 - (13 - 10)) = 24Input: 1 4 8 8 Steps: 8 / 4 = 2 (left: 1 2 8) 1 + 2 = 3 (left: 3 8) 3 \* 8 = 24 (left: 24) Let's do it step by step: f1 = 8 / 4 = 2. In this step, 8 and 4 are from the input. f2 = 1 + 2 = 3. In this step, 2 is from f1, and 1 is from the input. Thus, we replace 2 by f1: f2 = 1 + 2 = 1 + f1 = (1 + (8 / 4))

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#### = 3 $f3 = 3 \times 8 = 24$ . In this step, 3 is from f2, and 8 is from the input. Thus, we replace 3 by f2: f3 = 3 \* 8 = f2 \* 8 = 24Since $f_2 = 1 + f_1$ , we replace $f_2$ by $1 + f_1$ : $f_3 = 3 + 8 = (1 + f_2)$ f1) \* 8 = 24 Since f1 = 8 / 4, we replace f1 by 8 / 4: (1 + f1) \* 8 = (1 + (8 / 4)) \* 8 = 24Answer: (1 + (8 / 4)) \* 8 = 24 Input: 5 5 5 9 Steps: 5 + 5 = 10 (left: 5 9 10) 10 + 5 = 15 (left: 9 15) 15 + 9 = 24 (left: 24) Let's do it step by step: f1 = 5 + 5 = 10. In this step, 5 and 5 are from the input. f2 = 10 + 5 = 15. In this step, 10 is from f1, and 5 is from the input. Thus, we replace 10 by f1: f2 = 10 + 5 = f1 + 5 = 15f3 = 15 + 9 = 24. In this step, 15 is from f2, and 9 is from the input. Thus, we replace 15 by f2: f3 = 15 + 9 = f2 + 9 = 24Since $f_2 = f_1 + 5$ , we replace $f_2$ by $f_1 + 5$ : $f_3 = 15 + 9 = (f_1)$ + 5) + 9 = 24Since f1 = 5 + 5, we replace f1 by 5 + 5: f3 = 15 + 9 = ((5 + 5))5) + 5) + 9 = 24 Answer: ((5 + 5) + 5) + 9 = 24Input: {input}Let's do it step by step: f1 = '

### **F** Tables

Method	GPT-3.5	GPT-4
Direct	28.51	47.16
СоТ	79.53	94.09
ToT	81.88	96.00

Table 2: Figure 2a	Table	2:	Figure	2a
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Dataset size	Direct	CoT
1000	18.50	88.00
2000	22.50	88.00
3000	30.50	92.50
4000	35.00	93.50
5000	37.50	95.00
6000	46.50	95.00
7000	46.50	96.00
8000	48.50	96.50
9000	48.50	97.50
10000	58.00	96.50

Table 3: Figure 2b

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Method	InD	OoD	Total
Direct 0s	38.67	8.75	21.57
Direct 3s	68.67	35.25	49.57
Direct 6s	57.67	30.25	42.00
CoT 0s	59.33	35.25	45.57
CoT Implicit 3s	67.00	41.50	52.43
CoT Implicit 6s	65.00	36.25	48.57
CoT Explicit 3s	85.67	65.00	73.86
CoT Explicit 6s	86.67	66.50	75.14

Table 4: Figure 3 GPT-4

Method	InD	OoD	Total
Direct 0s	26.00	13.50	18.86
Direct 3s	32.33	10.50	19.86
Direct 6s	39.33	20.25	28.43
CoT 0s	24.33	8.75	15.43
CoT Implicit 3s	18.00	6.75	11.57
CoT Implicit 6s	20.33	5.00	11.57
CoT Explicit 3s	56.67	16.00	33.43
CoT Explicit 6s	63.33	28.75	43.57

Num of edges	Large cities	Mid-sized cities
1069	90.64±2.21	80.32±3.21
2138	$93.30 \pm 2.02$	$85.87 \pm 3.92$
4277	$97.07 \pm 0.94$	$90.16 \pm 1.45$
6415	97.90±1.20	93.79±1.13

Table 8: Figure 6 ToT-linear (Accuracy  $\% \pm$  standard error)

Num of edges	Large cities	Mid-sized cities
744	65.50±5.22	58.10±4.91
1489	$78.94 \pm 3.90$	$68.85 \pm 4.56$
2979	$80.19 \pm 4.12$	$74.59 \pm 4.11$
4468	$81.52 \pm 5.23$	$77.97 \pm 5.10$
5958	$83.04 \pm 3.54$	$81.98{\pm}3.41$

Table 9: Figure 6 CoT (Accuracy % ± standard error)

Method	GPT-4	GPT-3.5
ToT 5s	58	20
ToT-Decomp 5s	86	47
ToT-Decomp 3s	23	20
ToT-Decomp 1s	19	15
CoT 5s	6	2
Direct 5s	10	4

Table 10: Figure 7, main results (Accuracy, %).

Method	Large cities	Mid-sized cities
CoT 0s	71.35	64.75
CoT 3s	76.02	68.03
CoT 8s	85.38	70.49
ToT-linear 0s	54.24	47.54
ToT-linear 3s	87.13	69.67
ToT-linear 8s	84.80	68.85
ToT 0s	76.02	70.49
ToT 3s	88.30	78.69
ToT 8s	88.89	79.51

Table 7: Figure 5 GPT-4 (Accuracy, %)

Method	Transition error	Proposal error
TOT-GPT4-5s	7.12	2.04
TOT-GPT4-Decomp-5s	2.80	1.44
TOT-GPT3.5-5s	16.62	3.15
TOT-GPT3.5-Decomp-5s	3.06	0.30
Method	Missing action	Answer error
TOT-GPT4-5s	12.44	10.04
TOT-GPT4-Decomp-5s	6.63	1.56
TOT-GPT3.5-5s	23.63	19.03
TOT-GPT3.5-Decomp-5s	16.60	2.28

Table 11: Figure 7, main results (Error rate, %).

Table 5: Figure 3 GPT-3.5

Method	Large cities	Mid-sized cities
CoT 0s	70.76	50.00
CoT 3s	73.10	51.64
CoT 8s	72.51	53.27
ToT-linear 0s	75.43	69.67
ToT-linear 3s	81.29	77.05
ToT-linear 8s	78.36	72.95
ToT 0s	78.36	72.13
ToT 3s	80.70	75.41

Table 6: Figure 5 GPT-3.5 (Accuracy, %)

75.41

81.29

ToT 8s