Tree of Problems: Improving structured problem solving with compositionality

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Abstract

Large Language Models (LLMs) have demonstrated remarkable performance across multiple tasks through in-context learning. For complex reasoning tasks that require step-by-step thinking, Chain-of-Thought (CoT) prompting has given impressive results, especially when combined with self-consistency. Nonetheless, some tasks remain particularly difficult for LLMs to solve. Tree of Thoughts (ToT) and Graph of Thoughts (GoT) emerged as alternatives, dividing the complex problem into paths of subproblems. In this paper, we propose Tree of Problems (ToP), a simpler version of ToT, which we hypothesise can work better for complex tasks that can be divided into identical subtasks. Our empirical results show that our approach outperforms ToT and GoT, and in addition performs better than CoT on complex reasoning tasks. All code for this paper is publicly available here: [https://github.](https://github.com/ArmelRandy/tree-of-problems) [com/ArmelRandy/tree-of-problems](https://github.com/ArmelRandy/tree-of-problems).

1 Introduction

In-Context Learning (ICL) [\(Brown et al.,](#page-5-0) [2020\)](#page-5-0) is the ability of Large Language Models (LLMs) to perform a task with the help of a few demonstrations within their context. It is widely used to evaluate LLMs on various tasks. These models, whose number of parameters and training corpus size has increased massively over recent years, keep pushing the state of the art on a wide range of natural language tasks [\(Anil et al.,](#page-5-1) [2023;](#page-5-1) [Touvron et al.,](#page-9-0) [2023;](#page-9-0) [Gemma Team](#page-7-0) et al., [2024\)](#page-7-0). However, they still struggle to perform complex tasks, notably those requiring multiple reasoning steps [\(Hendrycks et al.,](#page-7-1) [2021a](#page-7-1)[,b;](#page-7-2) [Suzgun et al.,](#page-9-1) [2023\)](#page-9-1). Recently, Chain-of-Thought (CoT) prompting [\(Wei et al.,](#page-9-2) [2022;](#page-9-2) [Ko](#page-7-3)[jima et al.,](#page-7-3) [2022\)](#page-7-3) has greatly helped to enhance reasoning abilities of LLMs by helping them to mimic step-by-step reasoning. However, CoT implicitly requires the model to generalize beyond

the cases seen in its prompt, which often leads to poor out-of-domain performance [\(Zhou et al.,](#page-9-3) [2023\)](#page-9-3). Applying CoT with self-consistency [\(Wang](#page-9-4) [et al.,](#page-9-4) [2023b\)](#page-9-4) drives the model to explore multiple reasoning paths and to choose the most consistent answer, usually yielding better performance, but helping only marginally with out-of-distribution generalization. Moreover, solving complex problems involves understanding their underlying structure; this can help to avoid lengthy CoTs that are prone to reasoning errors.

In this paper, we propose to tackle complex problem-solving and out-of-distribution generalization by dividing complex tasks into a series of simpler sub-tasks. We draw inspiration from techniques such as dynamic programming and divide and conquer in order to efficiently guide LLMs through complex problem solving. Such problems have previously been tackled using approaches adding structure to CoT, such as Tree of Thoughts (ToT) [\(Yao et al.,](#page-9-5) [2023\)](#page-9-5) and Graph of Thoughts (GoT) [\(Besta et al.,](#page-5-2) [2024\)](#page-5-2), which consist in sampling diverse reasoning paths (where path states represent subproblems) and finding the optimal path. We argue that for a subset of complex reasoning problems, where an instance can be decomposed into multiple analogous subinstances, ToT and GoT are overly complex, and the tasks can be better solved by a simpler approach. This simpler approach, which we name Tree of Problems (ToP) consists in building a tree structure, where each node represents a problem instance similar to the main instance. The deepest instances, which correspond to atomic problems, are solved first with CoT prompting and the internal nodes are recursively solved by merging their children's solutions. Figure [1](#page-1-0) illustrates our method on the tasks of Last Letter Concatenation and Navigate from the BIG-Bench Hard benchmark [\(Suzgun et al.,](#page-9-1) [2023\)](#page-9-1).

We conduct a comprehensive evaluation on several LLMs, including GPT-3.5, on multiple hard

Figure 1: Overview of the Tree of Problems (ToP) framework for two tasks. On the left (a canonical task consisting of independent subproblems organised in a tree structure), the task is to concatenate the last letters of a list of names, accomplished by breaking the list in two, finding their solutions, and recombining them. On the right (an extension of the canonical structure to handle sequential tasks), the task is to determine the final position of an object after a series of steps. We first find its position after half of the steps, and then determine the final position by tracing the object through the remaining steps. See Section [3](#page-2-0) for a description of ToP.

tasks. We find that ToP improves LLMs' problem solving abilities on structured tasks outperforming CoT, ToT and GoT by a large margin.

2 Related Work

CoT prompting was proposed to enhance reasoning by incorporating step-by-step logic into fewshot prompt demonstrations [\(Wei et al.,](#page-9-2) [2022\)](#page-9-2). It showed significant improvement over standard input-output (IO) prompting across various mathematical and symbolic reasoning benchmarks. Building on this, [Kojima et al.](#page-7-3) [\(2022\)](#page-7-3) and [Wang](#page-9-6) [et al.](#page-9-6) [\(2023a\)](#page-9-6) *inter alia* demonstrated that zeroshot CoT could be achieved by using reasoninginducing words at the end of the zero-shot prompt. Other works showed that wisely designing the CoT demonstrations could yield further improvements [\(Zhang et al.,](#page-9-7) [2023;](#page-9-7) [Fu et al.,](#page-7-4) [2022\)](#page-7-4). CoT Self-Consistency (CoT-SC; [Wang et al.](#page-9-4) [2023b\)](#page-9-4) improved on CoT by sampling diverse reasoning steps and selecting the most consistent answer after marginalizing over the reasoning paths. Our research also builds on the body of work addressing problem-solving through compositionality, which involves teaching LLMs to tackle complex problems by breaking them down into a series of subproblems and recursively solving them to derive

the final answer, e.g. Least-to-Most [\(Zhou et al.,](#page-9-3) [2023\)](#page-9-3), decomposed [\(Khot et al.,](#page-7-5) [2023\)](#page-7-5) and successive [\(Dua et al.,](#page-5-3) [2022\)](#page-5-3) prompting. While these works align with our approach through their use of problem decomposition, we focus on breaking a main task into multiple similar subtasks, solvable using the same prompt. Moreover, our approach uses a tree structure that allows for greater flexibility and coverage in problem solving. The most closely related approaches are Tree of Thoughts (ToT) [\(Yao et al.,](#page-9-5) [2023\)](#page-9-5) and Graph of Thoughts (GoT) [\(Besta et al.,](#page-5-2) [2024\)](#page-5-2). ToT builds on the idea of sampling diverse reasoning paths but redefines problem solving as a search over a thought space, where states represent partial solutions. GoT extends ToT by including thought aggregation, which is analogous to our merge operation and by allowing refining [\(Madaan et al.,](#page-7-6) [2023\)](#page-7-6). While a "thought" represents a general reasoning step in their approach, we focus on reasoning through subproblems. We do not perform a search over a tree of thoughts, nor do we score or refine (improve) our tree nodes. Instead, each node in the tree of problems is directly relevant to solving the problem, and their bottom-up recombination produces the final solution. ToP is therefore a simpler and more cost-effective alternative to ToT and GoT.

3 Our method

Solving a complex problem often requires reasoning, partly explaining the success of CoT prompting for such problems. Reasoning involves understanding a problem's structure and design. This aspect is frequently overlooked in CoT because incorporating it can be challenging. Our method addresses this by constructing a tree of simpler, closely related subproblems to solve a more complex problem. We hypothesize that the capability of an LLM to solve simple instances can be extended to more complex ones. The ability of an LLM to solve a complex instance therefore lies in how accurately it can solve simpler ones and then combine their answers. The main class of problems we aim to tackle are complex problems that are divisible into independent subproblems resembling the initial one (we refer to these as canonical tasks). However, we also experiment with relaxing the independency constraint in order to tackle sequential tasks, which require finding the final state of a system after a series of independent processing steps (See the right of Figure [1\)](#page-1-0). Our method relies on the following components:

- A decomposer divides a problem instance into a series of smaller related instances, algorithmically or via few-shot prompting with a divide_prompt. We recursively build a tree of problems (nodes) considering 2 parameters: the *breadth* (the number of children of each internal node) and the *depth* of the tree, directly related to the granularity of the atomic subproblems. The root of the tree is the main problem. In this paper, ToP (b, d) refers to using breadth b and depth d.
- A solver is used to do the task of interest, namely the simplest instances obtained after decomposition (in our case an LLM with a task-specific solve_prompt).
- A merger receives the solved subproblems (problem statement and solution) at level *k* to build and solve the problem at level $k - 1$. It uses a specific merge_prompt to get the LLM to learn to combine the subproblems' solutions into the parent solution. As opposed to L2M, the prompt to get the solution of a problem at a level *k* only depends on the directly connected problems (at the level $k + 1$).

The workflow can be described as follows: The decomposer builds the tree of problems, the solver addresses the subproblems at the tree's leaves, and the merger recursively derives each node's solution by combining its children's solutions in a bottomup approach. The total number of inference calls (omitting the cost of problem decomposition) is equal to the number of nodes in the tree structure.

In addition to canonical tasks with a classic tree structure (see the left of Figure [1\)](#page-1-0), ToP can also be used for sequential tasks, where a given subproblem needs the result of a previous subproblem as an input (see the right of Figure [1\)](#page-1-0). Our standard ToP paradigm described above can be used to solve such problems by setting the breadth to 1. This has the effect that the problem is decomposed into a sequence of n subproblems organised as hierarchy of depth *n*. When solving the $(k + 1)$ -th subproblem, the solver will have access to its child subproblem's result, i.e. the result of subproblem k , thereby accounting for the sequentiality of the decomposition. The LLM is no longer required to merge subproblems' solutions; it is directly fed with a new problem formulation automatically computed using the corresponding child's solution. The final solution is obtained by solving the last subproblem, and so the main problem instance (root node) does not influence the inference cost.

For both tasks, all problems at the same level of the tree are solved in parallel to promote efficiency. We further detail the method with more examples in Appendix [A.](#page-9-8)

4 Experiments

We first compare ToP to ToT and GoT to test our hypothesis that our simpler approach is more adapted to canonical tasks. We do this using the GoT tasks proposed by [Besta et al.](#page-5-2) [\(2024\)](#page-5-2). We then show that ToP is more effective in comparison to IO (direct input-output) and CoT prompting across a wider ranger of canonical tasks, namely Last Letter Concatenation [\(Wei et al.,](#page-9-2) [2022\)](#page-9-2) and 5 BIG-Bench Hard [\(Srivastava et al.,](#page-7-7) [2023\)](#page-7-7) tasks fitting the description. Finally, we test ToP on sequential tasks.

4.1 Datasets

GoT tasks. [Besta et al.](#page-5-2) [\(2024\)](#page-5-2) compared GoT to ToT, IO, and CoT prompting on three tasks (each with 100 examples): (i) *Sorting*, which involves arranging a list of 32 numbers ranging from 0 to 9 (both inclusive) in order, (ii) *Set Intersection*, which involves finding the common elements between two sets, each containing 32 elements and (iii) *Keyword Counting*, which involves identifying countries mentioned in a text and counting how many times each country appears.

Symbolic Reasoning. We use two toy tasks introduced by [Wei et al.](#page-9-2) [\(2022\)](#page-9-2) (each with 500 examples): (i) *Last Letter Concatenation*, where the LLM is tasked with recovering the concatenation of the last letters from a list of names and (ii) *Coin Flip*, which evaluates if the LLM can deduce the final state of a coin (heads or tails) after people either flip it or not. During evaluation, we consider various list lengths (4, 8 and 16) for the first task, and different numbers of people involved (4, 8 and 16) for the second.

BIG-Bench Hard (BBH). BBH consists of 23 BIG-Bench [\(Srivastava et al.,](#page-7-7) [2023\)](#page-7-7) tasks that have been shown to benefit from CoT [\(Suzgun et al.,](#page-9-1) [2023\)](#page-9-1). We use 8 tasks:[1](#page-3-0) *Boolean Expressions*, *Hyperbaton*, *Multi-Step Arithmetic Two*, *Navigate*, *Object Counting*, *Tracking Shuffled Objects (3, 5, 7)*, *Web of Lies* and *Word Sorting*.

4.2 Language models and prompts

We experiment with gpt-3.5-turbo and $gpt-3.5$ -turbo-instruct.² For the solve_prompts, we use the CoT prompts^{[3](#page-3-2)} of [Suzgun et al.](#page-9-1) [\(2023\)](#page-9-1) on BBH tasks, with minor changes. The CoT prompts for *Symbolic Reasoning* are inspired by those in [\(Wei et al.,](#page-9-2) [2022\)](#page-9-2), which contain 8 examples of 2-letters or 2-flips and those for *GoT tasks* are the same as in [Besta](#page-5-2) [et al.](#page-5-2) [\(2024\)](#page-5-2). We report some implementation details in Appendix [D](#page-15-0) and Appendix [E.](#page-15-1)

4.3 Main results

GoT tasks. Table [1](#page-3-3) compares our results on the GoT tasks with those obtained by rerunning the CoT, ToT and GoT approaches from [\(Besta et al.,](#page-5-2) [2024\)](#page-5-2). More precisely, we use the highest accuracy achieved with ToT and GoT on each task with gpt-3.5-turbo-0125. For *Sorting*, we intuitively choose $b = 2$ as in merge sort and $d = 2$ for performance. We use the same b for *Keyword Counting*, with $d = 4$ to get simple atomic instances. In *Set Intersection*, we use $b = 4$ because each set is divided into two disjoint subsets, resulting in four pairs of subsets (one pair per subproblem). Such a large breadth was sufficient to produce simple atomic problems, so we used $d = 1$. ToP outperforms

²More results and analysis for LLaMA (different model versions and sizes) are provided in Appendices [B.1](#page-11-0) and [C.](#page-11-1)

ToT and GoT by a large margin on *sorting* with an absolute improvement of 40% over GoT. Similarly, ToP outperforms GoT by 19% and 5% respectively on *Set Intersection* and *Keyword Counting*.

GoT Tasks	$gpt-3.5-turbo$						
	CoT	ToT (best)	GoT (best)	ToP (ours)			
Sorting	0.02	0.17	0.28	0.68			
Set Intersection	0.07	0.25	0.46	0.65			
Keyword Counting	0.00	0.00	0.26	0.31			

Table 1: Results on 3 tasks from [\(Besta et al.,](#page-5-2) [2024\)](#page-5-2). In all results tables, best results are highlighted in bold.

Last Letter Concatenation. We consider ToP (2, 1). Subproblems are obtained by dividing the main list into $b = 2$ lists of equal length.

Last Letter Concatenation	gpt-3.5-turbo-instruct				
	Ю	CoT	ToP (ours)		
Four Eight Sixteen	0.032 0.000 0.000	0.900 0.662 0.252	0.990 0.854 0.444		

Table 2: Results on Symbolic Reasoning tasks.

Comparison to Least-to-Most Prompting and CoT with Self-consistency. Least-to-most (L2M) prompting has also been successfully applied to Last Letter Concatenation [\(Zhou et al.,](#page-9-3) [2023\)](#page-9-3). Given a list of L names, L2M requires $L-1$ inference calls, the first to concatenate the first 2 last letters and the $L-2$ other to add the remaining last letters one after the other. Following [Huang](#page-7-8) [et al.](#page-7-8) [\(2024\)](#page-7-8), we provide a fair comparison of L2M to ToP by adapting ToP's tree structure to require the same number of inference calls as L2M. This is done by using trees of breadth 2 and depth $log_2(L) - 1$ for lists of length L. We compare ToP to L2M as well as CoT self-consistency with L reasoning paths. The results (Table [3\)](#page-4-0) show that for $L = 4$ or $L = 8$, ToP (breadth = 2, depth = 1) achieves comparable performance to L2M while requiring half as many inference calls. When the number of inference calls is matched between the two methods, ToP demonstrates superior performance in all scenarios. CoT-SC lags behind both L2M and ToP.

Moreover, since L2M is similar to ToP $(1, L-1)$, we compare its accuracy to ToP (match) at each level of the tree. As illustrated in Figure [2,](#page-4-1) both methods start with a perfect score that gradually

¹See Appendix [E.2](#page-15-2) for more details.

 3 We report some results with IO in Appendix [C.3.](#page-13-0)

Last Letter Concatenation	gpt-3.5-turbo-instruct				
	CoT-SC	L2M	ToP	ToP (match)	
Four	0.908	0.988	0.990	0.990	
Eight	0.574	0.870	0.854	0.932	
Sixteen	0.116	0.742	0.444	0.858	

Table 3: Comparison of ToP to L2M and CoT-SC for Last Letter Concatenation. ToP (match) refers to ToP with the same number of inference calls as L2M.

Figure 2: Per-level accuracy of Least to Most prompting and ToP (match) for *Last Letter Concatenation*.

decreases as they approach the task's resolution. ToP (match) consistently outperforms L2M at each step across all three settings.

4.4 Complementary results

We have successfully applied ToP to problems that can be divided into multiple independent instances. In this section, we report additional results for more such tasks and sequential tasks.

4.4.1 Canonical BBH tasks

BBH tasks such as *Boolean Expressions*, *Hyperbaton*, *Multistep Arithmetic Two*, *Object Counting*, and *Word Sorting* can be decomposed into multiple independent instances, whose solutions are later combined. They therefore correspond to canonical ToP tasks. We apply ToP (2, 1) to them and report results in Table [4.](#page-4-2) ToP yields an absolute improvement over CoT of 21.2% on *Word Sorting* and 9.8% on *Hyperbaton*. However, it is slightly worse than CoT on *Boolean Expressions*, *Multistep Arithmetic Two* and *Object Counting* with an average deterioration of 3.6% on the 3 tasks. We attribute this loss of accuracy to reasoning inconsistencies and we explore this in more detail in Appendix [C.4.](#page-14-0)

	gpt-3.5-turbo-instruct			
	Ю	CoT	ToP	
Boolean Expressions	0.908	0.924	0.896	
Hyperbaton	0.528	0.804	0.902	
Multistep Arithmetic Two	0.032	0.780	0.736	
Object Counting	0.412	0.928	0.892	
Word Sorting	0.837	0.619	0.831	

Table 4: Results on the canonical BBH tasks.

4.4.2 Sequential tasks

Coin Flip is an example of a sequential task. Using ToP (1, 2), the problem at the leaves is to find the state of the coin after going through the first half of the people. The final solution is obtained by determining how this state changes as the coin goes through the remaining half of the people. *Navigate*, *Tracking Shuffled Objects*, and *Web of Lies* can be modeled in a similar way. ToP outperforms CoT on all tasks, as shown in Table [5.](#page-4-3) ToP reaches near perfect accuracy on *Coin Flip* with 4 and 8 people. Moreover, it is more robust to the out-ofdistribution setting than CoT, showing a lesser performance drop as the number of people increases. Compared to CoT, it yields an absolute improvement of 5.2% on *Web of Lies*, 5.9% on average on *Tracking Shuffled Objects* and 2% on *Navigate*.

	gpt-3.5-turbo-instruct				
	Ю	CoT	ToP		
Coin Flip					
Four	0.512	0.998	0.998		
Eight	0.502	0.840	0.998		
<i>Sixteen</i>	0.476	0.718	0.756		
BIG-Bench Hard					
<i>Navigate</i>	0.204	0.864	0.884		
Tracking Shuffled Objects (3)	0.004	0.536	0.524		
Tracking Shuffled Objects (5)	0.004	0.324	0.440		
Tracking Shuffled Objects (7)	0.000	0.044	0.118		
Web of Lies	0.528	0.920	0.972		

Table 5: Results on *Coin Flip* and sequential BBH tasks.

Conclusion

We use compositionality to grant the ability to solve complex and structured problems to LLMs via the Tree of Problems (ToP) framework. ToP is a simplification of the ToT framework, and involves decomposing complex tasks into identical subtasks. Our experiments demonstrate that LLMs can benefit from ToP and solve certain complex problems better than ToT, GoT and L2M approaches and generalize better than with CoT.

Acknowledgements

This work was partly funded by the last two authors' chairs in the PRAIRIE institute funded by the French national agency ANR as part of the "Investissements d'avenir" programme under the reference ANR-19-P3IA-0001. The authors are grateful to the OPAL infrastructure from Université Côte d'Azur for providing resources and support. We thank Maciej Besta for answering our questions regarding Graph of Thoughts and Lydia Nishimwe for her helpful feedback.

Limitations

Applicability of the Tree of Problems framework. Although ToP is a powerful prompting strategy that significantly widens the range of tasks that LLMs can handle accurately; it is limited to problems which have a structure (mathematical tasks, algorithmic tasks etc.) that can be decomposed into analogous subproblems. The founding hypothesis of ToP is the fact that LLMs can solve simple instances of a task and this ability can be efficiently translated to more complex instances.

Reasoning consistency of LLMs. LLMs can surprisingly fail to be robust to minor changes in a problem formulation. They can fail to solve a problem closely related to another one that they are capable to solve. We note this as a typical failure case of ToP in Appendix [C.4](#page-14-0) on *Object Counting* and *Multistep Arithmetic Two*.

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A Clarifications

A.1 Canonical Tasks

In Figure [1](#page-1-0) we showed how to apply $ToP(2, 1)$ to an instance of Last Letter Concatenation. We illustrate how $ToP(2, 2)$ would look for concatenating the last letters of a list of 8 words in Figure [3.](#page-10-0) The decomposition is done on two levels, the leaves being solved first and the merge operation being recursively applied from the bottom to the top.

A.2 Sequential tasks

Let us say that we have a system at state s_0 , and we want to find its state after going through m processing steps (p_1, \ldots, p_m) in this order (i.e. a sequential task). Applying ToP $(1, k)$ is equivalent to grouping the above steps into k groups $G_1 = \left(p_1, \ldots, p_{\lceil \frac{m}{k} \rceil} \right)$ $\Big), \ldots, G_k =$ $(p_{m-\lfloor \frac{m}{k} \rfloor+1}, \ldots, p_m)$. We build a path graph from top to bottom, where the root is the main instance, and the leaf is the instance defined by s_0 and G_1 . Solving it yields a state s_1 to which we apply the steps G_2 and so on until we reach G_k . *Tracking Shuffled Objects* is an example of such a task. At the start, L people are assigned one object each. We are interested in recovering the assignment between people and objects after L swaps (transpositions). Figure [4](#page-10-1) illustrates the application of $ToP(1,3)$ to an instance with 3 swaps. We first decompose the main instance into 3 subinstances; here, each instance corresponds to one swap. After decomposition, only the first instance has the correct initial assignment (grey part). For the remaining instances, placeholders are used, which will later be replaced by the solutions to the problems they depend on.

Figure 3: Overview of ToP (2, 2) for Last Letter Concatenation. The list of words is divided into 2 sublists which are recursively divided into two sublists. The problems at the leaves, which consist into concatenating the last letters of 2-word lists are solved first. The solutions are then merged in a bottom-up way until the main instance is solved.

Figure 4: Overview of $ToP(1,3)$ on an instance of *Tracking Shuffled Objects (three objects)*.

A.3 Comparison with Least-to-Most Prompting

Least-to-Most prompting also handles Last Letter Concatenation as a sequential task. In this regards, it is similar to $ToP(1, L)$ on list with L words. As illustrated in Figure [5,](#page-11-2) L2M uses all couples

instance-solution preceding an instance to build the prompt to solve it whereas ToP only uses the couples directly connected to it in the tree hierarchy.

Figure 5: Overview of L2M prompting on Last Letter Concatenation with 4 words.

B Additional Experiments

B.1 Scaling behaviour

In this section, we study how ToP behaves as we vary the model scale. In Figure [6,](#page-12-0) we plot the performance of both IO and CoT prompting and ToP as a function of model scale for LLaMA 2 models [\(Touvron et al.,](#page-9-0) [2023\)](#page-9-0) and 3 BBH tasks. We use ToP $(2, 1)$ for canonical tasks and ToP $(1, 2)$ for sequential tasks. For all tasks, scaling up model size improved the performance of ToP beyond CoT prompting. LLaMA 2 70B achieves a 98% accuracy on *Object Counting*, an absolute improvement of 18.8% over CoT. ToP improves over random accuracy of IO and CoT on *Web of Lies* with LLaMA 2 7B, with an accuracy of 72.8%.

We report IO prompting, CoT prompting and ToP performance on 8 BBH tasks in Table [6.](#page-12-1) ToP consistently yields an improvement of performance compared to IO and CoT prompting for most tasks and at all scales.

C Analysis

We aim to gain a comprehensive understanding of the performance improvements offered by the ToP framework. We theoretically derive an upper bound of expected ToP's performance, then we study the impact of the tree structure on the results obtained. For the experiments in this section, we use LLaMA 3 8B [\(Dubey et al.,](#page-5-4) [2024\)](#page-5-4) unless stated otherwise.

C.1 Theoretical Analysis

Let us consider a task with n problems. Each problem is further divided into k subproblems, resulting in a total of nk subproblems. If we evaluate an LLM on these nk subproblems and obtain m incorrect answers, we can infer the number of incorrect answers likely to occur when evaluating the original n problems. Assuming that an incorrect answer to a subproblem implies an incorrect answer to its corresponding main problem, we can analyze the outcomes in two scenarios. In the worst case, each of the m incorrect subproblems is associated with a distinct main problem and thus there would be m main problems with incorrect answers. The best case is when the m incorrect subproblems are distributed such that each affected main problem has k or $m\%k$ incorrect subproblems. Consequently, the number of main problems with incorrect answers would be at most $\lceil \frac{m}{k} \rceil$ $\frac{m}{k}$. From this analysis, we can deduce that the accuracy at any level l of the problem hierarchy is constrained by the accuracy at level $l - 1$. Therefore, the accuracy for the overall task (the root of the hierarchy) is bounded by the accuracy observed at the most granular level (the leaves of the hierarchy). We validate this analysis by comparing the accuracy at level 1 to the accuracy at level 0 (main problem) for some of the

Figure 6: Scaling behavior of ToP compared to IO and CoT with the LLaMA 2 family on 3 BBH tasks.

BBH Tasks		LLaMA 27B			LLaMA 213B		LLaMA 270B		
	IО	CoT	ToP	IO	CoT	ToP	IО	CoT	ToP
Boolean Expressions	0.680	0.628	0.672	0.728	0.768	0.728	0.812	0.868	0.924
Hyperbaton	0.530	0.550	0.562	0.508	0.666	0.700	0.530	0.684	0.830
Multistep Arithmetic Two	0.008	0.004	0.012	0.012	0.024	0.044	0.016	0.196	0.216
Navigate	0.272	0.164	0.088	0.340	0.308	0.156	0.336	0.400	0.284
Object Counting	0.404	0.476	0.516	0.492	0.532	0.616	0.540	0.792	0.98
Tracking Shuffled Objects									
Three	0.156	0.156	0.136	0.076	0.184	0.132	0.056	0.584	0.568
Five	0.000	0.000	0.000	0.012	0.044	0.048	0.080	0.528	0.664
Seven	0.000	0.000	0.000	0.000	0.000	0.004	0.000	0.288	0.592
Web of Lies	0.488	0.528	0.728	0.552	0.984	1.000	0.488	0.996	0.984
Word Sorting	0.418	0.146	0.244	0.538	0.261	0.320	0.788	0.445	0.717

Table 6: Few-shot prompting performance of the LLaMA 2 family on BIG-Bench Hard (BBH).

Figure 7: Comparison between CoT, ToP, ToP with an Oracle Merger and the leaves' accuracy on 3 BBH tasks.

aforementioned BBH tasks. The results are summarized in Figure [7.](#page-12-2) The Oracle Merger represents the accuracy that would be achieved if the merger process were flawless.

As expected, the accuracy at the leaves acts as an upper bound for ToP. Moreover, the Oracle Merger yields better performance than vanilla ToP. This suggests that there is a loss in accuracy when going from level k to level $k - 1$, which can prevent ToP from achieving an even higher performance. Interestingly, what happens with *Multistep Arithmetic Two* comes close to the worst case scenario that we depicted earlier. Despite the leaves' accuracy being 55%, ToP + Oracle Merger fails to outperform CoT's 34% accuracy, showing that the distribution of the correct leaves' instances inherently undermines ToP performance in this scenario.

C.2 Impact of the tree structure.

GoT Tasks. We analyze the impact of the tree structure on ToP's results. As shown previously, there may be a loss in accuracy during the merge operation. A deeper tree means more of these losses, but it also means easier subproblems. For the three GoT tasks, we analyze the impact of the tree's depth when the breadth is set to two with LLaMA 3 70B Instruct [\(Dubey et al.,](#page-5-4) [2024\)](#page-5-4).

As suggested by Figure [8,](#page-13-1) deeper trees led to a higher accuracy for all three tasks. This is because we observed very few errors during the merge operation performed by the LLM. Going deeper, even with a near perfect merger can negatively affect performance as observed with the Set Intersection task, which has an accuracy of 47% with $d = 4$ but 74% with $d = 3$ and 62% with $d = 2$. The small errors performed at the leaves being propa-

Figure 8: Impact of the tree structure (depth) on the accuracy on the 3 GoT Tasks with LLaMA 3 70B Instruct. Depth = 0 represents CoT prompting.

gated during the repetitive merge operations impact the overall accuracy of ToP. In terms of breadth, applying ToP (4, 1) to *Set Intersection* yields the same accuracy of 62% as ToP (2, 2). We observed ToP (4, 2) to have a 49% accuracy, comparable to ToP (2, 4)'s 47%.

BBH Tasks. *Tracking Shuffled Objects* involves recovering the final assignement of L objects given to L people ($L \in \{3, 5, 7\}$) after a series of L transpositions (pairwise swaps). Applying ToP $(1, d)$ to these tasks implies using d even subseries of swaps in a manner akin to *Navigate* (see Figure [1\)](#page-1-0). We study the impact of various depths and we report the results in Figure [9.](#page-13-2)

Across all settings, the task accuracy gradually increases with deeper trees and reaches its maximum when all the subproblems involve only one swap (depth = $L - 1$). The trade-off between the number of merge operations and the accuracy of simple instances is not at play here.

On *Multistep Arithmetic Two*, ToP (2, 1) and ToP (2, 2) respectively achieve 30.8% and 57.2% accuracy where CoT is at 34%. Similarly, ToP (1, 2) and ToP (1, 3) respectively achieve 60% and 66.4% where CoT is at 60.4% on *Navigate*. This suggests that the tree structure can greatly affect the quality of ToP.

C.3 Robustness to the solve prompt.

Throughout our experiments, we used CoT prompting to solve the most granular subproblems (the tree's leaves). In this section, we examine the impact of using IO prompting to solve the leaves. We conduct experiments on *Word Sorting*, which did not benefit from CoT prompting as shown in

Figure 9: Impact of the tree structure (depth) on the accuracy of ToP on *Tracking Shuffled Objects* $(L \in \{3, 5, 7\})$. Depth = 0 and depth = 1 represent CoT prompting.

Table [4.](#page-4-2) Additionally, we include *Tracking Shuffled Objects (3, 5)*, *Boolean Expressions*, *Multistep Arithmetic Two*, and *Object Counting*, where IO prompting produced much poorer results compared to CoT. The results are summarized in Table [7.](#page-13-3)

BBH tasks	LLaMA 3 8B			
	Ю	$IO + ToP$		
Boolean Expressions	0.824	0.876		
Multistep Arithmetic Two	0.008	0.036		
Object Counting	0.492	0.552		
Tracking Shuffled Objects				
Three	0.132	0.196		
Five	0.004	0.008		
Web of Lies	0.528	0.484		
Word Sorting	0.647	0.679		

Table 7: Comparison of IO prompting and IO + ToP on BBH tasks.

We observe that $IO + Top$ consistently outperforms standalone IO prompting on all the BBH tasks except *Web of Lies*. This is because the LLM's performance is random (0.528) on that specific task and dividing it into simpler instances does not resolve the issue (leaves' $EM = 0.496$). Moreover, applying IO + ToP on *Multistep Arithmetic Two* with a depth of 2 instead of 1 gives a 22% accuracy. These results demonstrate that ToP is robust to low-quality solve_prompt but achieves the best results with a good solve_prompt.

C.4 Analysis of failure cases

In Table [4,](#page-4-2) we showed that ToP induces considerable performance gains on various complex BBH tasks with gpt-3.5-turbo-instruct. However, ToP specifically failed to improve performance on *Multistep Arithmetic Two* and *Object Counting*. An analysis of the model's outputs suggests 2 main causes:

1. The founding hypothesis of ToP is not always

verified. The founding hypothesis of ToP is the ability of an LLM to perform better on simpler instances of a task compared to more complex ones. When this is not verified, ToP's performance tends to fall behind CoT prompting. We strikingly observe such a behaviour on *Object Counting*. For multiple instances, the LLM was able to count the relevant items in a given list but fails to do so in a subset of the same list, as illustrated in Table [8.](#page-14-1) This also frequently occurs with *Multistep Arithmetic Two* instances, where the 73.6% ToP's accuracy cannot be improved even with an Oracle merger.

MAIN INSTANCE

Q: I have three oranges, a pig, a frog, a cow, three bananas, a nectarine, and a snail. How many animals do I have?

Let's think step by step.

We first identify the animals on the list and include their quantity in parentheses: - pig (1) $-$ frog (1)

- $-$ cow (1)
- snail (1)
-

Now, let's add the numbers in parentheses: $1 + 1 + 1 + 1$ $= 4$. So the answer is 4.

SUBINSTANCE

Q: I have three bananas, a nectarine, and a snail. How many animals do I have?

Let's think step by step. We first identify the animals on the list and include their quantity in parentheses: - bananas (3) - nectarine (1) - snail (1) Now, let's add the numbers in parentheses: $3 + 1 + 1 =$

5. So the answer is 5.

Table 8: gpt-3.5-turbo-instruct is able to accurately count the number of animals in a given list but fails to count it in a sublist.

2. The LLM fails to merge subproblems' solutions into their parent's solution. In Appendix [C.1,](#page-11-3) we showed that the use of an oracle

merger leads to even greater improvements in the ToP framework. Additionally, a bad merger can bring ToP below CoT performance. Table [9](#page-14-2) shows an example on the *Object Counting* task, where the LLM accurately solve both subproblems but fail to combine their answers. We believe that such issues can be significantly alleviated with a better merge_prompt.

SUBINSTANCE 1

- garlic (1)

Now, let's add the numbers in parentheses: $1 + 1 + 2 + 1$ $= 5.$ So the answer is 5.

SUBINSTANCE 2

Q: I have a carrot, a head of broccoli, a potato, a stalk of celery, a lettuce head, and a toaster. How many vegetables do I have?

Let's think step by step.

We first identify the vegetables on the list and include their quantity in parentheses:

- $-$ carrot (1)
- broccoli (1)
- potato (1)
- celery (1)
- lettuce (1)

Now, let's add the numbers in parentheses: $1 + 1 + 1 + 1$ $+ 1 = 5$. So the answer is 5.

MAIN INSTANCE

11. So the answer is 11.

Q: I have a yam, a cauliflower, a bed, two cabbages, a garlic, an oven, a carrot, a head of broccoli, a potato, a stalk of celery, a lettuce head, and a toaster. How many vegetables do I have?

Let's think step by step. The list of words can be written as the concatenation of A and B where $-A = a$ yam, a cauliflower, a bed, two cabbages, and a garlic. $-B = an$ oven, a carrot, a head of broccoli, a potato, a stalk of celery, and a lettuce head. According to the premises, A contains 5 vegetables. According to the premises, B contains 6 vegetables. Then, the total number of vegetables is $A + B = 5 + 6 =$

Table 9: gpt-3.5-turbo-instruct is unable to use the information in its context to solve the given problem.

D Implementation details

D.1 Language Models and Datasets

In Table [10,](#page-16-0) we list the links to the relevant resources used to build this work.

D.2 Sampling scheme and evaluation metrics

For prompting strategies that require sampling, we use nucleus sampling with $T = 0.7$ and top-p = 0.95. Otherwise, we use greedy decoding $(T =$ 0.0). In all experiments, we generate at most 2000 new tokens and use Exact String Match (EM) as the evaluation metric.

D.3 Decomposition

All the decomposers are algorithmic. For sorting and set intersection, a list L is divided into $L[\emptyset:len(L)/2]$ and $L[\len(L)/2:]$. For keyword sorting, we decompose the input text based on its sentences with the help of a sentence splitter module.[4](#page-15-3)

D.4 How to choose the breadth and the depth

ToP depends on 2 parameters, the breadth and the depth of the tree structure. A quick analysis of the problem can lead to an informed guess about what a good breadth should be. This is typically the case of sorting problems when a breadth of 2 helps to mimic the merge sort algorithm. We mostly experimented with a breadth of 2 for canonical tasks and saw that it yielded very good results. When it comes to sequential problems, the breadth is 1 and the depth plays the role of the number of block of steps before reaching the final state (depth-wise decomposition). Using 2 blocks also gave good results, but deeper trees tend to always give better results for such problems.

E Prompts

E.1 GoT Tasks

We provide the links to all the prompts used to solve the GoT tasks in Table [11.](#page-16-1)

E.2 BBH tasks

We describe the modification applied to 3 BBH tasks: *Hyperbaton*, *Navigate* and *Tracking Shuffled Objects*. Instead of choosing which of two sentences has the right adjective ordering, we turned

4 [https://github.com/mediacloud/](https://github.com/mediacloud/sentence-splitter) [sentence-splitter](https://github.com/mediacloud/sentence-splitter)

each instance of *Hyperbaton* into 2 separate instances of Yes/No questions relative to adjectives ordering. Table [12](#page-16-2) shows an example instance before and after the modification (we only reported one separate instance for visibility). We modify *Navigate* to require to find the final position after a series of instructions instead of asking if they lead to the starting point. Table [13](#page-17-0) shows an example instance before and after modification. In *Tracking Shuffled Objects*, we ask the LLM to recover the final object assignments after the pairwise swaps as exemplified in Table [14.](#page-18-0)

We provide the links to all the prompts used to solve the BBH tasks in Table [15.](#page-18-1)

E.3 Symbolic Reasoning

We provide the links to all the prompts used to solve Coin Flip and Last Letter Concatenation in Table [16.](#page-19-0)

Table 10: Links to datasets, benchmarks and language models.

Table 11: Links to solve and merge prompts of the GoT Tasks.

BEFORE

Q: Which sentence has the correct adjective order:

Options:

(A) rubber terrible ship

(B) terrible rubber ship

IO Answer

(B)

CoT Answer

A: Let's think step by step.

When there is more than one adjective before a noun, the adjectives need to respect the following order before a noun: "[1. opinion] [2. size] [3. age] [4. shape] [5. color] [6. origin] [7. material] [8. purpose] noun".

Option (A): "rubber terrible ship". (1) rubber" falls into the material category. (2) "terrible" falls into the opinion category. Option (A) has the following adjective order: [7. material] [1. opinion] (or, in numeric terms, 7 1). Because $7 < 1$ is not correct, (A) does not have the correct ordering.

Option (B): "terrible rubber ship". Option (B) has the following adjective order: [1. opinion] [7. material] (or, in numeric terms, 1 7). Because $1 < 7$ is correct, (B) has the correct ordering. So the answer is (B) .

AFTER

Q: Answer with Yes or No. Does the following sentence have the correct adjective order? rubber terrible ship

IO Answer

No

CoT Answer

A: Let's think step by step.

When there is more than one adjective before a noun, the adjectives need to respect the following order before a noun: "[1.] opinion] [2. size] [3. age] [4. shape] [5. color] [6. origin] [7. material] [8. purpose] noun".

The sentence is "rubber terrible ship". (1) rubber" falls into the material category. (2) "terrible" falls into the opinion category. The sentence has the following adjective order: [7. material] [1. opinion] (or, in numeric terms, 7 1). Because 7 < 1 is not correct, the sentence does not have the correct ordering. So the answer is No.

Table 12: Modification applied to *Hyperbaton*.

BEFORE

Q: If you follow these instructions, do you return to the starting point? Turn left. Turn around. Turn left. Take 7 steps. Take 2 steps. Take 4 steps. Take 8 steps.

IO Answer

No

CoT Answer

A: Let's think step by step. We start at the origin (0, 0), facing the positive y-axis.

(1) Turn left: $(0, 0)$, facing the negative x-axis.

(2) Turn around: (0, 0), facing the positive x-axis.

 (3) Turn left: $(0, 0)$, facing the positive y-axis.

(4) Take 7 steps: (0, 7), facing the positive y-axis.

(5) Take 2 steps: (0, 9), facing the positive y-axis.

(6) Take 4 steps: (0, 13), facing the positive y-axis.

(7) Take 8 steps: (0, 21), facing the positive y-axis.

Since $(0, 21)$ is not $(0, 0)$, we are not where we started. So the answer is **No.**

AFTER

 Q : If you follow these instructions, what are the coordinates of the end point if you start at the point $(0, 0)$, facing the positive y-axis? Turn left. Turn around. Turn left. Take 7 steps. Take 2 steps. Take 4 steps. Take 8 steps.

IO Answer

 $(0, 21)$

CoT Answer

A: Let's think step by step. We start at the origin $(0, 0)$, facing the positive y-axis.

(1) Turn left: $(0, 0)$, facing the negative x-axis.

(2) Turn around: $(0, 0)$, facing the positive x-axis.

(3) Turn left: (0, 0), facing the positive y-axis.

(4) Take 7 steps: (0, 7), facing the positive y-axis.

(5) Take 2 steps: (0, 9), facing the positive y-axis.

(6) Take 4 steps: (0, 13), facing the positive y-axis.

(7) Take 8 steps: (0, 21), facing the positive y-axis.

So the answer is $(0, 21)$.

Table 13: Modification applied to *Navigate*.

BEFORE

Q: Alice, Bob, and Claire are friends and avid readers who occasionally trade books. At the start of the semester, they each buy one new book: Alice gets Ulysses, Bob gets Frankenstein, and Claire gets Lolita. As the semester proceeds, they start trading around the new books. First, Claire and Bob swap books. Then, Bob and Alice swap books. Finally, Claire and Bob swap books.

At the end of the semester, Bob has

Options:

(A) Ulysses

(B) Frankenstein

(C) Lolita

IO Answer

(B)

CoT Answer

A: Let's think step by step.

(0) At the start: Alice: Ulysses, Bob: Frankenstein, Claire: Lolita.

(1) Claire and Bob swap books: Alice: Ulysses, Bob: Lolita, Claire: Frankenstein.

(2) Bob and Alice swap books: Alice: Lolita, Bob: Ulysses, Claire: Frankenstein.

(3) Claire and Bob swap books: Alice: Lolita, Bob: Frankenstein, Claire: Ulysses.

At the end of the semester, Bob has Frankenstein. So the answer is (B).

AFTER

Q: Alice, Bob, and Claire are friends and avid readers who occasionally trade books. At the start of the semester, they each buy one new book: Alice gets Ulysses, Bob gets Frankenstein, and Claire gets Lolita. As the semester proceeds, they start trading around the new books. First, Claire and Bob swap books. Then, Bob and Alice swap books. Finally, Claire and Bob swap books.

At the end of the semester, what is the assignment of books?

IO Answer

Alice: Lolita, Bob: Frankenstein, Claire: Ulysses

CoT Answer

A: Let's think step by step.

(0) At the start: Alice: Ulysses, Bob: Frankenstein, Claire: Lolita.

(1) Claire and Bob swap books: Alice: Ulysses, Bob: Lolita, Claire: Frankenstein.

(2) Bob and Alice swap books: Alice: Lolita, Bob: Ulysses, Claire: Frankenstein.

(3) Claire and Bob swap books: Alice: Lolita, Bob: Frankenstein, Claire: Ulysses.

So the answer is Alice: Lolita, Bob: Frankenstein, Claire: Ulysses.

Table 15: Links to solve and merge prompts for the BBH tasks.

Table 16: Links to solve and merge prompts for Coin Flip and Last Letter Concatenation.