

Have Large Language Models Learned to Reason? A Characterization via 3-SAT

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Abstract

Large Language Models (LLMs) have been touted as AI models possessing advanced reasoning abilities. In theory, autoregressive LLMs with Chain-of-Thought (CoT) can perform more serial computations to solve complex reasoning tasks. However, recent studies suggest that, despite this capacity, LLMs do not truly learn to reason but instead fit on statistical features. To study the reasoning capabilities in a principled fashion, we adopt a computational theory perspective and propose an experimental protocol centered on 3-SAT – the prototypical NP-complete problem lying at the core of logical reasoning and constraint satisfaction tasks. Specifically, we examine the phase transitions in random 3-SAT and characterize the reasoning abilities of state-of-the-art LLMs by varying the inherent hardness of the problem instances. By comparing DeepSeek R1 with other LLMs, our findings reveal two key insights (1) LLM accuracy drops significantly on harder instances, suggesting all current models struggle when statistical shortcuts are unavailable (2) Unlike other LLMs, R1 shows signs of having learned the underlying reasoning. Following a principled experimental protocol, our study moves beyond the benchmark-driven evidence often found in LLM reasoning research. Our findings highlight important gaps and suggest clear directions for future research. [Link to our code.](#)

1 Introduction

The success and versatility of Large Language Models (LLMs) have sparked widespread interest and debate on whether LLMs are capable of reasoning. Recent studies suggest that LLMs are inherently capable of zero-shot reasoning (Kojima et al., 2022). This ability has been shown to *emerge* and improve with scale (Wei et al., 2022a; Srivastava et al., 2023), and can be further enhanced through prompting techniques that encourage LLMs to *think step-by-step* (Wei et al., 2022b; Yao et al., 2023b). Demonstrations include, inter alia, planning (Huang et al., 2022; Hazra et al., 2024b), theorem proving (Jiang et al., 2023; Welleck et al., 2022), search and optimization (Romera-Paredes et al., 2024; Hazra et al., 2024a), self-reflection (Yao et al., 2023a; Madaan et al., 2023), and tool usage (Schick et al., 2023).

Conversely, a growing body of research presents a more critical view of these reasoning abilities. For instance, LLMs may exhibit limitations in consistent logical reasoning (Arkoudas, 2023; Saparov & He, 2023), effective planning (Valmeekam et al., 2022), and accurate self-evaluation of their outputs (Stechly et al., 2023). So, to what extent can LLMs reason?

Recent works address this question by characterizing LLMs’ theoretical capabilities and limitations using worst-case complexity analysis. Peng et al. (2024) demonstrated that multi-layer transformers cannot solve problems such as Derivability, 2-SAT, and Horn SAT. However, with *T*-chain of thought (CoT) steps, transformers’ abilities can be extended up to those solvable by Boolean circuits of size *T* (Li et al., 2024). Moreover, with polynomially many *correct* intermediate CoT steps, an LLM can compute all circuits in polynomial size,

P/poly, a superclass of P. Therefore, LLMs should be able to solve reasoning problems falling into these complexity classes, like 2-SAT and Horn-SAT. It is also expected to solve some – but not all – 3-SAT instances since certain problems may require circuit complexities that exceed polynomial bounds. Empirically, this aligns with test-time compute scaling studies that show improved reasoning performance with increased computational resources (Lightman et al., 2024; Snell et al., 2025). **Thus, from a theoretical standpoint, LLMs equipped with CoT possess the capacity to solve reasoning problems falling in P or P/Poly.**

However, despite this, recent works have shown that LLMs are **not learning to reason**, by fitting on statistical features and not internalizing the logic (i.e. learning to reproduce the style and not logic) (Zhang et al., 2023) much like the *Clever Hans Cheat* (Bachmann & Nagarajan, 2024). With the advent of Large Reasoning Models (LRMs) like DeepSeek R1 (DeepSeek-AI, 2025a) which leverage more test-time compute, there is renewed optimism about enhancing reasoning capabilities. However, it is unclear if this marks a real step change, due to limitations in current reasoning benchmarks like (1) growing concerns about dataset contamination¹ (Zhang et al., 2024) that can inflate the reasoning performance; (2) conflation of commonsense reasoning rooted in *retrieving* world knowledge, and logical or deductive reasoning – requiring algebraic *manipulation* of knowledge (Genesereth & Nilsson, 1987) – making it challenging to decouple the two.

To move beyond these limitations, a more principled approach to evaluating reasoning is needed. We adopt Leon Bottou’s definition, which defines reasoning as “*algebraically manipulating previously acquired knowledge to answer a new question*” (Bottou, 2014). This closely aligns with Russell and Norvig’s description of AI as rational thinking (Russell & Norvig, 2010). Building on this, we ask: Have LLMs learned to reason, and if so, to what extent? We answer through the following contributions:

(1) Characterizing LLM-reasoning from a computational theory perspective. Adhering to Leon Bottou’s definition, we propose an experimental framework centered on 3-SAT, to evaluate reasoning. Introduced in Figure 1, 3-SAT is a foundational problem in computational complexity, and many problems in AI such as (propositional fragments of) logical reasoning, planning, and constraint satisfaction can be reduced to 3-SAT. We also extend our analysis to tractable fragments like 2-SAT (NL-Complete) (Bollobás et al., 2001) and 1-3 Horn-SAT (P-Complete) (Demopoulos & Vardi, 2006) which also exhibit phase transitions, revealing interesting observations across complexity classes. Our approach provides a formal and robust evaluation of reasoning abilities and bridges computational theory with modern AI.

(2) Studying Phase Transition Characteristics of LLMs. We investigate the phase transition characteristics of LLMs (Cheeseman et al., 1991), i.e., how LLMs’ performance varies in the easy and hard regions of the problem space, unlike standard reasoning benchmarks that overlook variations due to *inherent hardness* of problems. We observe that LLM performance declines in the hard region where statistical features are largely absent.

(3) Comprehensive evaluation of state-of-the-art LLMs. We conducted extensive experiments across state-of-the-art open-source and proprietary LLMs. We find a significant gap between the performances of DeepSeek R1 (DeepSeek-AI, 2025a) to other LLMs like GPT-4o (OpenAI, 2024), Claude 3.7 Sonnet (Anthropic, 2025), Gemini 2.0 Flash (Google, 2024), and DeepSeek V3 (DeepSeek-AI, 2025b). Interestingly, the CoT traces produced by DeepSeek R1 reveal patterns suggestive of an in-context tree search with backtracking, which may account for its superior performance. In contrast, the other models consistently fail to demonstrate comparable reasoning capabilities. This leads us to believe that LRMs like R1 could be a **step-change in reasoning abilities**.

2 Preliminaries

2.1 Phase Transitions in Random 3-SAT

We study the reasoning capabilities of LLMs on random 3-SAT problems. 3-SAT constitutes one of the most fundamental problems in computer science as it is the prototypical

¹Data closely resembling the benchmark leaks into the training data.

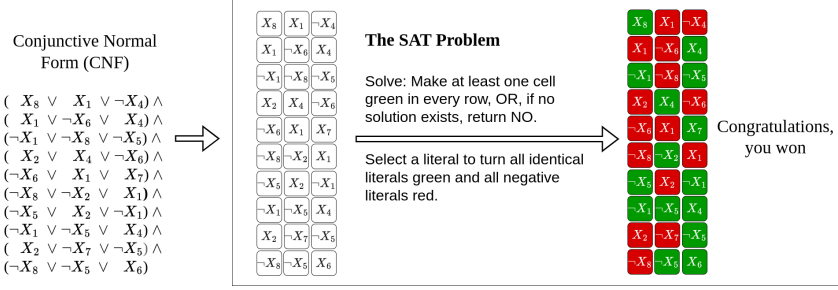


Figure 1: **The 3-SAT problem**, visualized using a variant of the SAT game (Roussel). In SAT, the goal is to return a truth assignment to Boolean variables that satisfies a Boolean formula in conjunctive normal form (CNF), or return unsAT if none exists. In the visualization, each row represents a clause—a disjunction (logical OR, \vee) of literals, where each literal is either positive (X_1) or negative ($\neg X_1$). A clause is satisfied if at least one of its literals is assigned true. Clauses are joined by logical AND (\wedge), so all must be satisfied for the formula to hold. If no such assignment exists, the formula is unsatisfiable.

NP-complete problem, lying at the foundation of computational complexity theory. Moreover, various prevalent reasoning problems in artificial intelligence, such as planning and constraint satisfaction, can be reduced to solving 3-SAT problems (Garey & Johnson, 1990).

By randomly sampling 3-SAT formulas², we avoid domain-specific biases, and it lets us control the complexity of the generated formulas. In fact, an interesting empirical observation is the presence of a *phase transition* in random 3-SAT problems (Cheeseman et al., 1991). When randomly sampling 3-SAT formulas, one can observe a sharp change in the probability of a 3-SAT formula being satisfiable when plotted against $\alpha = m/n$, where m is the number of clauses and n is the number of variables. For random 3-SAT, this phase transition occurs at $\alpha_c \approx 4.267$ (Mertens et al., 2006; Ding et al., 2015), i.e. the point at which a randomly sampled 3-SAT formula has equal probability to be satisfiable or unsatisfiable. This naturally divides 3-SAT problems into three regions: the under-constrained region below the threshold (Easy), the constrained region in the neighborhood of the threshold (Hard), and the over-constrained region above the threshold (Easy), cf. Figure 2.

2.2 SAT Solvers

SAT solvers are tools to automatically verify the satisfiability of propositional logic formulas. The Davis–Putnam–Logemann–Loveland (DPLL) algorithm (Davis et al., 1962) is a key component of modern SAT solvers. It consists of a backtracking-based algorithm, equipped with heuristics, to efficiently explore the search space and determine if a formula is satisfiable (Figure 2). The algorithm selects a literal and assigns a truth value to it. This is applied recursively until all clauses are satisfied, meaning that the original formula is satisfiable. Modern SAT solvers are based on Conflict-Driven Clause Learning (CDCL) (Silva & Sakallah, 1996) which enhances DPLL with conflict analysis and clause learning. In Figure 2, we show how the time to determine the satisfiability of a random 3-SAT formula varies in function of α . Most prominently, we see a pronounced peak in runtime around the α_c .

Analogously to characterizing SAT solvers by their behavior with varying α , we study the reasoning capabilities of LLMs with respect to the phase transition in random 3-SAT.

3 Related Work

Merrill & Sabharwal (2023) established that multi-layer transformers belong to the complexity class log-uniform TC⁰. Subsequently, Peng et al. (2024) demonstrated that multi-layer transformers cannot solve problems such as Derivability, 2-SAT, Horn SAT, and Circuit

²We use Selman et al. (1996) random model, where clauses are sampled with replacement.

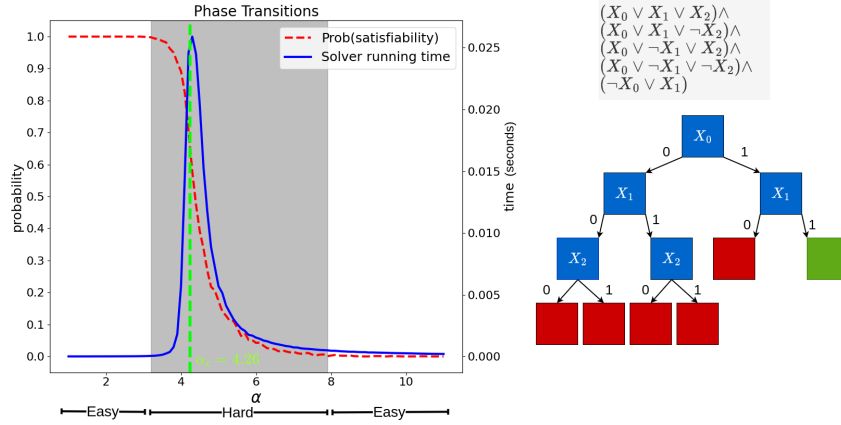


Figure 2: [Left]: **Random 3-SAT Phase Transitions** (Cheeseman et al., 1991). Plotted in red is the probability of a randomly sampled 3-SAT formula being satisfied against the hardness α of the formula. We can observe a clear phase transition occurring at $\alpha_c \approx 4.267$ (marked by a green -). We identify two Easy regions, one on either side of α_c . The gray area in the middle denotes the Hard region. The boundaries of the hard region are defined where the probability of the formula being satisfied ceases to be deterministically 1 (left) or 0 (right). The solid blue line shows the mean time taken by the MiniSAT solver to solve 3-SAT instances. Notably, there is a spike in the solver’s runtime near α_c . This is due to the absence of useful heuristics in this region, forcing the solver to resort to exhaustive searches. [Right]: **DPLL Search Trace** from a SAT Solver for the given formula. Red boxes denote unsatisfiable assignments; the green box highlights a satisfying one. 0, 1 are truth assignments.

Evaluation unless $L=NL$. While these results provide worst-case performance bounds for transformer architectures, their relevance to average-case complexity is limited (Coarfa et al., 2000), therefore, offering only partial insights into the practical reasoning capabilities of LLMs. Notably, recent works have shown that T chain of thought (CoT) steps can extend transformers’ abilities beyond TC^0 , up to those solvable by Boolean circuits of size T (Li et al., 2024). With T being polynomial in the input size, LLMs can in theory solve problems in P class like 2-SAT and Horn SAT. Our SAT experiments support this, showing improved reasoning with extended CoT steps. Yet, a central question remains: *can LLMs learn to reason effectively, given that they are theoretically capable?*

To this end, Dziri et al. (2023) investigate the performance of LLMs on compositional tasks with varying levels of complexity. Their experiments reveal a significant performance decline as task complexity increases, measured by problem size and reasoning depth. The findings indicate that while models can memorize single-step operations from training, they fail to compose these steps into correct reasoning paths. Similarly, Zhang et al. (2023) found that BERT-based models fail to generalize to out-of-distribution data even within a tractable (i.e., not NP-complete) problem class, overfitting to statistical features during training. Our results extend these findings by showing that performance declines are better explained by *inherent problem hardness* – as captured by phase transitions – rather than size or depth alone.

Closest to our work is the NPHardEval (Fan et al., 2024), which examines reasoning across various computational complexity classes. We extend this by analyzing phase transition characteristics and how performance varies with inherent problem hardness. Our evaluation focuses on classes with known phase transitions (Schaefer, 1978), including 2-SAT (NL-Complete), 1-3 Horn-SAT (P-Complete), and 3-SAT (NP-Complete). By comparing LRMs with LLMs, we gain deeper insights into the impact of longer reasoning traces, performance across easy and hard regions, and variation with model count (i.e., number of solutions).

Our findings also align with Xiang et al. (2025), who claim that classical CoT training data fails to capture the non-linear and iterative nature of complex reasoning. They propose Meta-CoT, which explicitly models this “thinking” process. We observe that DeepSeek R1

exhibits Meta-CoT-like behavior, autoregressively generating search trees that reflect latent reasoning steps – suggesting that the model has, to some extent, *learned to reason*.

4 Methodology

4.1 Using LLMs as 3-SAT Solvers

To use LLMs as 3-SAT solvers, we reframe the 3-SAT problem as a natural language menu-selection problem, termed as **SAT-Menu**. As shown in Box 1, the prompt input to the LLM consists of a task outline, along with a specific scenario detailing the dietary preferences of a set of people. The LLM’s objective is to identify a combination of orderable (akin to positive literals) and non-orderable (akin to negative literals) food items that meet these preferences; or declare the situation unsatisfiable (unSAT) if no valid combination exists. Note, that the prompt example in Box 1 constitutes a minimal example stripped of all details. The complete system prompt incorporates techniques known to enhance the apparent reasoning capabilities of LLMs, such as chain-of-thought (CoT) (Wei et al., 2022b) and in-context learning (Brown et al., 2020) (see Box 2 in Appendix for the full prompt).

Additionally, we introduce a second problem formulation where the LLM is directly given the underlying 3-SAT formula in Conjunctive Normal Form (CNF). We refer to this scenario as **SAT-CNF**. Specifically, in this setting, the problem is presented as a list of integers to the LLM, similar to the approach outlined in SAT Game (Figure 1). For more details about the prompt, we refer the reader to Box 3 in the Appendix.

Box 1: SAT-Menu Prompt

System Message

Your task is to output two distinct lists of food items, one denoting what can be ordered ('orderable') and the other what cannot ('not_orderable'), to meet the preferences of a group of individuals. Each person must find the selection satisfactory based on their likes and dislikes. The satisfaction criteria are: 1. A person is satisfied if at least one liked item is in 'orderable' list or one disliked item is in 'not_orderable' list. 2. No item can appear on both lists. 3. All participants must be satisfied by the combination of the two lists. 4. Importantly, if no such combination exists that satisfies all, output empty lists for both. Check carefully before finalizing. You always think step-by-step and show all your work in the explanation. Output your final solution as a comma-separated list of strings in Python code (`orderable = [...], not_orderable = [...]`).

Input for a new problem

Preferences: Jay: Likes nachos, ratatouille. Dislikes pie. Ada: Likes pie. Dislikes burger, ravioli. Zoe: Likes ravioli. Dislikes pie, burger. Arun: Likes ratatouille. Dislikes pie, nachos. Ula: Likes ratatouille. Dislikes ravioli, nachos. Ying: Likes nachos, ratatouille. Dislikes burger.

We consider two 3-SAT variants to evaluate reasoning – Decision problem (NP-complete) where the model determines satisfiability, answering “yes” or “no”; and the Search problem (NP-hard), where it should return a satisfying assignment if it exists, else return “no”.

Since we have theoretical bounds that apply specifically to autoregressive LLMs, we restrict our evaluation to state-of-the-art models that follow this paradigm – namely, GPT-4o (OpenAI, 2024), Gemini 2.0 Flash (Google, 2024), Claude 3.7 Sonnet (Anthropic, 2025), and DeepSeek V3 (DeepSeek-AI, 2025b). Additionally, we include DeepSeek R1 (DeepSeek-AI, 2025a) in our analysis, as (1) we have access to its chain-of-thought (CoT) “thinking” tokens, which we can confirm are generated autoregressively³; (2) it is one of the top models⁴. The generation configurations are listed in Appendix Table 2. To verify the LLM-generated solutions, we employed MiniSAT v2.2 (Eén & Sörensson, 2003) solver.

³Although other *thinking* models exist, they either do not expose their thinking tokens or only provide them through their respective user interface. As such, we cannot verify whether their reasoning is produced autoregressively or through search-based methods at test time.

⁴<https://huggingface.co/spaces/lmarena-ai/chatbot-arena-leaderboard>

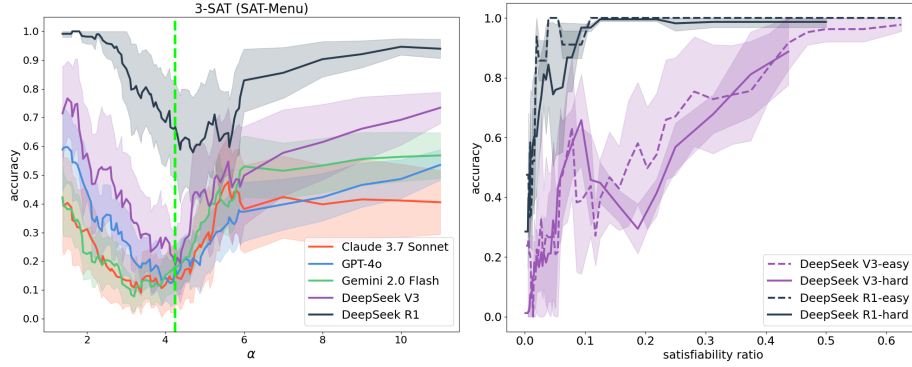


Figure 3: [Left] 3-SAT performance comparison for the **search** version of SAT-Menu. [Right] Accuracy vs. satisfiability ratio on the search version of SAT-Menu. We only include satisfiable instances and analyze hard (solid line) and easy regions (dashed line) separately. We use 90% confidence intervals to quantify uncertainty around the estimated accuracy. In the plots, these intervals help assess the reliability of accuracy estimates – narrow bands indicate high certainty, while wider bands suggest greater variability.

Notably, techniques such as Tree-of-Thoughts (Yao et al., 2023a), Best-of-N (Wang et al., 2023) sampling, or other tree-based search frameworks effectively wrap LLMs in an external symbolic search and are beyond the scope of our analysis. These methods use the LLM to generate ideas (nodes of the tree) while orchestrating search or backtracking over a tree data structure. Crucially, the graph algorithm (e.g., tree traversal, backtracking) is not internally generated or maintained by the LLM. Instead, it is externally imposed. **Our goal is to assess whether LLMs can natively reason** – for example, whether they can generate multiple candidate solutions, maintain them in memory, reason over them, and converge to a consistent answer entirely in context.

4.2 Dataset Generation

To generate 3-SAT data, we varied $\alpha = m/n$ as a parameter to guide the generation process. For each $n \in [1, 10]$, we selected $\alpha \in [1, 11]$ based on feasible values of m . Table 1 in the Appendix provides the full range of values. MiniSAT v2.2 (Eén & Sörensson, 2003) labels each instance as satisfiable or unsatisfiable. Additionally, each instance is annotated with model count (i.e. number of feasible solutions for a formula) using the D4 model counter (Lagniez & Marquis, 2017).

For SAT-Menu setup, we map each instance (i.e. CNF formula) to a menu selection puzzle. The goal is to select a combination of orderable and non-orderable food items in a way that satisfies everyone’s preferences. To this end, a food item is sampled without replacement corresponding to the list of variables in the formula. Then, every clause in the formula is treated as the preferences for an individual, leading to the creation of two distinct lists for each person: “Likes,” for food items linked to positive literals, and “Dislikes,” for those associated with negated literals, cf. Box 2.

Detailed statistics and data generation processes for 2-SAT and Horn-SAT are provided in Appendix A. All our experiments use a pool of randomly sampled ≈ 5000 formulas which include satisfiable and unsatisfiable instances.

5 Results

5.1 Do LLMs Reason?

We evaluate the performance of LLMs by measuring their accuracy in solving SAT Search across formulas with varying α . As shown in Figure 3 [Left], we find that all LLMs exhibit

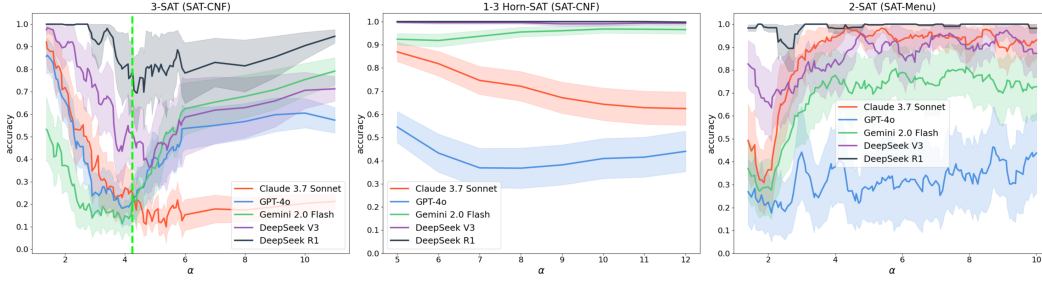


Figure 4: **Performance across all complexity classes for the search problem.** R1 outperforms all LLMs across all complexity classes. From left to right, 3-SAT (SAT-CNF), 1-3 Horn SAT (SAT-CNF), and 2-SAT (SAT-Menu). It can be observed that LLM performances are affected around the critical points for 3-SAT ($\alpha_c = 4.267$) and 2-SAT ($\alpha_c = 1.0$). We use 90% confidence intervals to quantify uncertainty around the estimated accuracy – narrow bands indicate high certainty.

inverted phase transitions (Easy-Hard-Easy pattern) in the SAT Search problem. Their performance is high in the easy regions, while it significantly drops to $\approx 10\%$ in the hard region. The hard region performance remains unaffected by in-context learning (Appendix Figure 10). We also observe that R1 significantly outperforms other LLMs where **R1’s accuracy in the hard region surpasses even the easy-region performance of LLMs.**

A similar performance trend is observed for SAT-Decision (Appendix Figure 10). From the confusion matrix (Appendix Figure 12), we observe that R1 accurately detects satisfiable formulas, **demonstrating a higher degree of soundness** in its reasoning. However, it often fails to find the satisfying assignment itself, indicating **limited completeness in the hard region**. Other LLMs, by contrast, exhibit lower levels of both soundness and completeness.

In Figure 3 [Right], we plot the performance of LLMs against the *satisfiability ratio*, defined as $\frac{\text{model count}}{2^n}$, where the model count is the number of satisfying assignments and n is the number of variables. This denotes the probability that a randomly selected variable assignment satisfies the given 3-SAT theory⁵. We can observe a clear dependence between the accuracy and satisfiability ratio: **formulas with more satisfying assignments tend to be easier for LLMs.** This holds across both easy and hard regions. **R1, however, maintains consistent accuracy regardless of satisfiability ratio, much like a classical SAT solver.** Similar plots comparing other LLMs are shown in Appendix Figure 11.

We also test 2-SAT (Figure 4), where we observe a distinct dip in LLM performance around the known phase transition at $\alpha_c = 1$ (Bollobás et al., 2001), indicating sensitivity to structural hardness even in problems within NL class. However, LLMs show no clear patterns on 1–3 Horn-SAT. In contrast, **R1 achieves near-perfect accuracy on both 2-SAT and Horn-SAT**, showing no degradation near the phase transition. This suggests that R1 handles problems in the lower complexity classes with ease.

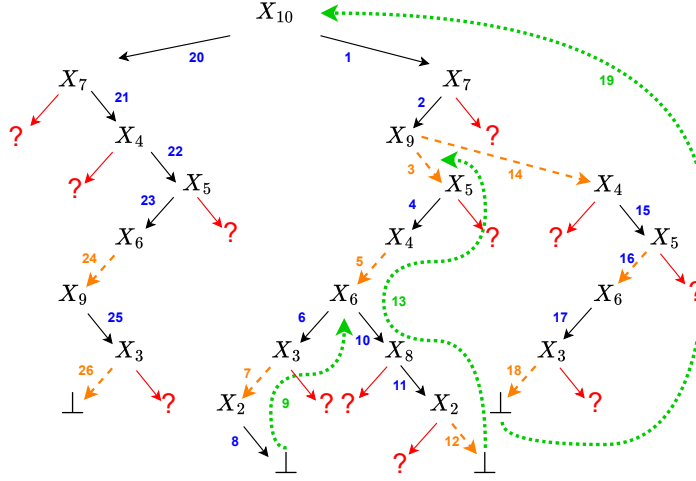
5.2 Has R1 internalized search?

We qualitatively analyzed the search traces generated by R1 and other LLMs on SAT-CNF (Figure 5) and SAT-Menu tasks (Figure 8). Specifically, we annotated the “thinking” traces and attempted to map them to known symbolic search algorithms to better understand the type and depth of search strategies employed, particularly by R1.

In Figure 5, we highlight a failure case where both R1 and GPT-4o incorrectly conclude that a satisfiable formula is unsatisfiable. Despite such failures, our analysis reveals that **R1 consistently exhibits surprisingly coherent and interpretable search behaviors**, including:

⁵Note, this is different from the probability that at least one satisfying assignment exists. Two formulas can both be satisfiable but have different model counts, hence different satisfiability ratios.

[[-9, 10, -7], [7, 5, 6], [3, -2, -7], [-4, -8, 6], [-10, -7, -4], [-6, -9, 3], [9, -4, 5], [-8, -4, 6], [3, -6, 1], [-4, -1, 2], [-6, -4, -10], [4, -3, -6], [4, -7, -5], [7, -10, 3], [-9, 5, -1], [-5, 1, 6], [5, -4, -8], [-10, 5, 4], [1, -3, -4], [7, 6, 9], [-6, -4, 8], [-6, 1, -4], [7, 2, -6], [4, -9, 3], [-7, 6, -10], [6, -5, 4], [-2, -7, -3], [6, -1, 4], [-10, -6, -9], [2, 7, 3]]



Let me start by checking for unit clauses, but wait, all clauses here are disjunctions of three literals. So, there are no unit clauses. (Heuristic Usage: Unit Clauses)
Another approach is to look for pure literals. A pure literal appears only in positive or only in negative form throughout all clauses. (Heuristic Usage: Pure Literals)

Next approach: look for variables that appear frequently. Let's count the occurrences of each variable (ignoring sign). (Heuristic Usage: Maximum Occurrences in Minimum Size clauses)

Now, let's check clause 4: [-4 (False), -8, 6]. So need -8 or 6. Let's see if we can set 6 to True. Let's check clauses involving 6. So if we set 6=True, then clauses 4,8,16,20,25,26,28 are satisfied. But clauses 21 and 22 would require 8 and 1 respectively. (Heuristic Usage: Lookahead in step 6)

... Wait, clause 6: [-6, -9, 3]. Since 6 is True, -6 is False. -9 is True (since 9=False). So clause 6 requires 3 to be True. So 3 must be True. (Mistake: Clause 6 is already satisfied in step 7, however, it's not wrong to set X3)

... Clause 10: [-4 (False), -1, 2 (False)]. So need -1= True \rightarrow 1=False. Wait, but earlier in clause 22, we needed 1=True. So we have a conflict: 1 must be both True and False. This means our current assignments lead to a contradiction. We need to backtrack. (Backtracking: Step 9)

Where did we go wrong? Let's see. The conflict arises from setting 6=True, which leads to clause 22 requiring 1=True, but clause 10 requiring 1=False. Let's backtrack to where we set 6=True. Maybe instead of setting 6=True, we should set 6=False and see what happens. Wait, but when we set 4=True, clause 4: [-4, -8, 6] \rightarrow -4 is False, so need -8 or 6. If we set 6=False, then we need -8 to be True \rightarrow 8=False. So let's try setting 6=False. Let's backtrack to where we set 4=True and 5=True, but then instead of setting 6=True, set 6=False. (Self-Reflection: In step 9, deciding what node to backtrack to)

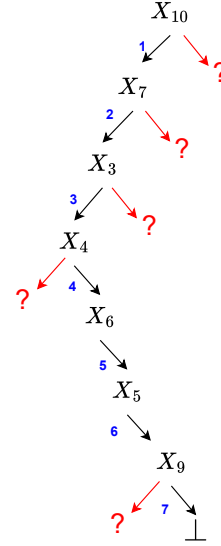
... Clause 27: [-2, -7 (False), -3 (False)]. So need 2=False. (Mistake: In step 11, X3 is unset due to backtracking.)

10=False, 7=True, 9=False, 5=True, 4=True, 6=False, 8=False, 2=False. But 1 must be both True and False. So this path is invalid. Hmm. Let's backtrack further. Maybe setting 5=True was the wrong choice. Let's try setting 5=False instead. Let's backtrack to where we set 10=False, 7=True, 9=False. (Backtracking: Step 14)

So setting 4=False leads to several clauses being satisfied. Clause 18: [-10, 5, 4]. 4=False \rightarrow need 5=True. (Mistake: Unit propagation mistake in step 14. Clause 18 is already satisfied by X10=False.)

Alternatively, maybe the formula is unsatisfiable. But I need to check thoroughly. Let me check another path. Suppose instead of setting 10=False, what if we set 10=True? (Self Correction: Step 20)

It seems that every path I try leads to a contradiction. Therefore the original formula may be unsatisfiable.



We'll make guesses when necessary, but backtrack if a contradiction arises. We can try a greedy approach — assign a variable to make the clause True if not yet assigned. If already assigned, check if it satisfies the clause.

Clause 1: Assign: 10: True
Clause 2: Assign: 7: True
Clause 3: Assign: 3: True
Clause 4: Assign: 4: False
Clauses 5,6,7,8,9,10,11
Clause 12: Assign: 6: False
Clause 14: Assign: 5: False
Clause 14 is satisfied
Clause 15: Assign: 9: False
Clauses 16,17 are satisfied
Clause 18 not satisfied
This means our current assignment is invalid. To satisfy clause 18, at least one of:
x10 = False contradicts earlier
x5 = True contradicts
x4 = True contradicts.

So no way to satisfy clause 18 without violating previous assignments.

Since we have reached a contradiction and the conflicting variables are already fixed, there is no satisfying assignment possible.

Figure 5: **Failure Cases:** SAT-CNF traces for DeepSeek-R1 and GPT-4o. Although the input formula is satisfiable, both models incorrectly predict it as unsat. Colored boxes indicate model behaviors: cyan for heuristic variable selection, orange --- for mistakes, green ... for backtracking, yellow for self-reflection, and violet for self-correction. Left branch always represents a *True* assignment. \perp marks unsatisfiability, and ? indicates an unexplored subtree. Integers are denoted as variables ($10 \rightarrow X_{10}$). Numbers show the order of steps. The input formula is in CNF, where each list of integers represents a clause (e.g., [-9, 10, -7] $\mapsto (\neg X_9 \vee X_{10} \vee \neg X_7)$), and the full formula is a conjunction (\wedge) of these clauses.

- **Tree search:** R1 constructs and logically navigates a search tree. It maintains an awareness of its current position in the search space and builds upon previous decisions.
- **Heuristic usage:** R1 actively applies classical SAT-solving heuristics, including: (1) Unit Clause Elimination: Identifies and assigns values to literals that appear alone in a clause.

- (2) Pure Literal Elimination: Searches for literals that appear with only one polarity across all clauses and assigns them accordingly. (3) MOMS (Maximum Occurrences in Minimum Size clauses) (Crawford & Auton, 1996; Hooker & Vinay, 1995): Prioritizes variables that occur most frequently in the smallest clauses. (4) Lookahead (Heule et al., 2012; Heule & Kullmann, 2017): Anticipates the downstream consequences of assignments before committing. (5) Unit Propagation: Deduces necessary assignments implied by current decisions and propagates them through the formula.
- **Backtracking:** Upon encountering conflicts, R1 identifies the source of the inconsistency and backtracks. In many cases, it performs *backjumping* (i.e., jumping to the most recent conflicting node) to return to the most recent cause of failure (Steps 9, 13).
 - **Self-reflection:** When conflicts arise, R1 engages in reasoning about why the contradiction occurred, revisits earlier decisions, and identifies the specific variable assignments that led to inconsistency.
 - **Self-correction:** R1 demonstrates the ability to recognize flawed strategies or inconsistent outcomes, revise previous decisions, and explore alternative branches in the search space.

Overall, R1 seems to have learned the underlying logic of search and not just the style – unlike, **GPT-4o which performs a greedy search without backtracking**. We examined why R1 occasionally fails despite structured behavior, identifying key failure modes:

- **Incomplete.** Despite initiating a structured search process, **R1 often terminates prematurely** without fully exploring the search tree. Consequently, it fails to guarantee finding a satisfying assignment even if one exists. This is depicted by ? in Figure 5.
- **Limited soundness.** R1 sometimes generates logically inconsistent intermediate states by overlooking clauses (e.g., considering only 47 out of 48 clauses) or incorrectly handling variable assignments after backtracking (e.g., treating a previously unset variable as assigned in Step 11). This results in invalid reasoning states (Steps 3, 14 in Figure 5).
- R1 uses human-like narration in its reasoning trace – expressing internal dialogue, or narrative-style thinking. While this makes the trace more interpretable for humans, it introduces **redundant and verbose explanations** that do not advance the logical search.

We also analyze SAT-Menu traces in Figure 8 (Appendix) and observe that the search process is noticeably more unstructured compared to SAT-CNF. While R1 still displays many abovementioned behaviors such as tree search, heuristic application, backtracking, self-correction, and reflection, it struggles to map SAT-Menu inputs into structured CNF-like representations, which it could potentially handle more effectively. This limitation suggests that **R1’s reasoning ability is still closely tied to familiar input formats, and its generalization to more natural or abstract representations remains a challenge**.

We find that R1’s output tokens grow polynomially with input tokens (Figure 13, Appendix), unlike other LLMs whose outputs remain largely constant. This suggests that **R1 adapts its reasoning depth based on input size** – aligning with theoretical work showing that polynomially many CoT steps can boost a LLMs’ reasoning power (Li et al., 2024). We hypothesize that merely training LLMs to produce longer CoT traces via next-token prediction may still encourage statistical patterns in learning rather than true reasoning as highlighted in Bachmann & Nagarajan (2024). In contrast, R1’s improved performance may stem from reinforcement learning, which can guide models to develop coherent and goal-directed thought processes, rather than just mimicking token sequences (as evidenced by the performance difference between DeepSeek R1 and its base model V3, cf. Figure 3)

6 Discussion

In this section, we analyze the LLM performance by drawing analogies with SAT solvers and discuss the implications for the reasoning capabilities of LLMs.

Why are Easy regions easy? The reason why MiniSAT is capable of solving problems in the easy regions faster than problems around α_c is due to the heuristics built into the solver that guide the search for satisfying solutions (e.g. unit propagation, MOMS). That is, heuristics work well when they can exploit statistical features in the problem instance to be solved.

LLMs, too, appear to perform well in these easy regions. However, this performance can be reinterpreted as statistical pattern matching rather than genuine reasoning. For example, LLMs may associate a high number of input tokens with unsatisfiability – an assumption that often holds for overconstrained formulas (see Appendix B). In such cases, the model is not solving the problem logically but reacting to superficial cues in the input.

Why is the Hard region hard? Around the critical phase transition threshold (α_c), known heuristics fail due to the complexity and combinatorial explosion of possible assignments inherent to NP-hard problems such as 3-SAT. As a result, solvers resort to exhaustive or extended search procedures. In this hard region, statistical patterns are weak or nonexistent, making heuristic guidance less effective.

Without statistical patterns, LLMs must rely on multi-step reasoning – a task at which they typically struggle. This aligns with Bottou’s definition of reasoning. **Specifically, these models struggle to compose known functions (such as variable selection, assignment, backtracking) into longer, novel reasoning chains that generalize beyond their training distribution.** Similar observations have been made by Dziri et al. (2023) for function composition and by Zhang et al. (2023) for logical reasoning using BERT (Devlin et al., 2019).

In contrast, **R1 shows signs of having learned the underlying reasoning.** Its ability to generalize to longer or harder reasoning problems – potentially outside its training distribution – suggests a shift from pattern matching to structured search. While its reasoning process remains *incomplete*, this progress marks a **step-change in LLM reasoning abilities** – something that is not immediately apparent in standard reasoning benchmarks, which are increasingly saturated (cf., Figure 7 in Appendix). It opens up a promising path, encouraging the community to build on its training recipe.

What if the tested models were trained on SAT data? We suspect that all models have likely encountered SAT data during pretraining. This is evidenced by their immediate use of terminology and strategies (e.g., DPLL, tree search, backtracking) when presented with SAT instances in CNF form. **However, the core concern is not whether SAT-related content exists in the training data (which it likely does), but whether our specific evaluation is compromised by data leakage.** We address this by considering two scenarios:

- **Exact data overlap.** The strongest form of data leakage occurs when the evaluation set contains identical instances present in the model’s training data. This scenario is highly unlikely in our case. We use a custom SAT data generator, and neither the data nor the generator was open-sourced before publication. This rules out direct memorization.
- **In-distribution, but non-identical data.** The most plausible scenario is that the evaluation data shares a distributional similarity with pretraining data. Even in this case, our evaluation results on the Hard region minimize reliance on shallow statistical patterns.

A third possibility is out-of-distribution generalization, where models must rely on reasoning rather than statistical shortcuts. This is consistent with prior work (Zhang et al., 2024; Dziri et al., 2023), which demonstrates that LLMs trained on reasoning tasks suffer sharp performance degradation under even modest distribution shifts when fitting on statistical patterns. We also highlight our SAT-Menu setup, where the problem is reframed as a menu-based preference selection task. It is extremely unlikely that such a format appears in pretraining data, yet we still observe a clear performance gap between R1 and other models.

7 Conclusion

While R1 shows promising results in reasoning, it should be noted that our experiments were conducted on bounded 3-SAT problems with a maximum of 10 variables and 110 clauses. In contrast, classical solvers can solve problems with thousands of variables with perfect accuracy. Moreover, R1 still struggles in the hard region and its reasoning is neither perfectly *sound* (i.e. produces incorrect conclusions), nor *complete* (i.e. it cannot guarantee finding a solution). For better reliability and accuracy, it is advisable to use search scaffolds with LLMs, aligned with neurosymbolic techniques (De Raedt et al., 2020) – recognizing the ability of LLMs as approximate idea-generators for problems as against directly solving them (Kambhampati et al., 2024) – while invoking solvers for completeness (cf. Appendix C).

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References

- Anthropic. Claude 3.7 sonnet and claude code. 2025. URL <https://www.anthropic.com/news/claude-3-7-sonnet>.
- Konstantine Arkoudas. Gpt-4 can’t reason. *arXiv*, 2308.03762, 2023. URL <https://api.semanticscholar.org/CorpusID:260704128>.
- Gregor Bachmann and Vaishnavh Nagarajan. The pitfalls of next-token prediction. *arXiv*, 2403.06963, 2024. URL <https://api.semanticscholar.org/CorpusID:268364153>.
- Béla Bollobás, Christian Borgs, Jennifer T Chayes, Jeong Han Kim, and David B Wilson. The scaling window of the 2-sat transition. *Random Structures & Algorithms*, 18(3):201–256, 2001.
- Léon Bottou. From machine learning to machine reasoning: An essay. *Machine learning*, 94: 133–149, 2014.
- Tom Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared D Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, Sandhini Agarwal, Ariel Herbert-Voss, Gretchen Krueger, Tom Henighan, Rewon Child, Aditya Ramesh, Daniel Ziegler, Jeffrey Wu, Clemens Winter, Chris Hesse, Mark Chen, Eric Sigler, Mateusz Litwin, Scott Gray, Benjamin Chess, Jack Clark, Christopher Berner, Sam McCandlish, Alec Radford, Ilya Sutskever, and Dario Amodei. Language models are few-shot learners. In *Advances in Neural Information Processing Systems*, volume 33, pp. 1877–1901, 2020. URL https://proceedings.neurips.cc/paper_files/paper/2020/file/1457c0d6bfc4967418bfb8ac142f64a-Paper.pdf.
- Peter Cheeseman, Bob Kanefsky, and William M. Taylor. Where the really hard problems are. In *Proceedings of the 12th International Joint Conference on Artificial Intelligence - Volume 1*, IJCAI’91, pp. 331–337. Morgan Kaufmann Publishers Inc., 1991.
- Cristian Coarfa, Demetrios D Demopoulos, Alfonso San Miguel Aguirre, Devika Subramanian, and Moshe Y Vardi. Random 3-sat: The plot thickens. In *International Conference on Principles and Practice of Constraint Programming*, pp. 143–159. Springer, 2000.
- James M Crawford and Larry D Auton. Experimental results on the crossover point in random 3-sat. *Artificial intelligence*, 81(1-2):31–57, 1996.
- Martin Davis, George Logemann, and Donald Loveland. A machine program for theorem-proving. *Communications of the ACM*, 5(7):394–397, 1962.
- Luc De Raedt, Sebastijan Dumančić, Robin Manhaeve, and Giuseppe Marra. From statistical relational to neuro-symbolic artificial intelligence. In *Proceedings of the Twenty-Ninth International Joint Conference on Artificial Intelligence, IJCAI-20*, pp. 4943–4950. International Joint Conferences on Artificial Intelligence Organization, 7 2020. doi: 10.24963/ijcai.2020/688. URL <https://doi.org/10.24963/ijcai.2020/688>. Survey track.
- DeepSeek-AI. Deepseek-r1: Incentivizing reasoning capability in llms via reinforcement learning, 2025a. URL <https://arxiv.org/abs/2501.12948>.

- DeepSeek-AI. Deepseek-v3 technical report, 2025b. URL <https://arxiv.org/abs/2412.19437>.
- Demetrios D Demopoulos and Moshe Y Vardi. The phase transition in the random hornsat problem. In *Computational Complexity and Statistical Physics*. Oxford University Press, 2006.
- Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. BERT: Pre-training of deep bidirectional transformers for language understanding. In *Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers)*, pp. 4171–4186. Association for Computational Linguistics, June 2019. doi: 10.18653/v1/N19-1423. URL <https://aclanthology.org/N19-1423>.
- Jian Ding, Allan Sly, and Nike Sun. Proof of the satisfiability conjecture for large k. In *Proceedings of the forty-seventh annual ACM symposium on Theory of computing*, pp. 59–68, 2015.
- Nouha Dziri, Ximing Lu, Melanie Sclar, Xiang (Lorraine) Li, Liwei Jiang, Bill Yuchen Lin, Sean Welleck, Peter West, Chandra Bhagavatula, Ronan Le Bras, Jena Hwang, Soumya Sanyal, Xiang Ren, Allyson Ettinger, Zaid Harchaoui, and Yejin Choi. Faith and fate: Limits of transformers on compositionality. In *Advances in Neural Information Processing Systems*, volume 36, pp. 70293–70332, 2023. URL https://proceedings.neurips.cc/paper_files/paper/2023/file/deb3c28192f979302c157cb653c15e90-Paper-Conference.pdf.
- Niklas Eén and Niklas Sörensson. An extensible sat-solver. In *International conference on theory and applications of satisfiability testing*, pp. 502–518. Springer, 2003.
- Lizhou Fan, Wenyue Hua, Lingyao Li, Haoyang Ling, and Yongfeng Zhang. Nphardeval: Dynamic benchmark on reasoning ability of large language models via complexity classes, 2024. URL <https://arxiv.org/abs/2312.14890>.
- Michael R. Garey and David S. Johnson. *Computers and Intractability; A Guide to the Theory of NP-Completeness*. W. H. Freeman & Co., USA, 1990. ISBN 0716710455.
- Michael R. Genesereth and Nils J. Nilsson. *Logical foundations of artificial intelligence*. Morgan Kaufmann Publishers Inc., 1987.
- Google. Introducing gemini 2.0: Our new ai model for the agentic era. 2024. URL <https://blog.google/technology/google-deepmind/google-gemini-ai-update-december-2024/>.
- Rishi Hazra, Alkis Sygkounas, Andreas Persson, Amy Loutfi, and Pedro Zuidberg Dos Martires. REvolve: Reward Evolution with Large Language Models for Autonomous Driving, 2024a. URL <https://arxiv.org/abs/2406.01309>.
- Rishi Hazra, Pedro Zuidberg Dos Martires, and Luc De Raedt. SayCanPay: Heuristic Planning with Large Language Models using Learnable Domain Knowledge. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 38, pp. 20123–20133, 2024b.
- Marijn J. H. Heule and Oliver Kullmann. The science of brute force. *Commun. ACM*, 60(8): 70–79, July 2017. ISSN 0001-0782. doi: 10.1145/3107239. URL <https://doi.org/10.1145/3107239>.
- Marijn J. H. Heule, Oliver Kullmann, Siert Wieringa, and Armin Biere. Cube and conquer: Guiding cdcl sat solvers by lookaheads. In Kerstin Eder, João Lourenço, and Onn Shehory (eds.), *Hardware and Software: Verification and Testing*, pp. 50–65. Springer Berlin Heidelberg, 2012.
- John N Hooker and V Vinay. Branching rules for satisfiability. *Journal of Automated Reasoning*, 15(3):359–383, 1995.
- Wenlong Huang, Pieter Abbeel, Deepak Pathak, and Igor Mordatch. Language models as zero-shot planners: Extracting actionable knowledge for embodied agents. In *Proceedings of the 39th International Conference on Machine Learning*, volume 162, pp. 9118–9147, 2022.

- Albert Qiaochu Jiang, Sean Welleck, Jin Peng Zhou, Timothee Lacroix, Jiacheng Liu, Wenda Li, Mateja Jamnik, Guillaume Lample, and Yuhuai Wu. Draft, sketch, and prove: Guiding formal theorem provers with informal proofs. In *The Eleventh International Conference on Learning Representations*, 2023. URL <https://openreview.net/forum?id=SMA9EAovKMC>.
- Subbarao Kambhampati, Karthik Valmeekam, L. Guan, Kaya Stechly, Mudit Verma, Sidhant Bhambri, Lucas Saldyt, and Anil Murthy. Llms can’t plan, but can help planning in llm-modulo frameworks. *arXiv*, 2402.01817, 2024. URL <https://api.semanticscholar.org/CorpusID:267413178>.
- Takeshi Kojima, Shixiang (Shane) Gu, Machel Reid, Yutaka Matsuo, and Yusuke Iwasawa. Large language models are zero-shot reasoners. In *Advances in Neural Information Processing Systems*, volume 35, pp. 22199–22213, 2022. URL https://proceedings.neurips.cc/paper_files/paper/2022/file/8bb0d291acd4acf06ef112099c16f326-Paper-Conference.pdf.
- Jean-Marie Lagniez and Pierre Marquis. An improved decision-dnnf compiler. In *Proceedings of the Twenty-Sixth International Joint Conference on Artificial Intelligence, IJCAI-17*, pp. 667–673, 2017. doi: 10.24963/ijcai.2017/93. URL <https://doi.org/10.24963/ijcai.2017/93>.
- Zhiyuan Li, Hong Liu, Denny Zhou, and Tengyu Ma. Chain of thought empowers transformers to solve inherently serial problems. In *The Twelfth International Conference on Learning Representations*, 2024. URL <https://openreview.net/forum?id=3EWTEy9MTM>.
- Hunter Lightman, Vineet Kosaraju, Yuri Burda, Harrison Edwards, Bowen Baker, Teddy Lee, Jan Leike, John Schulman, Ilya Sutskever, and Karl Cobbe. Let’s verify step by step. In *The Twelfth International Conference on Learning Representations*, 2024. URL <https://openreview.net/forum?id=v8L0pN6EOi>.
- B. Liu, Yuqian Jiang, Xiaohan Zhang, Qian Liu, Shiqi Zhang, Joydeep Biswas, and Peter Stone. Llm+p: Empowering large language models with optimal planning proficiency. *arXiv*, 2304.11477, 2023. URL <https://api.semanticscholar.org/CorpusID:258298051>.
- Aman Madaan, Niket Tandon, Prakhar Gupta, Skyler Hallinan, Luyu Gao, Sarah Wiegrefe, Uri Alon, Nouha Dziri, Shrimai Prabhumoye, Yiming Yang, Shashank Gupta, Bodhisattwa Prasad Majumder, Katherine Hermann, Sean Welleck, Amir Yazdanbakhsh, and Peter Clark. Self-refine: Iterative refinement with self-feedback. In *Advances in Neural Information Processing Systems*, volume 36, pp. 46534–46594, 2023. URL https://proceedings.neurips.cc/paper_files/paper/2023/file/91edff07232fb1b55a505a9e9f6c0ff3-Paper-Conference.pdf.
- William Merrill and Ashish Sabharwal. The parallelism tradeoff: Limitations of log-precision transformers. *Transactions of the Association for Computational Linguistics*, 11:531–545, 2023. doi: 10.1162/tacl_a-00562. URL <https://aclanthology.org/2023.tacl-1.31>.
- Stephan Mertens, Marc Mézard, and Riccardo Zecchina. Threshold values of random k-sat from the cavity method. *Random Structures & Algorithms*, 28(3):340–373, 2006.
- Cristopher Moore, Gabriel Istrate, Demetrios Demopoulos, and Moshe Y Vardi. A continuous–discontinuous second-order transition in the satisfiability of random horn-sat formulas. *Random Structures & Algorithms*, 31(2):173–185, 2007.
- OpenAI. Gpt-4o system card. 2024. URL <https://cdn.openai.com/gpt-4o-system-card.pdf>.
- Binghui Peng, Srini Narayanan, and Christos Papadimitriou. On limitations of the transformer architecture. *arXiv*, 2402.08164, 2024. URL <https://api.semanticscholar.org/CorpusID:267636545>.
- Bernardino Romera-Paredes, Mohammadamin Barekatain, Alexander Novikov, Matej Balog, M. Pawan Kumar, Emilien Dupont, Francisco J. R. Ruiz, Jordan S. Ellenberg, Pengming Wang, Omar Fawzi, Pushmeet Kohli, and Alhussein Fawzi. Mathematical discoveries from program search with large language models. *Nature*, 625(7995):

- 468–475, Jan 2024. ISSN 1476-4687. doi: 10.1038/s41586-023-06924-6. URL <https://doi.org/10.1038/s41586-023-06924-6>.
- Olivier Roussel. The SAT Game. <https://www.cril.univ-artois.fr/en/software/satgame/>.
- Stuart Russell and Peter Norvig. *Artificial Intelligence: A Modern Approach*. Prentice Hall, 3 edition, 2010.
- Abulhair Saparov and He He. Language models are greedy reasoners: A systematic formal analysis of chain-of-thought. In *The Eleventh International Conference on Learning Representations*, 2023. URL <https://openreview.net/forum?id=qFVBzXxR2V>.
- Thomas J. Schaefer. The complexity of satisfiability problems. In *Proceedings of the Tenth Annual ACM Symposium on Theory of Computing*, STOC ’78, pp. 216–226, New York, NY, USA, 1978. Association for Computing Machinery. doi: 10.1145/800133.804350. URL <https://doi.org/10.1145/800133.804350>.
- Timo Schick, Jane Dwivedi-Yu, Roberto Dessi, Roberta Raileanu, Maria Lomeli, Eric Hambro, Luke Zettlemoyer, Nicola Cancedda, and Thomas Scialom. Toolformer: Language models can teach themselves to use tools. In *Advances in Neural Information Processing Systems*, volume 36, pp. 68539–68551, 2023. URL https://proceedings.neurips.cc/paper_files/paper/2023/file/d842425e4bf79ba039352da0f658a906-Paper-Conference.pdf.
- Bart Selman, David G Mitchell, and Hector J Levesque. Generating hard satisfiability problems. *Artificial intelligence*, 81(1-2):17–29, 1996.
- JP Marques Silva and Karem A Sakallah. Grasp-a new search algorithm for satisfiability. In *Proceedings of International Conference on Computer Aided Design*, pp. 220–227. IEEE, 1996.
- Charlie Victor Snell, Jaehoon Lee, Kelvin Xu, and Aviral Kumar. Scaling LLM test-time compute optimally can be more effective than scaling parameters for reasoning. In *The Thirteenth International Conference on Learning Representations*, 2025. URL <https://openreview.net/forum?id=4FWAwZtd2n>.
- Aarohi Srivastava, Abhinav Rastogi, Abhishek Rao, Abu Awal Md Shoeb, Abubakar Abid, Adam Fisch, Adam R. Brown, Adam Santoro, Aditya Gupta, Adrià Garriga-Alonso, Agnieszka Kluska, Aitor Lewkowycz, Akshat Agarwal, Alethea Power, Alex Ray, Alex Warstadt, Alexander W. Kocurek, Ali Safaya, Ali Tazarv, Alice Xiang, Alicia Parrish, Allen Nie, Aman Hussain, Amanda Askell, Amanda Dsouza, Ambrose Slone, Ameet Rahane, Anantharaman S. Iyer, Anders Johan Andreassen, Andrea Madotto, Andrea Santilli, Andreas Stuhlmüller, Andrew M. Dai, Andrew La, Andrew Lampinen, Andy Zou, Angela Jiang, Angelica Chen, Anh Vuong, Animesh Gupta, Anna Gottardi, Antonio Norelli, Anu Venkatesh, Arash Gholamidavoodi, Arfa Tabassum, Arul Menezes, Arun Kirubarajan, Asher Mullokandov, Ashish Sabharwal, Austin Herrick, Avia Efrat, Aykut Erdem, Ayla Karakaş, B. Ryan Roberts, Bao Sheng Loe, Barret Zoph, Bartłomiej Bojanowski, Batuhan Özyurt, Behnam Hedayatnia, Behnam Neyshabur, Benjamin Inden, Benno Stein, Berk Ekmekci, Bill Yuchen Lin, Blake Howald, Bryan Orinon, Cameron Diao, Cameron Dour, Catherine Stinson, Cedrick Argueta, Cesar Ferri, Chandan Singh, Charles Rathkopf, Chenlin Meng, Chitta Baral, Chiyu Wu, Chris Callison-Burch, Christopher Waites, Christian Voigt, Christopher D Manning, Christopher Potts, Cindy Ramirez, Clara E. Rivera, Clemencia Siro, Colin Raffel, Courtney Ashcraft, Cristina Garbacea, Damien Sileo, Dan Garrette, Dan Hendrycks, Dan Kilman, Dan Roth, C. Daniel Freeman, Daniel Khashabi, Daniel Levy, Daniel Moseguí González, Danielle Perszyk, Danny Hernandez, Danqi Chen, Daphne Ippolito, Dar Gilboa, David Dohan, David Drakard, David Jurgens, Debajyoti Datta, Deep Ganguli, Denis Emelin, Denis Kleyko, Deniz Yuret, Derek Chen, Derek Tam, Dieuwke Hupkes, Diganta Misra, Dilyar Buzan, Dimitri Coelho Mollo, Diyi Yang, Dong-Ho Lee, Dylan Schrader, Ekaterina Shutova, Ekin Dogus Cubuk, Elad Segal, Eleanor Hagerman, Elizabeth Barnes, Elizabeth Donoway, Ellie Pavlick, Emanuele Rodolà, Emma Lam, Eric Chu, Eric Tang, Erkut Erdem, Ernie Chang, Ethan A Chi, Ethan Dyer, Ethan Jerzak, Ethan Kim, Eunice Engefu Manyasi, Evgenii Zheltonozhskii, Fanyue Xia, Fate-meh Siar, Fernando Martínez-Plumed, Francesca Happé, Francois Chollet, Frieda Rong,

Gaurav Mishra, Genta Indra Winata, Gerard de Melo, Germán Kruszewski, Giambattista Parascandolo, Giorgio Mariani, Gloria Xinyue Wang, Gonzalo Jaimovitch-Lopez, Gregor Betz, Guy Gur-Ari, Hana Galijasevic, Hannah Kim, Hannah Rashkin, Hannaneh Hajishirzi, Harsh Mehta, Hayden Bogar, Henry Francis Anthony Shevlin, Hinrich Schuetze, Hiromu Yakura, Hongming Zhang, Hugh Mee Wong, Ian Ng, Isaac Noble, Jaap Jumelet, Jack Geissinger, Jackson Kernion, Jacob Hilton, Jaehoon Lee, Jaime Fernández Fisac, James B Simon, James Koppel, James Zheng, James Zou, Jan Kocon, Jana Thompson, Janelle Wingfield, Jared Kaplan, Jarema Radom, Jascha Sohl-Dickstein, Jason Phang, Jason Wei, Jason Yosinski, Jekaterina Novikova, Jelle Bosscher, Jennifer Marsh, Jeremy Kim, Jeroen Taal, Jesse Engel, Jesujoba Alabi, Jiacheng Xu, Jiaming Song, Jillian Tang, Joan Waweru, John Burden, John Miller, John U. Balis, Jonathan Batchelder, Jonathan Berant, Jörg Froberg, Jos Rozen, Jose Hernandez-Orallo, Joseph Boudeman, Joseph Guerr, Joseph Jones, Joshua B. Tenenbaum, Joshua S. Rule, Joyce Chua, Kamil Kanclerz, Karen Livescu, Karl Krauth, Karthik Gopalakrishnan, Katerina Ignatyeva, Katja Markert, Kaustubh Dhole, Kevin Gimpel, Kevin Omondi, Kory Wallace Mathewson, Kristen Chiafullo, Ksenia Shkaruta, Kumar Shridhar, Kyle McDonell, Kyle Richardson, Laria Reynolds, Leo Gao, Li Zhang, Liam Dugan, Lianhui Qin, Lidia Contreras-Ochando, Louis-Philippe Morency, Luca Moschella, Lucas Lam, Lucy Noble, Ludwig Schmidt, Luheng He, Luis Oliveros-Colón, Luke Metz, Lütfti Kerem Senel, Maarten Bosma, Maarten Sap, Maartje Ter Hoeve, Maheen Farooqi, Manaal Faruqi, Mantas Mazeika, Marco Baturan, Marco Marelli, Marco Maru, Maria Jose Ramirez-Quintana, Marie Tolkiehn, Mario Giulianelli, Martha Lewis, Martin Potthast, Matthew L Leavitt, Matthias Hagen, Mátyás Schubert, Medina Orduna Baitemirova, Melody Arnaud, Melvin McElrath, Michael Andrew Yee, Michael Cohen, Michael Gu, Michael Ivanitskiy, Michael Starritt, Michael Strube, Michał Śwkedrowski, Michele Bevilacqua, Michihiro Yasunaga, Mihir Kale, Mike Cain, Mimeo Xu, Mirac Suzgun, Mitch Walker, Mo Tiwari, Mohit Bansal, Moin Amnaseri, Mor Geva, Mozhdah Gheini, Mukund Varma T, Nanyun Peng, Nathan Andrew Chi, Nayeon Lee, Neta Gur-Ari Krakover, Nicholas Cameron, Nicholas Roberts, Nick Doiron, Nicole Martinez, Nikita Nangia, Niklas Deckers, Niklas Muennighoff, Nitish Shirish Keskar, Niveditha S. Iyer, Noah Constant, Noah Fiedel, Nuan Wen, Oliver Zhang, Omar Agha, Omar Elbaghdadi, Omer Levy, Owain Evans, Pablo Antonio Moreno Casares, Parth Doshi, Pascale Fung, Paul Pu Liang, Paul Vicol, Pegah Alipoormolabashi, Peiyuan Liao, Percy Liang, Peter W Chang, Peter Eckersley, Phu Mon Htut, Pinyu Hwang, Piotr Miłkowski, Piyush Patil, Pouya Pezeshkpour, Priti Oli, Qiaozhu Mei, Qing Lyu, Qinlang Chen, Rabin Banjade, Rachel Etta Rudolph, Raefer Gabriel, Rahel Habacker, Ramon Risco, Raphaël Millièvre, Rhythm Garg, Richard Barnes, Rif A. Saurous, Riku Arakawa, Robbe Raymaekers, Robert Frank, Rohan Sikand, Roman Novak, Roman Sitelew, Ronan Le Bras, Rosanne Liu, Rowan Jacobs, Rui Zhang, Russ Salakhutdinov, Ryan Andrew Chi, Seungjae Ryan Lee, Ryan Stovall, Ryan Teehan, Rylan Yang, Sahib Singh, Saif M. Mohammad, Sajant Anand, Sam Dillavou, Sam Shleifer, Sam Wiseman, Samuel Gruetter, Samuel R. Bowman, Samuel Stern Schoenholz, Sanghyun Han, Sanjeev Kwatra, Sarah A. Rous, Sarik Ghazarian, Sayan Ghosh, Sean Casey, Sebastian Bischoff, Sebastian Gehrmann, Sebastian Schuster, Sepideh Sadeghi, Shadi Hamdan, Sharon Zhou, Shashank Srivastava, Sherry Shi, Shikhar Singh, Shima Asaadi, Shixiang Shane Gu, Shubh Pachchigar, Shubham Toshniwal, Shyam Upadhyay, Shyamolima Shammie Debnath, Siamak Shakeri, Simon Thormeyer, Simone Melzi, Siva Reddy, Sneha Priscilla Makini, Soo-Hwan Lee, Spencer Torene, Sriharsha Hatwar, Stanislas Dehaene, Stefan Dovic, Stefano Ermon, Stella Biderman, Stephanie Lin, Stephen Prasad, Steven Piantadosi, Stuart Shieber, Summer Mishnerghi, Svetlana Kiritchenko, Swaroop Mishra, Tal Linzen, Tal Schuster, Tao Li, Tao Yu, Tariq Ali, Tatsunori Hashimoto, Te-Lin Wu, Théo Desbordes, Theodore Rothschild, Thomas Phan, Tianle Wang, Tiberius Nkinyili, Timo Schick, Timofei Kornev, Titus Tunduny, Tobias Gerstenberg, Trenton Chang, Trishala Neeraj, Tushar Khot, Tyler Shultz, Uri Shaham, Vedant Misra, Vera Demberg, Victoria Nyamai, Vikas Raunak, Vinay Venkatesh Ramasesh, vinay uday prabhu, Vishakh Padmakumar, Vivek Srikumar, William Fedus, William Saunders, William Zhang, Wout Vossen, Xiang Ren, Xiaoyu Tong, Xinran Zhao, Xinyi Wu, Xudong Shen, Yadollah Yaghoobzadeh, Yair Lakretz, Yangqiu Song, Yasaman Bahri, Yejin Choi, Yichi Yang, Yiding Hao, Yifu Chen, Yonatan Belinkov, Yu Hou, Yufang Hou, Yuntao Bai, Zachary Seid, Zhuoye Zhao, Zijian Wang, Zijie J. Wang, Zirui Wang, and Ziyi Wu. Beyond the imitation game: Quantifying and extrapolating the capabilities of

- language models. *Transactions on Machine Learning Research*, 2023. ISSN 2835-8856. URL <https://openreview.net/forum?id=uyTL5Bvosj>.
- Kaya Stechly, Matthew Marquez, and Subbarao Kambhampati. GPT-4 doesn't know it's wrong: An analysis of iterative prompting for reasoning problems. In *NeurIPS 2023 Foundation Models for Decision Making Workshop*, 2023. URL <https://openreview.net/forum?id=PmtZjDYB68>.
- Karthik Valmeekam, Alberto Olmo, Sarath Sreedharan, and Subbarao Kambhampati. Large language models still can't plan (a benchmark for LLMs on planning and reasoning about change). In *NeurIPS 2022 Foundation Models for Decision Making Workshop*, 2022. URL <https://openreview.net/forum?id=wUU-7XTL5X0>.
- Xuezhi Wang, Jason Wei, Dale Schuurmans, Quoc V Le, Ed H. Chi, Sharan Narang, Aakanksha Chowdhery, and Denny Zhou. Self-consistency improves chain of thought reasoning in language models. In *The Eleventh International Conference on Learning Representations*, 2023. URL <https://openreview.net/forum?id=1PL1NIMMrw>.
- Jason Wei, Yi Tay, Rishi Bommasani, Colin Raffel, Barret Zoph, Sebastian Borgeaud, Dani Yogatama, Maarten Bosma, Denny Zhou, Donald Metzler, Ed H. Chi, Tatsunori Hashimoto, Oriol Vinyals, Percy Liang, Jeff Dean, and William Fedus. Emergent abilities of large language models. *Transactions on Machine Learning Research*, 2022a. ISSN 2835-8856. URL <https://openreview.net/forum?id=yzkSU5zdwD>.
- Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, brian ichter, Fei Xia, Ed Chi, Quoc V Le, and Denny Zhou. Chain-of-thought prompting elicits reasoning in large language models. In *Advances in Neural Information Processing Systems*, volume 35, pp. 24824–24837, 2022b. URL https://proceedings.neurips.cc/paper_files/paper/2022/file/9d5609613524ecf4f15af0f7b31abca4-Paper-Conference.pdf.
- Sean Welleck, Jiacheng Liu, Ximing Lu, Hannaneh Hajishirzi, and Yejin Choi. Naturalprover: Grounded mathematical proof generation with language models. In *Advances in Neural Information Processing Systems*, volume 35, pp. 4913–4927, 2022. URL https://proceedings.neurips.cc/paper_files/paper/2022/file/1fc548a8243ad06616eee731e0572927-Paper-Conference.pdf.
- Violet Xiang, Charlie Snell, Kanishk Gandhi, Alon Albalak, Anikait Singh, Chase Blagden, Duy Phung, Rafael Rafailov, Nathan Lile, Dakota Mahan, Louis Castricato, Jan-Philipp Franken, Nick Haber, and Chelsea Finn. Towards system 2 reasoning in llms: Learning how to think with meta chain-of-thought, 2025. URL <https://arxiv.org/abs/2501.04682>.
- Shunyu Yao, Dian Yu, Jeffrey Zhao, Izhak Shafran, Tom Griffiths, Yuan Cao, and Karthik Narasimhan. Tree of thoughts: Deliberate problem solving with large language models. In *Advances in Neural Information Processing Systems*, volume 36, pp. 11809–11822, 2023a. URL https://proceedings.neurips.cc/paper_files/paper/2023/file/271db9922b8d1f4dd7aaef84ed5ac703-Paper-Conference.pdf.
- Shunyu Yao, Jeffrey Zhao, Dian Yu, Nan Du, Izhak Shafran, Karthik R Narasimhan, and Yuan Cao. React: Synergizing reasoning and acting in language models. In *The Eleventh International Conference on Learning Representations*, 2023b. URL https://openreview.net/forum?id=WE_vluYUL-X.
- Xi Ye, Qiaochu Chen, Isil Dillig, and Greg Durrett. SATLM: Satisfiability-aided language models using declarative prompting. *Advances in Neural Information Processing Systems*, 36, 2024.
- Honghua Zhang, Liunian Harold Li, Tao Meng, Kai-Wei Chang, and Guy Van den Broeck. On the paradox of learning to reason from data. In *Proceedings of the Thirty-Second International Joint Conference on Artificial Intelligence, IJCAI-23*, pp. 3365–3373, 8 2023. doi: 10.24963/ijcai.2023/375. URL <https://doi.org/10.24963/ijcai.2023/375>.

Hugh Zhang, Jeff Da, Dean Lee, Vaughn Robinson, Catherine Wu, Will Song, Tiffany Zhao, Pranav Raja, Dylan Slack, Qin Lyu, Sean Hendryx, Russell Kaplan, Michele, Lunati, and Summer Yue. A careful examination of large language model performance on grade school arithmetic. *arXiv*, 2405.00332, 2024.

Appendix for “Have Large Language Models Learned to Reason? A Characterization via 3-SAT”

The appendix is organized as follows. Dataset Statistics § A, Output analysis of LLMs § B, LLM + Solver integration § C, and Full Prompts § D.

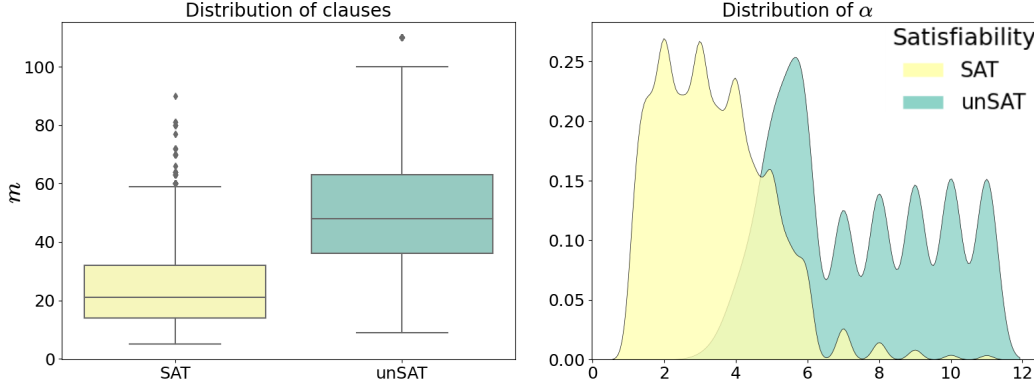


Figure 6: **3-SAT Dataset Statistics.** Figures depict clauses m (left) and α (right) distribution across SAT and unSAT instances, highlighting that unSAT problems typically feature more clauses and higher α values.

A Dataset Statistics

A.1 3-SAT

Table 1 lists all values of the range of α corresponding to each n . For α values within the $(6, 11]$ interval, we incremented α by 1. For the $[1, 6]$ interval, which contains the most “interesting problems,” we aimed for finer granularity by choosing the smallest possible α increment. This increment ensures that, given the number of variables n , we obtain an integer number of clauses m . For example, with $n = 3$, the minimum increment is $\alpha_{inc} = 1$, and for $n = 4$, it is $\alpha_{inc} = 0.25$. For each α_{inc} we generated 300 formulas.

The distribution of formulas according to the number of variables is detailed as follows: 3,000 formulas with 3 variables, 7,500 with 4 variables, 9,000 with 5 variables, 4,500 with 6 variables, 3,000 with 7 variables, 13,500 with 8 variables, 3,000 with 9 variables, and 16,500 with 10 variables.

As shown in Figure 6, the range of clauses (m) varies in $[5, 90]$, and the alpha ($\alpha = m/n$) ranges in $[1.1, 11.0]$. For unSAT instances, the clauses range from 9 to 110, with the alpha varying in $[2.60, 11.0]$. Across the entire dataset, the average number of variables (n) is 7.2, the average number of clauses (m) is 33, and the mean α is 4.7. This diverse dataset provides a broad spectrum for analyzing the impact of variable and clause distribution on formula satisfiability.

A.2 2-SAT

For the experiments on 2-SAT, we followed the same formula generation procedure used for 3-SAT. However, the α range was reduced to $[1, 10]$, as the unsatisfiability transition occurs earlier in 2-SAT problems. This adjustment allowed us to reduce the dataset size while preserving relevant data for analysis. For each α value, detailed in Table 1, we generated 100 formulas. The resulting dataset comprises a total of 29,600 formulas, of which 4,860 are satisfiable.

Table 1: Table shows the range of alpha value for each n (i.e. number of variables) in the generated dataset. We generate 300 formulas per α value.

n	Range of α
3	1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0
4	1.0, 1.25, 1.5, 1.75, 2.0, 2.25, 2.5, 2.75, 3.0, 3.25, 3.5, 3.75, 4.0, 4.25, 4.5, 4.75, 5.0, 5.25, 5.5, 5.75, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0
5	1.0, 1.2, 1.4, 1.6, 1.8, 2.0, 2.2, 2.4, 2.6, 2.8, 3.0, 3.2, 3.4, 3.6, 3.8, 4.0, 4.2, 4.4, 4.6, 4.8, 5.0, 5.2, 5.4, 5.6, 5.8, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0
6	1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0, 5.5, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0
7	1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0
8	1.0, 1.125, 1.25, 1.375, 1.5, 1.625, 1.75, 1.875, 2.0, 2.125, 2.25, 2.375, 2.5, 2.625, 2.75, 2.875, 3.0, 3.125, 3.25, 3.375, 3.5, 3.625, 3.75, 3.875, 4.0, 4.125, 4.25, 4.375, 4.5, 4.625, 4.75, 4.875, 5.0, 5.125, 5.25, 5.375, 5.5, 5.625, 5.75, 5.875, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0
9	1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0
10	1.0, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0, 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7, 2.8, 2.9, 3.0, 3.1, 3.2, 3.3, 3.4, 3.5, 3.6, 3.7, 3.8, 3.9, 4.0, 4.1, 4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 5.0, 5.1, 5.2, 5.3, 5.4, 5.5, 5.6, 5.7, 5.8, 5.9, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0

Table 2: Configuration Parameters for LLMs

Model	Temperature	Top_p	Max Tokens
GPT-4o	0.3	1	16000
Claude 3.7 Sonnet	0.3	1	8192
Gemini 2.0 Flash	0.3	1	8192
DeepSeek V3	0.3	1	8000
DeepSeek R1	0.3	1	8000 (up to 32,000 for CoT)

A.3 Horn-SAT

We generate formulas for random 1-3 Horn SAT, following the methodology outlined by Moore et al. (2007). Intuitively, 1-3-HornSAT formulas contain clauses with only 1 and 3 literals and correspond to 3-SAT in the Horn category, which are P-complete rather than NP-complete.

Specifically, we sampled formulas from H_{n,d_1,d_2}^2 and $H_{n,d_1,0,d_3}^3$ distributions, where d_1 was fixed to 0.5 to simplify the sampling space, and d_2 and d_3 (referred to as α) were varied to analyze formula behavior. For consistency with 2-SAT and 3-SAT analyses, α was incremented from 0 to 12 in steps of 1, resulting $m = \alpha n + 0.5n + 1$ clauses for these Horn formulas. Notice that for $\alpha = 0$, the formulas still contain $0.5n + 1$ clauses due to the fixed d_1 parameter. The choice of $d_1 = 0.5$ ensures we can observe a satisfiability threshold across different α values and small n . Lower values produced trivially satisfiable formulas at small n , for all α values, and were therefore avoided. We empirically explored d_1 values starting at 0.2 in increments of 0.1 before selecting 0.5.

We generated 300 formulas for each α value and formula type, with n ranging from 3 to 10. This range aligns with our other experimental settings, as opposed to the significantly larger $n = 20,000$ used by Moore et al. (2007). Each dataset contains 31,200 formulas. Among these, 5,036 formulas are satisfiable.

B LLMs as Solvers: Output Analysis

We observed the following behaviors in the generated outputs, including chain-of-thought (CoT) reasoning:

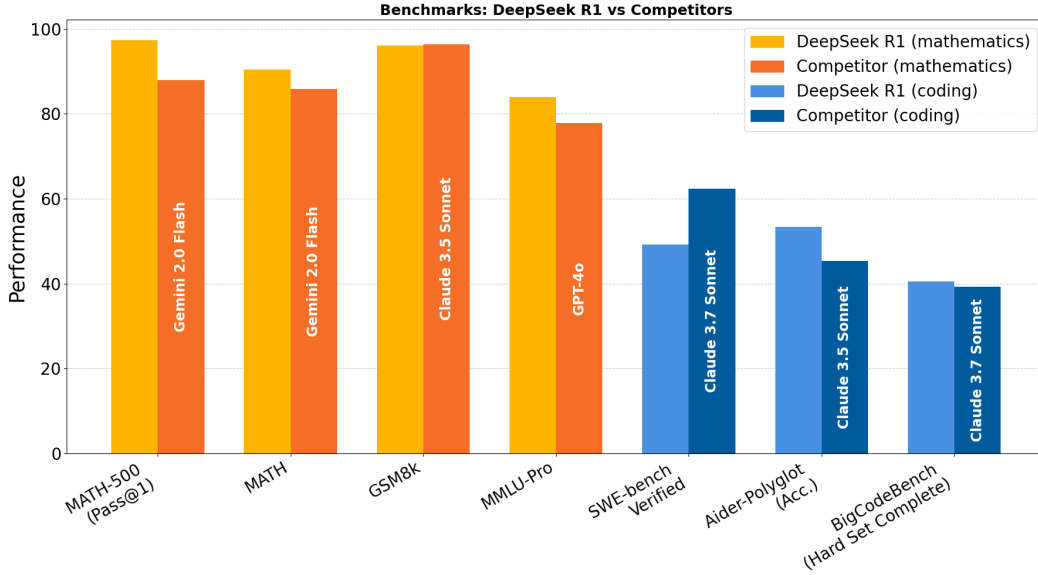


Figure 7: Performance comparison of DeepSeek R1 with the next best LLM for math and coding benchmarks. The figure shows the narrow performance margin between models suggesting that benchmarks are saturated. Sources: (DeepSeek-AI, 2025a; Anthropic, 2025; Google, 2024; OpenAI, 2024; DeepSeek-AI, 2025b)

Diverse Reasoning Techniques: LLMs employ varying reasoning techniques depending on the prompt type (SAT-CNF vs. SAT-Menu) and even adapt their approach across individual problems within the same prompt type.

SAT-CNF Reasoning: The dominant strategy involves backtracking, as illustrated in Box 5. Occasionally, LLMs employ local search, where it assigns items to “orderable” and “not-orderable” lists and iteratively modifies these based on detected conflicts (e.g., *We can create two sets for liked and disliked items and then compare them to find any conflicts. Let’s begin by creating a list of all the likes and dislikes to identify conflicts.*).

SAT-Menu Reasoning: The primary strategy here is trial-and-error. Occasionally, LLMs apply heuristics such as the Maximum Occurrence in Minimum-sized clauses (MOMS) heuristic to prioritize variables appearing most frequently in the smallest clauses (e.g., *We start by making a tally of how many people like or dislike each food item... If we put ‘macaron’ on the ‘orderable’ list, we will satisfy many people who like it.*”).

“Lazy” Solutions: As noted in subsequent text, LLMs often produce “lazy” solutions in many cases, either providing an outline of how to solve the problem or asking to be delegated to a solver.

We also discuss some interesting failure cases we observed during our experiments. In the SAT-CNF context, it was observed that LLMs, often opt to pass the task to an external SAT solver rather than solving it themselves. Additionally, when attempting to find a solution, these models tend to provide only a conceptual outline of the solution instead of a concrete answer, a tendency that becomes more pronounced with larger formulas. When prompted explicitly for a solution, LLMs might simplistically conclude that the problem is unsatisfiable due to its complexity, as shown in Box 4. Although this reasoning is not entirely sound – as over-constrained formulas can still potentially be solvable – it appears that LLMs might be leveraging this as a statistical feature.

In contrast, R1 always attempts to solve all problems. We discuss a failure case of R1 for SAT-Menu input where R1 finds a satisfying assignment even though none exists. We note interesting search-based behaviors as shown in Figure 8.

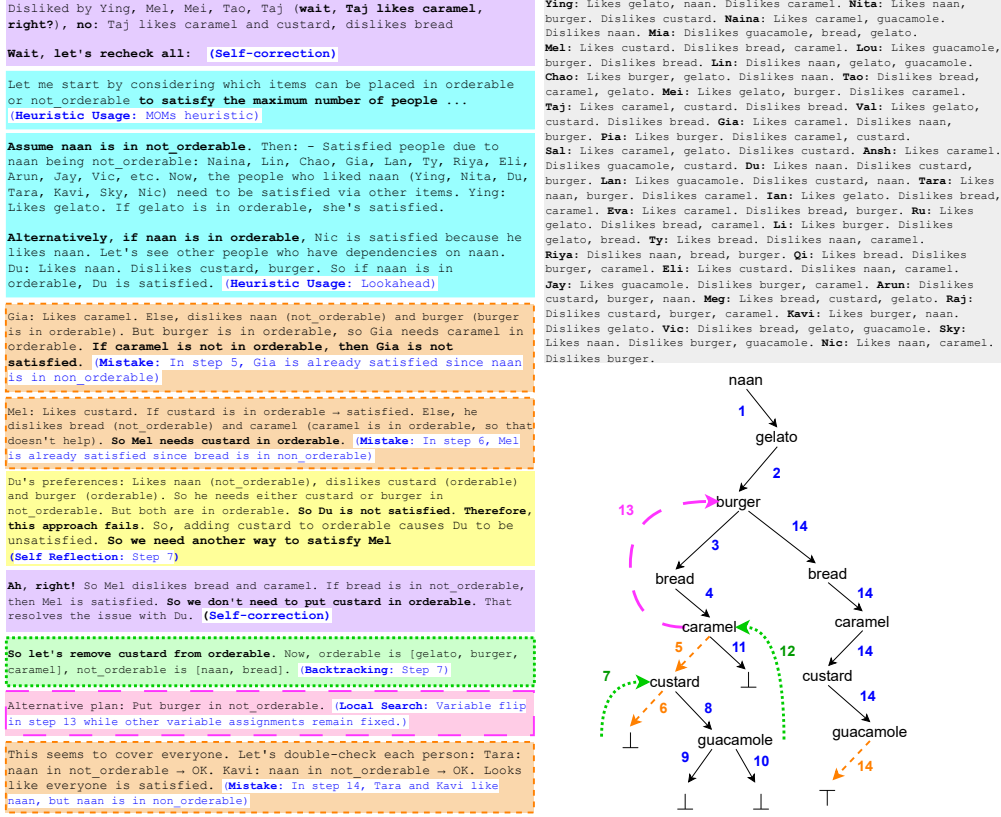


Figure 8: **Failure Cases:** SAT-Menu traces for DeepSeek-R1. Although the input formula is unsatisfiable, R1 incorrectly predicts it as satisfiable. Colored boxes indicate model behaviors: cyan for heuristic variable selection, orange - - - for mistakes, green ... for backtracking, yellow for self-reflection, violet for self-correction, and magenta for local search. Left branch always represents an assignment to the *orderable* list and vice versa. \perp marks unsatisfiability. Numbers show the order of steps.

C Can an LLM + Solver boost performance?

To aid LLMs in reasoning tasks, recent studies have explored pipelined approaches using LLMs to parse inputs into solver-compliant outputs, leveraging off-the-shelf solvers to derive the final answer (Ye et al., 2024; Liu et al., 2023). This approach is aligned with neurosymbolic techniques (De Raedt et al., 2020), which combine the universal function approximation capabilities of neural networks with the precision of symbolic systems.

To explore a similar setting in the context of 3-SAT, we ask whether we can augment LLMs with an external solver wherein the LLM translates (pseudo)-natural language into a format that a symbolic SAT solver, such as MiniSAT, can process. To this end, we prompt the LLM to translate 3-SAT formulas, which we provide in the SAT-Menu input format, into solver-compliant 3-SAT formulas. We then use a 3-SAT solver to solve the translated instance (see Box 5 in Appendix). We dub this approach **SAT-Translate** and plot GPT-4 Turbo’s performance in Figure 9.

We observe that when LLMs have access to an external solver, there is a significant increase in their accuracy, reaching at best, in GPT-4’s case, $\approx 100\%$ across the entire range of α . We attribute this to the relatively lower computational complexity of translating 3-SAT formulas compared to solving them (i.e. finding satisfying assignments). Interestingly, we

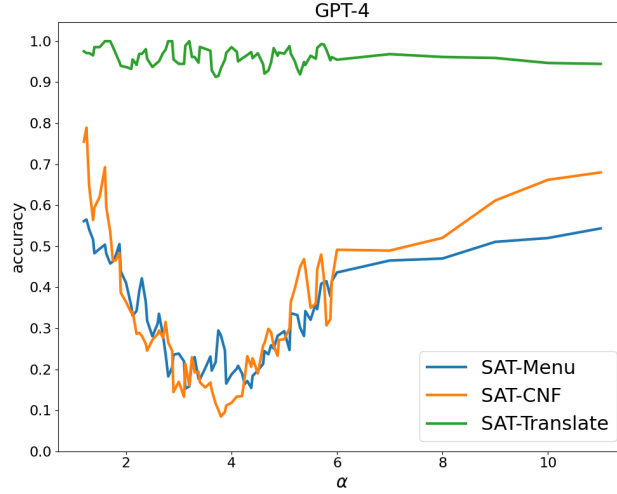


Figure 9: The figure compares LLM-Modulo frameworks (denoted as SAT-Translate) – here, GPT-4 Turbo equipped with a solver – with standalone GPT-4 using SAT-Menu and SAT-CNF inputs. SAT-Translate approach (in green) outperforms the rest, showing the significance of augmenting LLMs with symbolic solvers.

find that varying the input format between SAT-CNF and SAT-Menu does not significantly enhance LLMs inherent reasoning capabilities. The marked improvement in performance is primarily observed when they are equipped with an external solver. While ours is a straightforward approach, one could also explore tighter integrations as proposed in LLM-Modulo frameworks (Kambhampati et al., 2024) which augments LLMs with critics and verifiers (Hazra et al., 2024b), recognizing the ability of LLMs as *approximate* idea-generators for problems as against directly solving them.

It should be noted that the input to the LLM is based on fixed templates, the rules of which can be captured using regular grammar. Thus, one could write a simple parser to map the menu input to a CNF formula. However, mapping from ambiguous natural language to solver-compliant input may be non-trivial for the LLMs. Generally, outputs from LLMs often require additional post-processing to meet specific guidelines.

D Full Prompts

Here, we provide full prompts used in our experiments for SAT-Menu (Box 2) and SAT-CNF (Box 3).

Box 2: SAT-Menu Prompt

System Message

Your task is to output two distinct lists of food items, one denoting what can be ordered ('orderable') and the other what cannot ('not_orderable'), to meet the preferences of a group of individuals. Each person must find the selection satisfactory based on their likes and dislikes. SATISFACTION CRITERIA: : 1. A person is satisfied if at least one liked item is in 'orderable' list or one disliked item is in 'not_orderable' list. 2. No item can appear on both lists. 3. All participants must be satisfied by the combination of the two lists. 4. Importantly, if NO such combination exists that satisfies all, output empty lists for both. Check carefully before finalizing. You always think step-by-step and show all your work in the explanation. Output your final solution as a comma-separated list of strings in Python code (`orderable = [...], not_orderable = [...]`).

Pairs of Preferences and Solutions for in-context learning

Few-shot Examples ...

Input for a new problem

Preferences: Jay: Likes nachos, ratatouille. Dislikes pie. Ada: Likes pie. Dislikes burger, ravioli. Zoe: Likes ravioli. Dislikes pie, burger. Arun: Likes ratatouille. Dislikes pie, nachos. Ula: Likes ratatouille. Dislikes ravioli, nachos. Ying: Likes nachos, ratatouille. Dislikes burger.

Generated Solution for the given problem

Solution: First, let's list out the likes and dislikes of each person and then categorize the food items based on their preferences.

Jay: Likes nachos, ratatouille. Dislikes pie.
Ada: Likes pie. Dislikes burger, ravioli.
Zoe: Likes ravioli. Dislikes pie, burger.
Arun: Likes ratatouille. Dislikes pie, nachos.
Ula: Likes ratatouille. Dislikes ravioli, nachos.
Ying: Likes nachos, ratatouille. Dislikes burger.

Now, let's categorize the items as 'orderable' and 'not_orderable' based on the given preferences.

From the above preferences, we can create the following lists:

Orderable: pie, ratatouille, nachos
Not orderable: burger, ravioli

Let's examine if this combination satisfies all the participants' preferences.

1. Jay: Satisfied by ratatouille in orderable list.
2. Ada: Satisfied by pie in orderable list.
3. Zoe: Satisfied by burger in not_orderable list.
4. Arun: Satisfied by ratatouille in orderable list.
5. Ula: Satisfied by ratatouille in orderable list.
6. Ying: Satisfied by nachos in orderable list.

All participants are satisfied with this combination, and no item appears in both lists. So the final lists are:

```
```python
orderable=[pie, ratatouille, nachos]
not_orderable=[burger, ravioli]
```
```

Box 3: SAT-CNF Prompt**# System Message**

Let's play the SAT (satisfiability) game. The input is a list of clauses, where each clause is represented as a disjunction of literals (variables or their negation connected by logical OR). Your task is to find valuation of Boolean variables such that a Boolean CNF formula evaluates to True. The solution should be in form of a dictionary where keys are variables and values are Boolean (True or False). SATISFACTION CRITERIA: 1. At least one literal in each clause should be True. 2. A variable can't be both True and False in the dictionary. 3. MOST IMPORTANTLY, if NO satisfying assignment exists, you MUST output an EMPTY dictionary. Check carefully before finalizing. You always think step-by-step and show all your work in the explanation. Output the solution in Python code dictionary, enclosed within `<output : ...>`.

Input for a new problem**Formula:**

```
[[ -3, 1, -4], [ -4, -2, 1], [ -1, -4, 5], [ 5, 1, 2], [ -5, 4, 2], [ -4, 3, 1],
[ 1, 5, -3], [ -2, 1, 3], [ 1, -5, -4], [ 4, -3, -1], [ -2, 5, -3]]
```

Generated Solution for the given problem

Solution: To find a satisfying assignment for this CNF (Conjunctive Normal Form) formula, we will use a simple approach and try to construct a solution iteratively while checking at each step if the clauses are satisfied or not. We will go through the clauses one by one and make arbitrary decisions on the truth values of the literals. We have to ensure that no variable is assigned both True and False, and each clause must have at least one True literal.

We start with the first clause $[-3, 1, -4]$. Let's arbitrarily decide:

3 is False (so -3 is True),

1 is True (so we satisfy the clause $[-3, 1, -4]$ because 1 is True or -3 is True),

4 is True (since we haven't made any decision on 4, we do not yet satisfy the clause with -4, but that won't be an immediate issue).

Our current assignments are now: 1: True, 3: False, 4: True.

Next, we consider the second clause $[-4, -2, 1]$. Since 1 is True, this clause is already satisfied.

Next is $[-1, -4, 5]$. We need to satisfy this clause without changing the truth value of 1 or 4, so we choose to make 5 True.

Our assignments are now: 1: True, 3: False, 4: True, 5: True.

Next, we look at $[5, 1, 2]$. Since 5 is True, this clause is already satisfied.

Next is $[-5, 4, 2]$. We need to satisfy this without changing 5 or 4, so we set 2 to True.

Our current assignments are: 1: True, 2: True, 3: False, 4: True, 5: True.

Now the next clause is $[-4, 3, 1]$. Since 4 is True, -4 is False, but 1 is True, so the clause is satisfied.

For the clause $[1, 5, -3]$. This clause is already satisfied by 1 being True.

For $[-2, 1, 3]$. This clause is also satisfied because 1 is True.

For $[1, -5, -4]$. This is again satisfied because 1 is True.

Next clause is $[4, -3, -1]$. This clause is satisfied with 4 being True.

The last clause is $[-2, 5, -3]$. This is satisfied because 5 is True.

All clauses are satisfied with our current assignments, so we return:

```
```python
output: {1: True, 2: True, 3: False, 4: True, 5: True}
```
```

Box 4: SAT-CNF (Lazy Solution)**# System Message**

Let's play the SAT (satisfiability) game. The input is a list of clauses, where each clause is represented as a disjunction of literals (variables or their negation connected by logical OR). Your task is to find valuation of Boolean variables such that a Boolean CNF formula evaluates to True. The solution should be in form of a dictionary where keys are variables and values are Boolean (True or False). The satisfaction criteria are: 1. At least one literal in each clause should be True. 2. A variable can't be both True and False in the dictionary. 3. If no satisfying assignment exists, you should output an empty dictionary. You always think step-by-step and show all your work in the explanation. Output the solution in Python code dictionary, enclosed within `<output : ...>`.

Input for a new problem**Formula:**

```
[ [7, 9, -4], [1, -8, -4], [-1, 3, -8], [10, 3, -8], [9, -1, -8], [-4, 10, 6], [-7, 1, -8], [-3, 5, -6],
  [-5, 8, 6], [8, -9, 5], [8, -5, -9], [5, -8, -9], [-2, 4, 9], [8, -2, 6], [9, -5, 6], [-10, -4, -2], [-1, 2, -8],
  [-3, -5, -4], [-8, -2, -3], [1, 3, 9], [8, -10, -1], [-8, -2, -10], [4, -10, 3], [-9, 4, -8], [7, 8, -10],
  [-4, 5, -3], [7, 6, 2], [-5, -7, -4], [-4, 7, -9], [-10, 2, 5], [3, -1, 10], [-5, -4, -7], [-3, 8, 4],
  [-10, -3, -4], [6, 4, -1], [8, 7, 9], [1, 3, 10], [10, 8, 9], [-3, 9, 4], [-5, 9, -1], [-4, 8, 9], [2, -4, -1],
  [-4, 10, -7], [5, -7, -10], [2, 8, 7], [9, -2, 10], [-7, 2, -4], [5, -3, 4], [1, -5, 4]]
```

Generated Solution for the given problem

Solution: To solve this satisfiability problem, we need to determine an assignment of truth values to the variables such that all clauses are satisfied. With such a large and complex problem, an efficient systematic approach or use of an algorithm like the DPLL (Davis–Putnam–Logemann–Loveland) algorithm would be ideal. However, since we're expected to think step-by-step, let's attempt a simplified analysis.

We start by looking for unit clauses, which contain only one literal, or pure literals, which appear in one polarity only throughout the formula. Observing the clauses, we can't immediately spot such helpful shortcuts due to the complexity. Instead, we can iterate through the clauses, and try to assign truth values to the variables in a way that satisfies as many clauses as possible. We might need to backtrack if we reach a contradiction.

We must make some initial choices and see if those choices can lead to a consistent solution. Let's start with the first clause '[7, 9, -4]'. We can begin by setting 7 to True, 9 to True, or the negation of 4 (-4) to True. Let's decide to set 7 to True. This is an arbitrary choice at the beginning, and we may need to backtrack if this leads to a contradiction later.

Now, we need to check other clauses and see if this choice is consistent with them and try to fill in further values. We will need to iterate through each clause and see if it's possible to satisfy it given our previous choices.

Given the complexity of the problem and the large number of variables and clauses involved, solving it by hand or by a step-by-step explanation is impractical. In practice, we would use a SAT solver software to find the satisfying assignment, if one exists. A SAT solver automatically handles the process of proposing variable assignments, backtracking, and deducing necessary assignments based on the structure of the formula.

For the purposes of this answer, since I cannot run a SAT solver in real-time, I will have to state that solving this problem by hand is unfeasible within this format. The output, given the complexity, cannot be determined without the use of algorithmic assistance. If no satisfying assignment exists (meaning the formula is unsatisfiable), or we cannot solve it by a simple theoretical process within this framework, the output would be an empty dictionary.

```
```python
output: {}
```
```

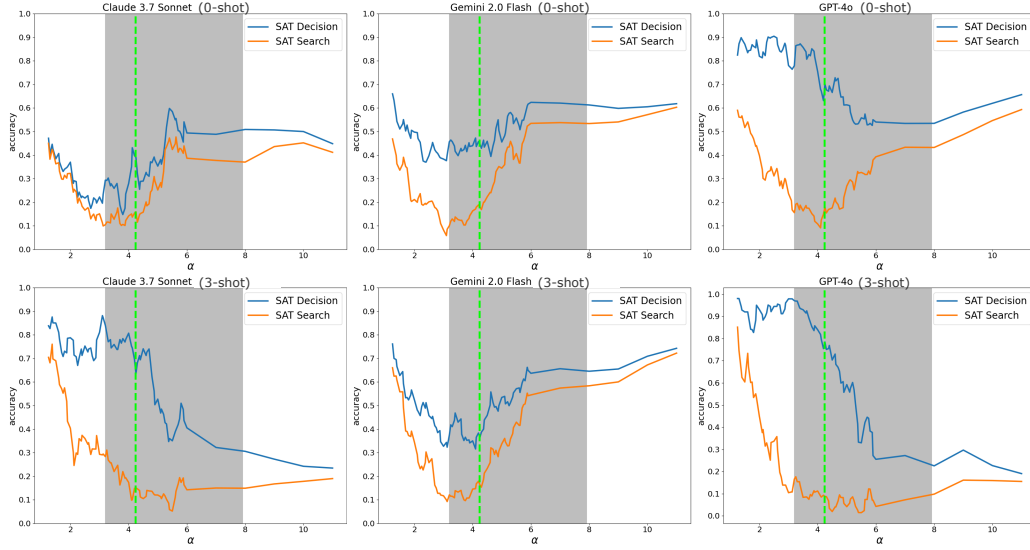


Figure 10: **0-shot vs. 3-shot accuracy.** The figure compares 0-shot and 3-shot performance comparing all LLMs. It can be observed that in-context learning does not enhance performance in the hard region. The setup SAT-Menu. The plot was generated using a size 4 moving window on α values.

Box 5: SAT-Translate Prompt

System Message

You are provided with a list of preferences from different individuals, each specifying items they like and dislike. Create a logical expression in Conjunctive Normal Form (CNF) that satisfies a set of individual preferences regarding likes and dislikes of certain items. The condition for an individual's satisfaction is that either at least one item they like is included, or at least one item they dislike is excluded in your selection. Format the final CNF expression in LaTeX. Ensure all item names are retained in the final output. Do not include any explanation.

Input for a new problem

Preferences: Om: Likes naan, curry. Dislikes tandoori. Bao: Likes curry. Dislikes naan, tandoori. Nic: Likes naan. Dislikes curry, tandoori. Pat: Likes curry. Dislikes naan, tandoori. Du: Likes tandoori, naan, curry. Kim: Likes curry. Dislikes tandoori, naan.

Generated Solution for the given problem

Solution:

$$(\text{naan} \vee \text{curry} \vee \neg \text{tandoori}) \wedge (\text{curry} \vee \neg \text{naan} \vee \neg \text{tandoori}) \wedge (\text{naan} \vee \neg \text{curry} \vee \neg \text{tandoori}) \wedge (\text{curry} \vee \neg \text{naan} \vee \neg \text{tandoori}) \wedge (\text{tandoori} \vee \text{naan} \vee \text{curry}) \wedge (\text{curry} \vee \neg \text{tandoori} \vee \neg \text{naan})$$

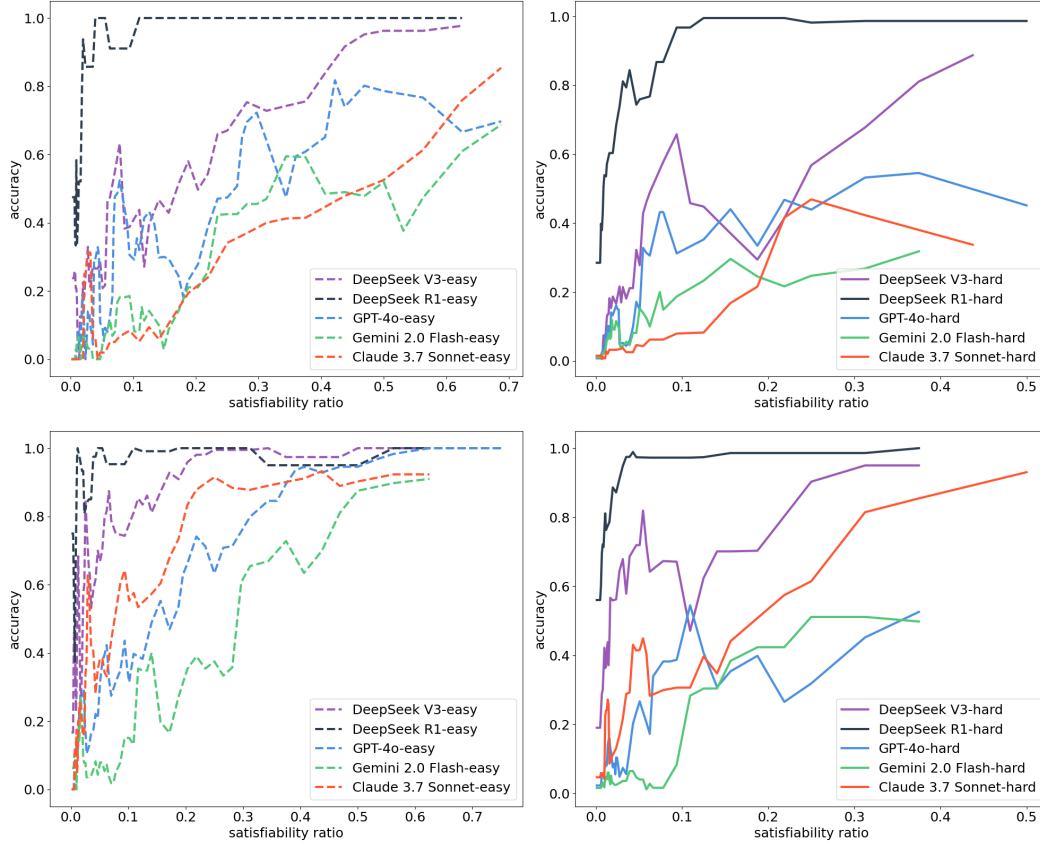


Figure 11: **Accuracy vs. satisfiability ratio.** R1 maintains consistent accuracy regardless of satisfiability ratio. In contrast, the performance of other LLMs is impacted by the number of satisfying assignments – more the satisfying assignments, higher the performance. The first row is for SAT-Menu and the second row is for SAT-CNF. We only include satisfiable instances and analyze easy (dashed line) and hard regions (solid line) separately.

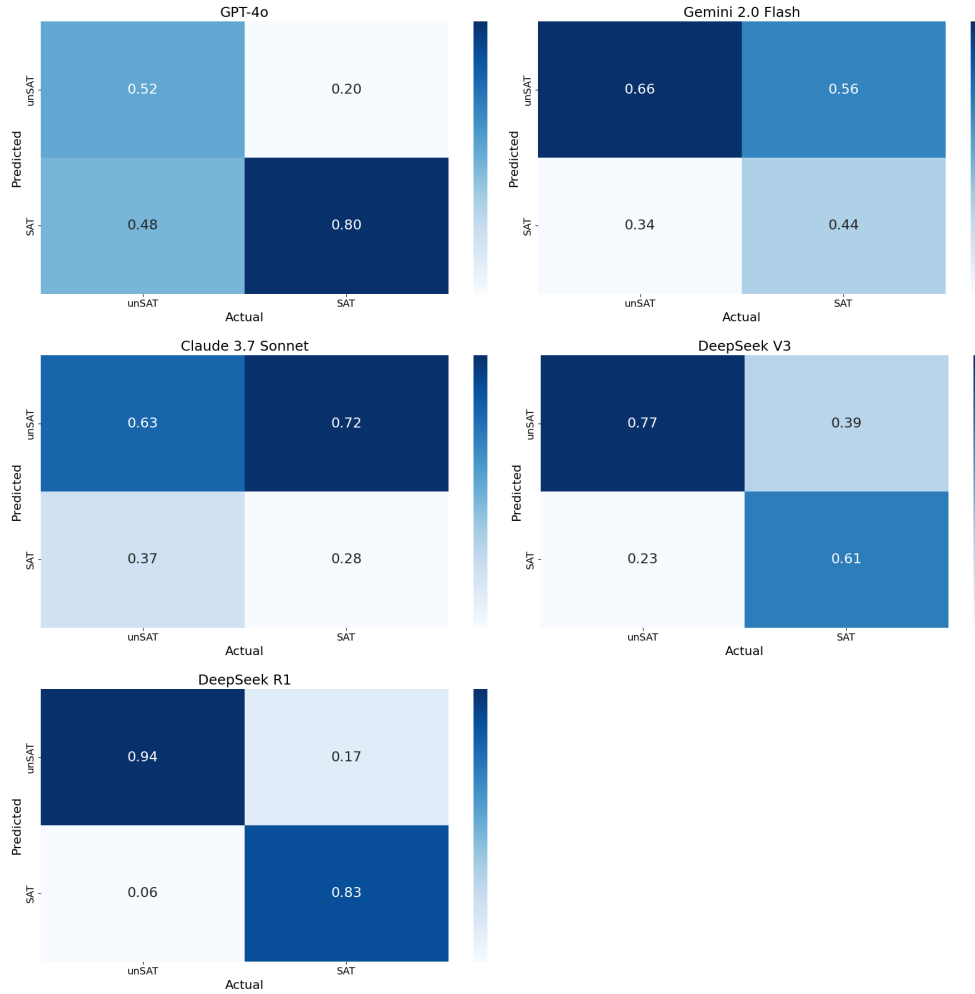


Figure 12: **Confusion matrices for the decision version of 3-SAT.** It can be observed that, except R1, all other LLMs struggle to correctly classify unsatisfiable instances. This suggests that R1 is more sound (detects sat/unsat correctly) than complete (cannot guarantee to find a solution). The cell annotations reflect classification accuracy, normalized over the true counts (column) to account for the imbalance between SAT and unSAT instances. The setup is SAT-Menu with 0-shot prompting.

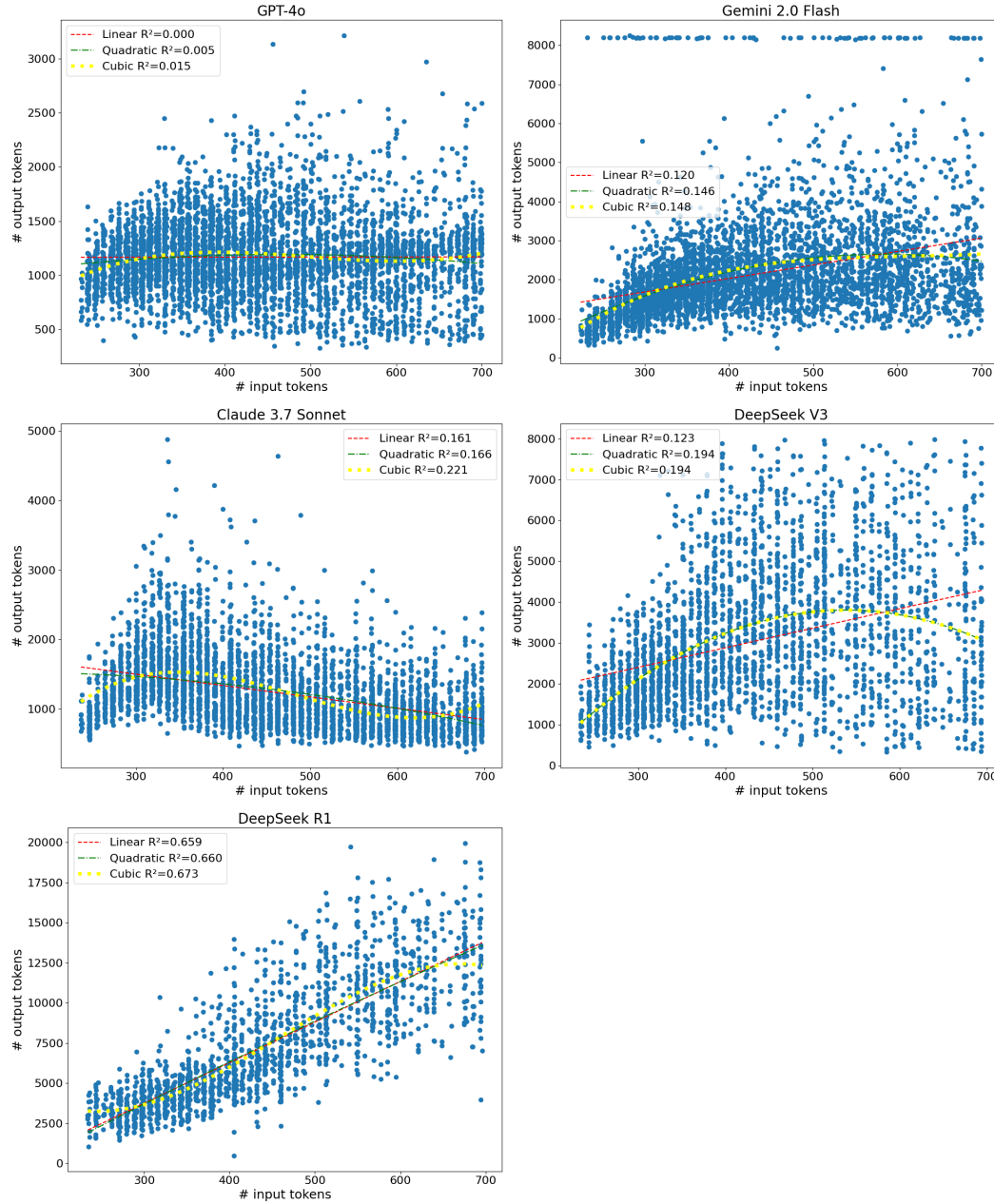


Figure 13: **Correlation between output (generated) and input tokens.** R1 output tokens grows polynomially with the input tokens. In contrast, the generated tokens of other LLMs remain largely unchanged.