

# Can Large Language Models Reason? A Characterization via 3-SAT

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## Abstract

Large Language Models (LLMs) are said to possess advanced reasoning abilities. However, some skepticism exists as recent works show how LLMs often bypass true reasoning using shortcuts. Current methods for assessing the reasoning abilities of LLMs typically rely on open-source benchmarks that may be overrepresented in LLM training data, potentially skewing performance. We instead provide a computational theory perspective of reasoning, using 3-SAT – the prototypical NP-complete problem that lies at the core of logical reasoning and constraint satisfaction tasks. By examining the phase transitions in 3-SAT, we empirically characterize the reasoning abilities of LLMs and show how they vary with the inherent hardness of the problems. Our experimental evidence shows that LLMs cannot perform true reasoning, as is required for solving 3-SAT problems.

**Keywords:** Large Language Models, Reasoning, Computational Complexity Theory

## Introduction

The success and versatility of Large Language Models (LLMs) have sparked widespread interest and debate on whether LLMs are capable of reasoning. The answer to this question may depend on the perspective on reasoning one takes, whether it

is more oriented toward commonsense reasoning [1] or towards logical or deductive reasoning [2]. We will adhere to Leon Bottou’s definition, which defines reasoning as “*algebraically manipulating previously acquired knowledge in order to answer a new question*” [3]. This is aligned with Russell and Norvig’s description of artificial intelligence as rational thinking [4].

Recent studies suggest that LLMs are inherently capable of zero-shot reasoning [5] (i.e. performing multi-step inference processes in previously unseen situations). This ability has been shown to *emerge* and improve with scale [6], and can be further enhanced by using smart prompting techniques that encourage LLMs to think step-by-step [7]. Demonstrations include, *inter alia*, planning [8, 9], theorem proving [10], search and optimization [11], self-reflection [12], and tool usage [13].

Conversely, a growing body of research presents a more critical view of these emergent abilities. For instance, LLMs may exhibit limitations in consistent logical reasoning [14], effective planning [15], and accurate self-evaluation of their outputs [16]. During training, language models can fit on statistical features [17] or identify reasoning shortcuts, much like the *Clever Hans Cheat* [18], thus bypassing true reasoning. There is also growing concern about dataset contamination<sup>1</sup> from open-source benchmarks [19] that can inflate the reasoning performance of LLMs. During inference, the autoregressive nature of LLMs makes them prone to snowballing errors over time [20]. Furthermore, these models can often generate unfaithful and biased explanations in their chains of thought [21]. Additionally, their greedy approach to reasoning often falls short in contexts with multiple valid reasoning steps [22]. On the architectural side of LLMs, findings reveal that the transformer layer is incapable of function composition for large domains [20, 23]. From a theoretical standpoint, transformer computations have been shown to lie in the complexity class log-uniform  $\text{TC}^0$ , which is too restrictive even for simple logical reasoning tasks such as 2-SAT<sup>2</sup>. Given these limitations, it has been suggested that the emergent abilities are but a mere *mirage* stemming from the choice of metric [25]. This inevitably leads to the question: “**Can Large Language Models reason**”, and if so, to what extent?

## Methods

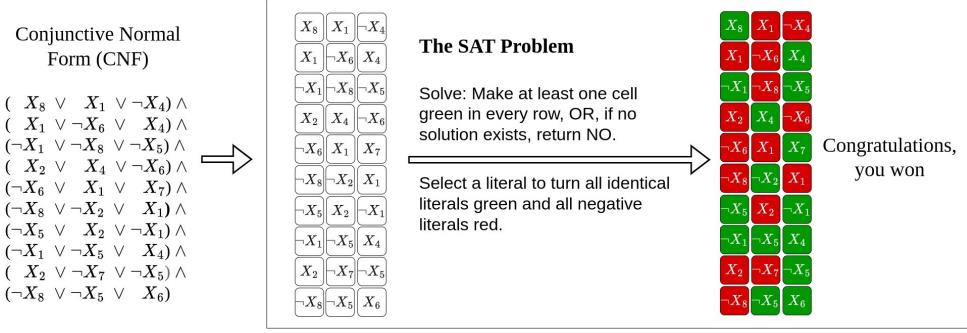
### 3-SAT Phase Transition

We study the reasoning capabilities of LLMs on 3-SAT problems, introduced in Figure 1. 3-SAT constitutes one of the most fundamental problems in computer science as it is the prototypical NP-complete problem lying at the foundation of computational complexity theory. To date, it is unknown whether efficient (i.e., polynomial time) algorithms for NP-complete problems exist (c.f. P vs. NP). Importantly, the different problems within the NP-complete class can be translated efficiently to each other [29]. Consequently, any polynomial time algorithm for 3-SAT would result in an efficient algorithm for any other NP-complete problem, e.g. graph coloring or the

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<sup>1</sup>Data closely resembling the benchmark leaks into the training data.

<sup>2</sup>More specifically,  $\text{TC}^0$  is more restrictive than the logarithmic memory class L [24]. Given that the 2-SAT problem is NL-complete (i.e., the class of non-deterministic logarithmic space algorithms), multi-layer transformers cannot solve 2-SAT instances, unless L=NL [23].



**Fig. 1 The 3-SAT problem**, visualized using a variant of the SAT game [26]. In SAT, one must return a truth assignment to Boolean variables that satisfy a Boolean formula in conjunctive normal form (CNF) if one exists, and return unSAT otherwise. A row in the visualization represents a clause, which is a disjunction (connected by a logical OR  $\vee$ ) of literals, wherein a literal can be positive ( $X_1$ ) or negative ( $\neg X_1$ ). An assignment satisfies a clause if one of its literals is assigned the value true. Since clauses are conjunctively connected (by a logical AND  $\wedge$ ), all clauses must be satisfied for the formula to be satisfied. If no satisfying assignment exists, then the formula is unsatisfiable.

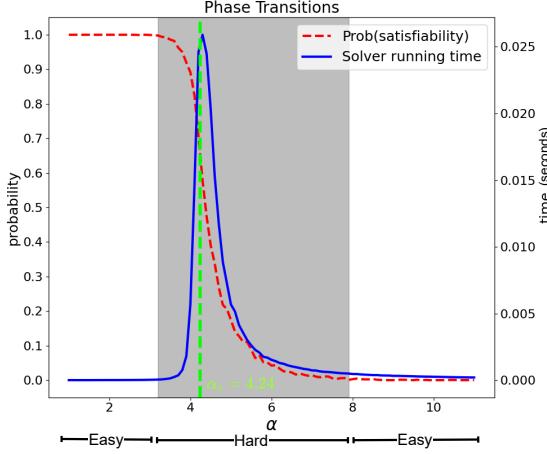
traveling salesman problem. Furthermore, various prevalent reasoning problems in artificial intelligence, such as planning and constraint satisfaction, can be reduced to solving 3-SAT problems [30].

An interesting empirical observation is the presence of a *phase transition* in 3-SAT problems [27]. 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 3-SAT, this phase transition occurs at  $\alpha_c \approx 4.24$  [31], 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.

Analogously to characterizing SAT solvers by their behavior on solving problems with varying  $\alpha$ , we study the reasoning capabilities of LLMs with respect to the phase transition in 3-SAT problems. A similar thought experiment framework was also proposed by Kambhampati et al [32]. Note that our goal is *not* to build 3-SAT solvers powered by LLMs. On the contrary, we use the 3-SAT phase transition to assess the reasoning abilities of LLMs using a well-established experimental protocol. This contrasts with other works that characterize reasoning by evaluating performance on benchmark datasets [33].

## 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



**Fig. 2 3-SAT Phase Transitions** [27]. Plotted in red is the probability of a randomly sampled 3-SAT formula being satisfied against the hardness  $\alpha$  of the formula. We can observe a clear phase transition occurring at  $\alpha_c \approx 4.24$  (marked by the green dotted line). We identify two easy regions, one on either side of  $\alpha_c$ . 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 one (left) or zero (right). The solid blue line shows the mean time taken by the MiniSAT solver [28] to solve a 3-SAT instance. Notably, there is a spike in the solver’s runtime near the critical  $\alpha_c$  value. This is attributed to the absence of useful heuristics in this region, forcing the solver to resort to essentially exhaustive searches.

items that meet these preferences, or declare the situation unsatisfiable (unSAT) if no valid combination exists. For details of dataset generation, see Figure 6 in materials and methods. 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) [7] and in-context learning [34] (see Box 2).

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 materials and methods.

To assess the reasoning capabilities of LLMs, we analyze their performance on two variants of the 3-SAT problem. The first variant is the 3-SAT Decision problem, where the LLM acts as a solver and must determine whether or not a given 3-SAT problem is satisfiable. If the problem has a satisfiable assignment, the LLM should respond with “yes” and with “no” if it is unsatisfiable. The second variant is the 3-SAT Search problem, where the LLM’s task extends beyond providing a simple “yes” or “no” response. If the formula is satisfiable, the LLM should also return an assignment to the variables that satisfies the formula. However, if the formula is found to be unsatisfiable, the LLM should once again respond with “no.”

### Box 1: SAT-Menu Prompt

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# 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. If no such combination exists that satisfies all, output empty lists for both. 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.
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Due to the wide-spread adoption and best-in-class performance<sup>3</sup> we use GPT-4 Turbo (specifically, GPT-4 1106-preview model) as the reference LLM to perform our experimental evaluation. In § B.2 of supplementary text, we also report extended comparisons of GPT-4 to additional state-of-the-art LLMs, including both open-source (Llama 2 70B chat-hf [35], Mixtral 8 × 7B [36]) as well as proprietary models (GPT-3.5 Turbo [37], Gemini 1.0 Pro [38], PaLM 2 text-bison [39]). The results of these comparisons can be found in Figures 7 to 13.

## Results

### Can LLMs solve 3-SAT problems?

We evaluate GPT-4’s performance by measuring its accuracy (of solving for SAT Search and prediction for SAT Decision) across formulas with varying  $\alpha$ . We present these results in Figure 3. GPT-4 demonstrates an apparent reasoning competence in the easy regions, while its accuracy significantly drops to  $\approx 10\%$  in the hard region for SAT Search. We also observe that SAT Search poses a slightly greater challenge for GPT-4 than SAT Decision.

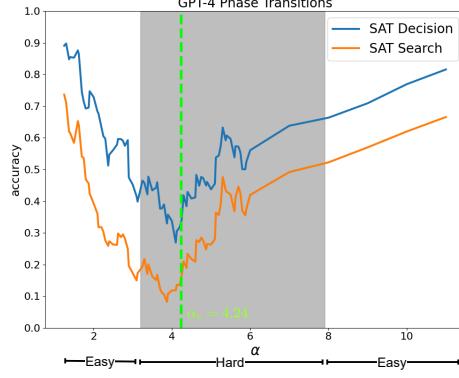
In Figure 4 we also plot GPT-4’s performance against the *satisfiability ratio*, defined as  $\frac{\text{model count}}{2^n}$ , where model count is the number of satisfying assignments and  $n$  is the number of variables. This ratio denotes the probability that a randomly selected variable assignment satisfies the given 3-SAT theory<sup>4</sup>. We can observe a clear dependence between the accuracy and the satisfiability ratio: formulas with more satisfying assignments tend to be easier for GPT-4 to solve. This holds across both easy and hard regions.

### Can LLM-Modulo frameworks boost performance?

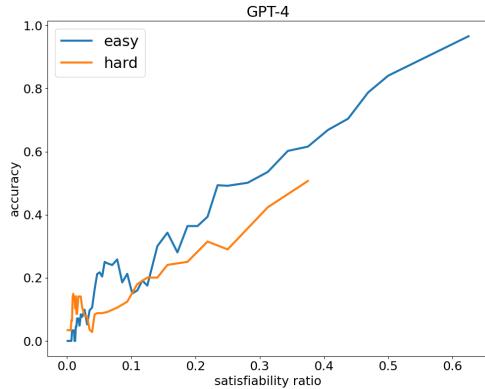
To enhance reasoning capabilities, recent studies have explored so-called *LLM-Modulo frameworks* coined by Kambhampati et al. [40]. The main idea is to augment LLMs

<sup>3</sup><https://huggingface.co/spaces/lmsys/chatbot-arena-leaderboard>

<sup>4</sup>Note that this is different from the probability that at least one satisfying assignment exists – two formulas can both be satisfiable but have different model counts and therefore different satisfiability ratios.



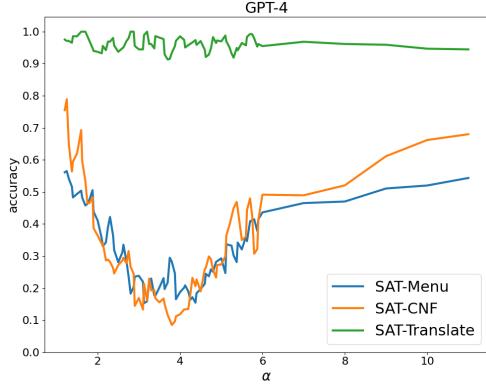
**Fig. 3 GPT-4 accuracy on 3-SAT Search and Decision variants.** We plot the accuracy of GPT-4 against  $\alpha$  for both SAT Decision and SAT Search. Notably, GPT-4’s accuracy for both variants exhibits a significant decline around the critical point ( $\alpha_c \approx 4.24$ ) aligning with the hard region. The dip in the performance mimics the increased solving time of the MiniSAT solver in the hard region. The setting is SAT-CNF. The curves are smoother for higher  $\alpha$  as they have been sampled more sparsely in that regime. The plot was generated using a size 4 moving window on  $\alpha$  values.



**Fig. 4 GPT-4 accuracy vs. satisfiability ratio.** We plot the accuracy of GPT-4 against the satisfiability ratio. We only include satisfiable instances and analyze problems from the hard and easy regions separately. Note that in our dataset, the 3-SAT problems exhibited maximum satisfiability ratios of approximately 0.4 for the hard region and 0.62 for the easy regions. The setting is the search version of SAT-CNF. The plot was generated using a size 4 moving window on accuracy.

with critics and verifiers [9, 41], recognizing the ability of LLMs as *approximate* idea-generators for problems as against directly solving them. This approach is aligned with neurosymbolic techniques [42], 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 GPT-4 to translate 3-SAT formulas, which we provide in the



**Fig. 5 LLM vs. LLM-Modulo frameworks.** We compare the SAT Search performance of LLM-Modulo frameworks (SAT-Translate) with standalone LLM on SAT-Menu and SAT-CNF variants. Remarkably, the SAT-Translate approach (plotted in green), achieves near-perfect accuracy across the entire  $\alpha$  range. The accuracy curves for SAT-CNF and SAT-Menu, which utilize a standalone GPT-4, are represented in orange and blue, respectively. The plot was generated using a size 4 moving window on  $\alpha$  values.

SAT-Menu input format, into solver-compliant 3-SAT formulas. We then use a 3-SAT solver to solve the translated instance (see Box 4 in materials and methods). We dub this approach **SAT-Translate** and plot its performance in Figure 5.

We observe that when GPT-4 has access to an external solver, there is a significant increase in GPT-4's accuracy reaching  $\approx 100\%$  across the entire range of  $\alpha$ . 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 find that varying the input format between SAT-CNF and SAT-Menu does not significantly enhance GPT-4's inherent reasoning capabilities. The marked improvement in performance is primarily observed only when GPT-4 is equipped with an external solver. While not typically an LLM-Modulo framework (requiring tighter integration), this is a simpler pipelined version explored in recent works [43].

## Discussion

At first sight, our experimental evaluation can be interpreted as indicating that LLMs, specifically GPT-4, exhibit a certain degree of reasoning capabilities: in the easy regions, GPT-4 solves some 3-SAT problems. One might then argue that GPT-4 does not reach perfect accuracy in these regions because of the scale of the model, and that simply increasing this will resolve the issue. For the hard region, however, it is unlikely that scaling up the model will result in radical improvements.

To explain this, reconsider Figures 2 and the time vs.  $\alpha$  plot specifically. The reason why MiniSAT is capable of solving problems in the easy regions faster than problems around  $\alpha_c$  is due to the heuristics built into the solver that guide the search for satisfying solutions (e.g. unit propagation and clause learning [44]). That is, heuristics work well when they can exploit statistical features in the problem instance to be solved. To date, there are no known heuristics that work well around  $\alpha_c$  (and they are

unlikely to exist due to the NP-hardness of 3-SAT). Solvers therefore have to resort to brute force search around  $\alpha_c$ .

In this light, we can reinterpret the experimental performance of GPT-4 on 3-SAT problems: GPT-4’s apparent reasoning capabilities (in the easy regions) is due to the presence of statistical features that it can leach onto. Conversely, in the hard region, the drop in performance can be attributed to GPT-4’s – and by extension current transformer-based LLMs’ – inability to reason according to Bottou’s definition. A similar observation has been made for a computationally tractable class of problems (not NP-complete) using BERT-style language models [17].

Our fine-grained empirical study also complements the theoretical results of LLM reasoning capabilities, c.f. log-uniform  $\text{TC}^0$  complexity class. As these findings only provide bounds on worst-case performance, they have a rather limited significance with regard to average-case complexity [45] and, as such, a limited significance for the reasoning capabilities of LLMs in practice.

Even though the basic 3-SAT phase transition provides a rigorous framework for studying the reasoning capabilities of LLMs, we need to point out that there exists many more results about 3-SAT that might be considered as well. For instance, it has been found that certain aspects of the hardness of 3-SAT instances cannot be explained using the easy-hard-easy regimes induced by the phase transition [46]. Nevertheless, the phase transition seems to be adequate in our settings as demonstrated by the drop in performance of LLMs in the vicinity of  $\alpha_c$ <sup>5</sup>.

## Conclusion

A superficial analysis of the reasoning capabilities of LLMs suggests they possess strong and complex reasoning capabilities – a common fallacy [47]. However, our detailed experimental analysis indicates that what appears as reasoning capabilities could be a mirage, with LLMs predominantly exploiting statistical features present in the data and would explain why LLMs have been termed “statistical parrots” [48].

This is not to say that LLMs lack value – quite the opposite. LLMs are highly effective at translating problems into a formal language and then passing these problems on to solvers. This utility is demonstrated by the relatively superior performance of SAT-Translate over SAT-Menu and SAT-CNF. In a more general context, it would require that the class of the problem is recognized correctly – here 3-SAT – and that the right solvers are available.

Furthermore, LLMs can serve as valuable knowledge bases, leveraging their extensive commonsense and world knowledge through natural language queries to guide search processes. This can be utilized by either solvers guiding LLMs [9] or vice versa, where LLMs assist solvers [43].

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<sup>5</sup>It should however be noted that, in practice, encountered 3-SAT instances often fall into the easy regions. Therefore, decision problems of interest do not usually exhibit worst-case complexity.

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# Supplementary Materials for Can Large Language Models Reason? A Characterization via 3-SAT Phase Transitions

The supplementary materials are organized as follows.

Materials and Methods

Supplementary Text

Figs. S1 to S8

Tables S1 and S2

References (69–70)

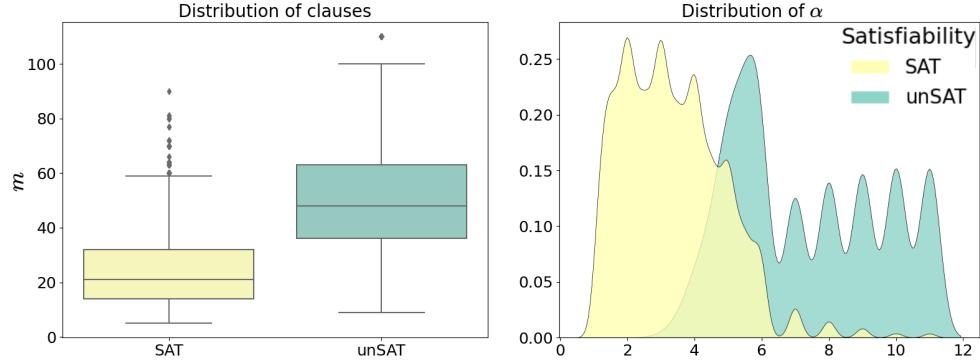
## A Materials and Methods

The section is organized as follows: § A.1 where we outline the dataset (SAT-CNF, SAT-Menu) statistics and generation details. § A.2 where we discuss the working of SAT solvers. § A.3 where we provide generation hyperparameters § A.3.1, discuss failure cases § A.3.2, and illustrate complete prompts for our experiments § A.4.

### A.1 Dataset

#### A.1.1 Generation

In this section, we outline the dataset employed for our study and the methodology behind its generation.



**Fig. 6 Dataset Statistics.** Figures depict clauses  $m$  (left) and  $\alpha$  (right) distribution across SAT and unSAT instances, highlighting that unSAT problems typically feature more clauses and higher  $\alpha$  values.

- We generated a dataset with  $k = 3$  for NP-complete problems (3-SAT).

**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  $\alpha$  value.

$n$	Range of $\alpha$
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

- We employed  $\alpha = m/n$  as a parameter to guide dataset generation across the  $\alpha$  range of [1, 11]. Here,  $m$  is the number of clauses, and  $n$  is the number of variables.
- For  $\alpha$  values within the (6, 11] interval, we incremented  $\alpha$  by 1. For the [1, 6] interval, which contains the most “interesting problems,” we aimed for finer granularity by choosing the smallest possible  $\alpha$  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  $\alpha_{inc} = 0.25$ .
- We generated formulas with  $n \in [1, 10]$  variables. For each  $\alpha_{inc}$  we generated 300 formulas.
- In the dataset with  $k = 2$ , we applied the same methodology but generated formulas within an  $\alpha$  range of [1, 10], always using the smallest feasible increment for each  $\alpha$ . All other parameters remained consistent.
- Each instance is labeled either as satisfiable or unsatisfiable using MiniSAT v2.2.
- Each instance in the dataset is annotated with model count (i.e. number of feasible solutions for a formula). We used D4 [49] for model counting.

**SAT-Menu Data.** 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. This approach is exemplified in Table 2.

### A.1.2 Statistics

Our dataset is comprised of 60,000 formulas, among which 39,909 are satisfiable (SAT) and the remaining 20,091 are unsatisfiable (unSAT) instances. For the purposes of our experiments, we randomly selected approximately 6,000 samples from this pool. 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.

In the case of SAT instances, 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  $\alpha$  is 4.7. This diverse dataset provides a broad spectrum for analyzing the impact of variable and clause distribution on formula satisfiability.

## A.2 SAT Solvers

SAT solvers are tools to automatically verify the satisfiability of propositional logic formulas. The Davis–Putnam–Logemann–Loveland (DPLL) algorithm [50] is a key component of modern SAT solvers. It consists of a backtracking-based search algorithm, enriched with deductive rules and heuristics to efficiently explore the search space and determine whether a formula is satisfiable. The core backtracking algorithm simply selects a literal and assigns a truth value to it. This step produces a simplified formula where all the parts made true by the assignment are removed. This step can be applied recursively until all clauses are removed, meaning that the original formula is satisfiable. Model checkers generalize SAT solvers by counting all the models that satisfy the formula.

Given the CNF in dimacs format, we employed MiniSAT v2.2 for both solution generation (for SAT-Translate) and verification (SAT-Menu, SAT-CNF).

## A.3 LLMs as Solvers

### A.3.1 Generation Hyperparameters

The open-source models were run on 4 NVIDIA-DGX A-100 GPUs using a distributed (model parallel) framework.

### A.3.2 Failure Cases

Here, we discuss some interesting failure cases we observed during our experiments. In the SAT-CNF context, it was observed that LLMs, including GPT-4, 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, GPT-4 might simplistically conclude that the problem is unsatisfiable due to its complexity, as shown in Box 5. Although this reasoning is not entirely sound – as over-constrained

**Table 2** Configuration Parameters

Parameter	Value
<b>GPT-*</b>	
temperature	1
max_tokens	4096
top_p	1
frequency_penalty	0
presence_penalty	0
<b>Llama 2 70B</b>	
4-bit quantization	True
tokenizer type	Fast
max_new_tokens	2048
batch_size	20
<b>Mixtral 8 × 7B</b>	
4-bit quantization	True
attention	Flash
max_new_tokens	4096
batch_size	30

formulas can still potentially be solvable – it appears that LLMs might be leveraging this as a statistical feature.

In the SAT-Translate approach, it was observed that LLMs (with the exception of GPT-4) frequently deviated from the specific requirements of the prompt, generating solutions that did not adhere to the syntax expected by the solver. These inconsistencies in translation led to suboptimal accuracy levels within the LLM-Modulo frameworks.

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 postprocessing to meet specific guidelines. For details on the parsing patterns used in this postprocessing, please refer to the `utils/results_analysis.py` code file.

## A.4 Full Prompts

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. 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. If no such combination exists that satisfies all, output empty lists for both. 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). 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:

```
[[−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.

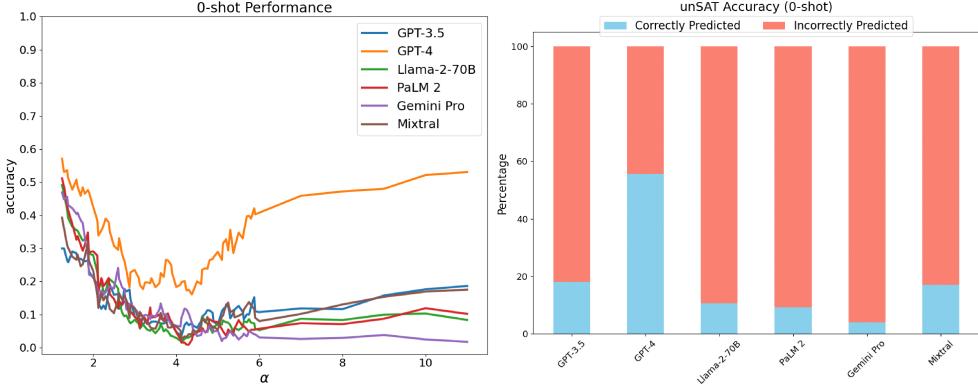
For  $[1, −5, −4]$ . This is again satisfied because 1 is True.

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}  
```
```



**Fig. 7 Comparing GPT-4 with SOTA LLMs.** [Left] Phase transition characteristics for all LLMs. [Right] Comparison of unSAT accuracy (i.e. accuracy of correctly predicting unsatisfiable problems) on 3-SAT decision problem. GPT-4 outperforms all other models in detecting unsatisfiable problems. Both plots are on the search version of SAT-Menu setup with zero-shot prompting. The left plot was generated using a size 4 moving window on  $\alpha$  values.

#### Box 4: 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:
(naan V curry V  $\neg$ tandoori)  $\wedge$  (curry V  $\neg$ naan V  $\neg$ tandoori)  $\wedge$  (naan V  $\neg$ curry V  $\neg$ tandoori)  $\wedge$ 
(curry V  $\neg$ naan V  $\neg$ tandoori)  $\wedge$  (tandoori V naan V curry)  $\wedge$  (curry V  $\neg$ tandoori V  $\neg$ naan)
```

## Box 5: 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: {}  
```
```

## B Supplementary Text

The section is organized as follows: § B.1 where we discuss how GPT-4 performance is impacted by prompt engineering methods. § B.2 where we compare GPT-4 with other state-of-the-art LLMs and discuss the common and divergent performance trends.

### B.1 Impact of Prompt Engineering

We explored 3-shot learning<sup>6</sup> using three chain-of-thought input/output (I/O) demonstrations. These were randomly selected from a set of accurate solutions generated by the LLM and manually checked for consistency between solutions and their explanations. Each I/O example included the input and the output solution, along with its chain-of-thought explanation. From Figure 11, we saw performance gains in the initial Easy-Hard phase but observed a decrease in the subsequent Easy phase.

### B.2 Are there differences in the solving ability w.r.t. state-of-the-art LLMs?

We compared GPT-4 Turbo against some of the best and most advanced LLMs, including both open-source (Llama 2 70B chat-hf, Mixtral 8 × 7B) as well as proprietary models (GPT-3.5 Turbo, Gemini 1.0 Pro, PaLM 2 text-bison). In these evaluations, GPT-4 emerges as a notable exception, outshining other LLMs across various metrics (cf. Appendix). We identify both common and divergent performance patterns.

#### B.2.1 Common Performance Trends

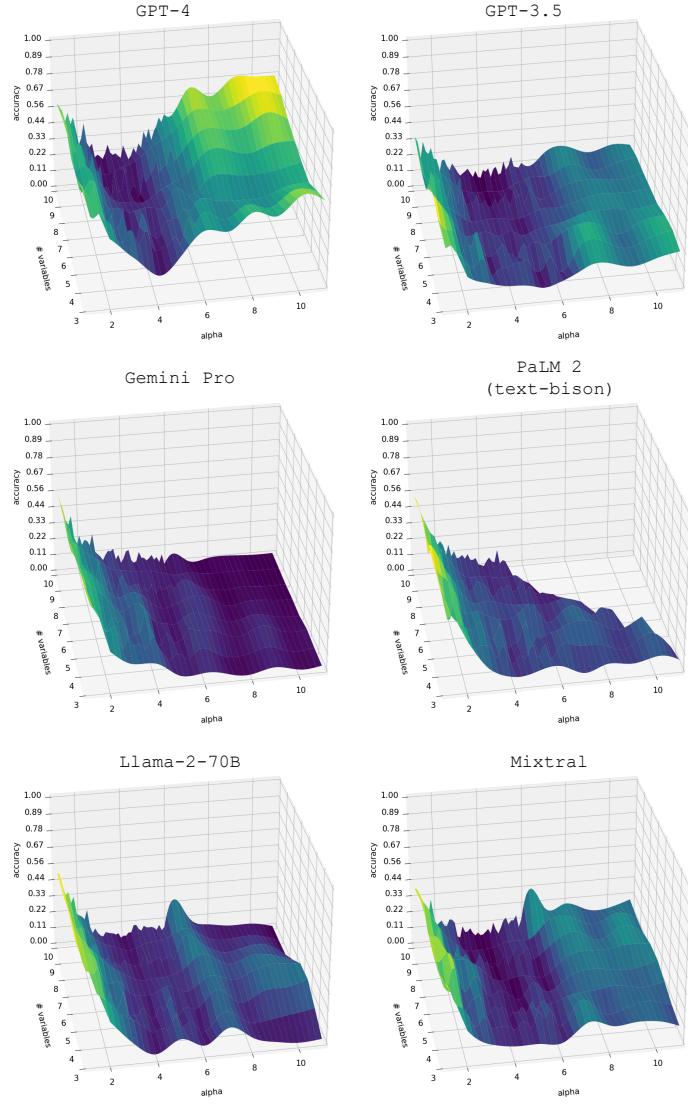
Firstly, the performance consistently correlates with the satisfiability ratio across LLMs, as depicted in Figure 9. Secondly, the performance of LLMs remains unchanged regardless of the input type, as illustrated in Figure 10. Lastly, in general, LLM-Modulo frameworks can enhance performance, as demonstrated in Figure 10.

#### B.2.2 Divergent Performance Trends

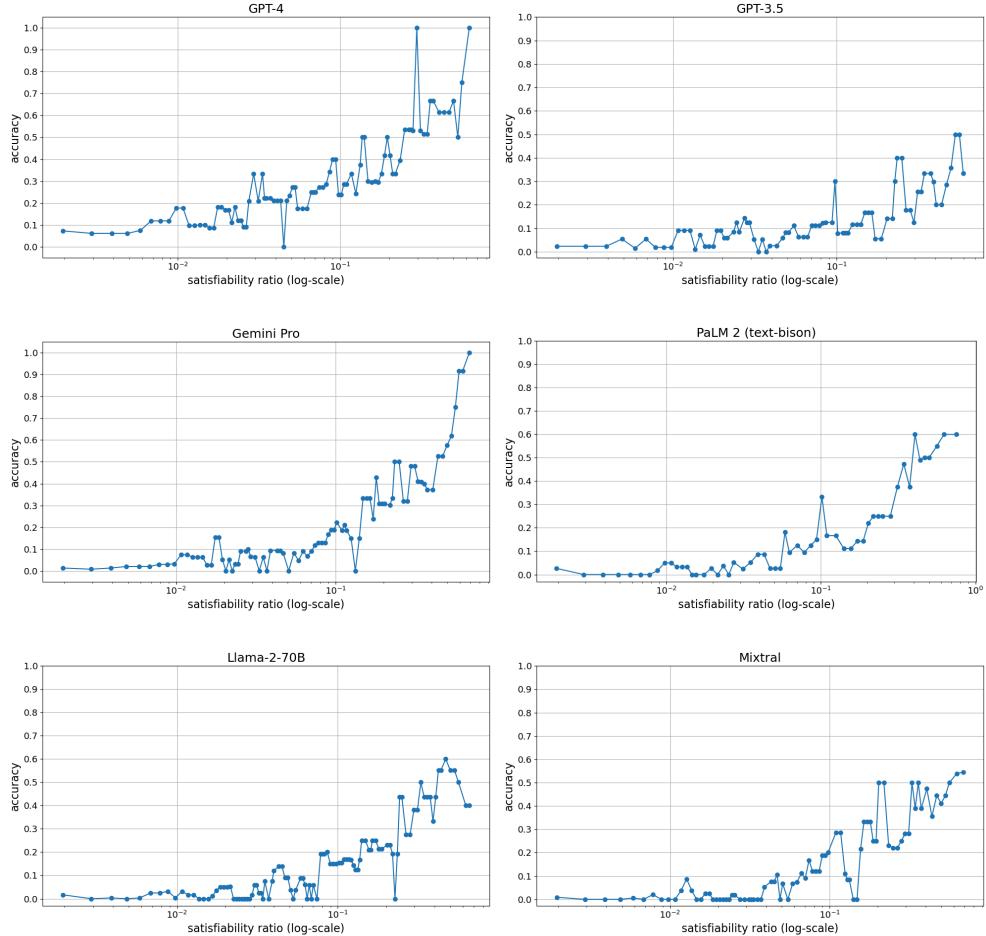
In the 3-SAT Search Problem, as shown in Appendix Figure 7 [Left], GPT-4 uniquely reflects solver-like phase transitions. In contrast, other LLMs exhibit a marked decline in performance in the high  $\alpha$  region, displaying an Easy-Hard-Hard pattern. For the 3-SAT Decision Problem, while all LLMs perform significantly better on the decision variant, only GPT-4 displays an Easy-Hard-Easy phase transition pattern on the decision problem, as shown in Figure 13. Moreover, GPT-4 is more accurate in detecting unsatisfiable instances, as detailed in Figure 7[Right] and Figure 12. Finally, in contrast with GPT-4, other LLMs show no performance change with in-context learning, as demonstrated in Figure 11.

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<sup>6</sup> $k$ -shot learning is a machine learning approach where models learn from just  $k$  labeled examples.



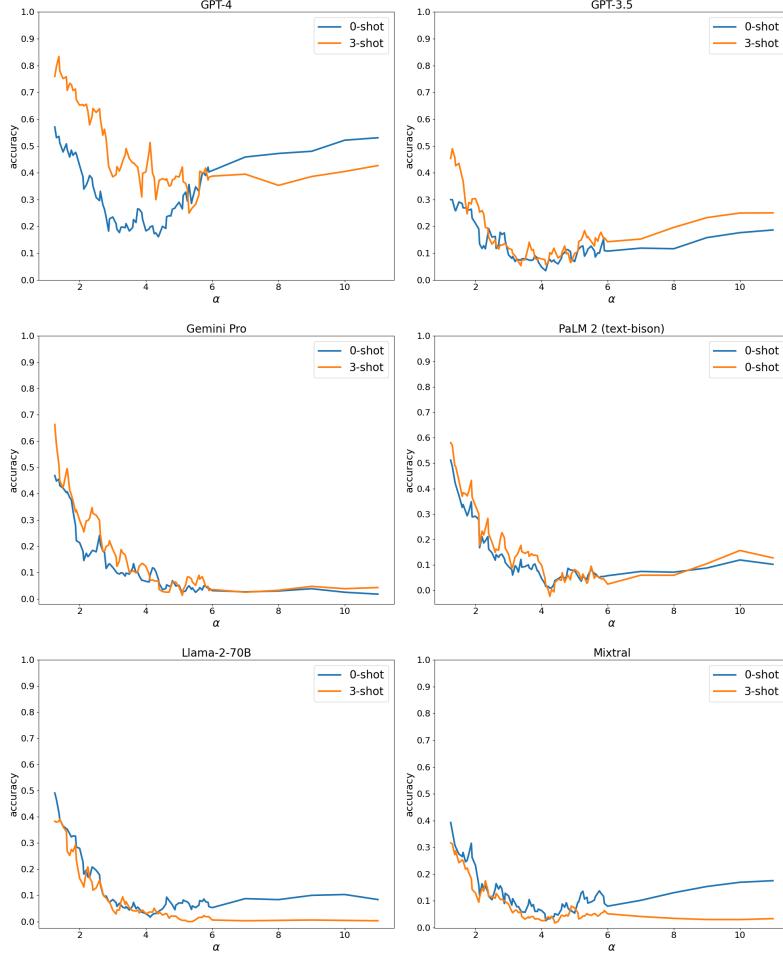
**Fig. 8 LLM Phase Transitions.** Surface plots depict phase transition characteristics, comparing the accuracy in the range  $[0, 1]$  against  $\# \text{variables}$  and  $\alpha$ . The setup is the search version of SAT-Menu with zero-shot prompting. Unlike solvers, the surface plot does not show steepness with an increase in  $\# \text{variables}$ .



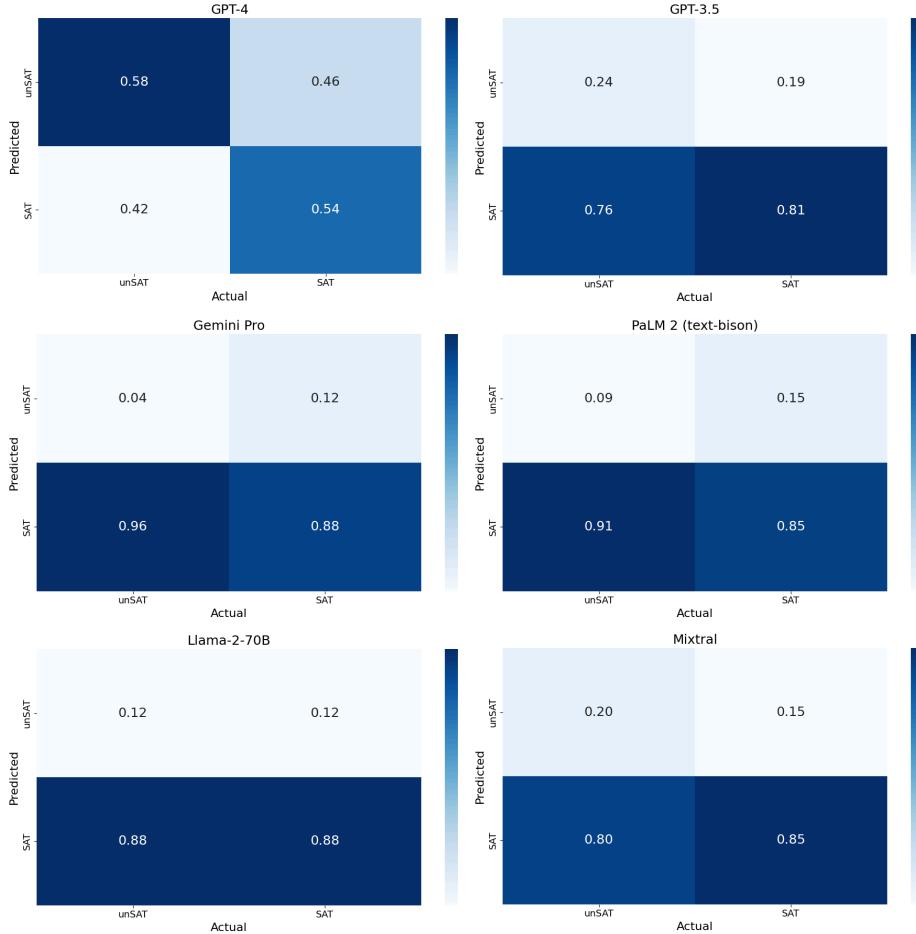
**Fig. 9 LLM accuracy vs. satisfiability ratio.** Figure shows how accuracy improves with satisfiability ratio (in log-scale) across all LLMs. The setup used is the search version of SAT-Menu with 0-shot prompting.



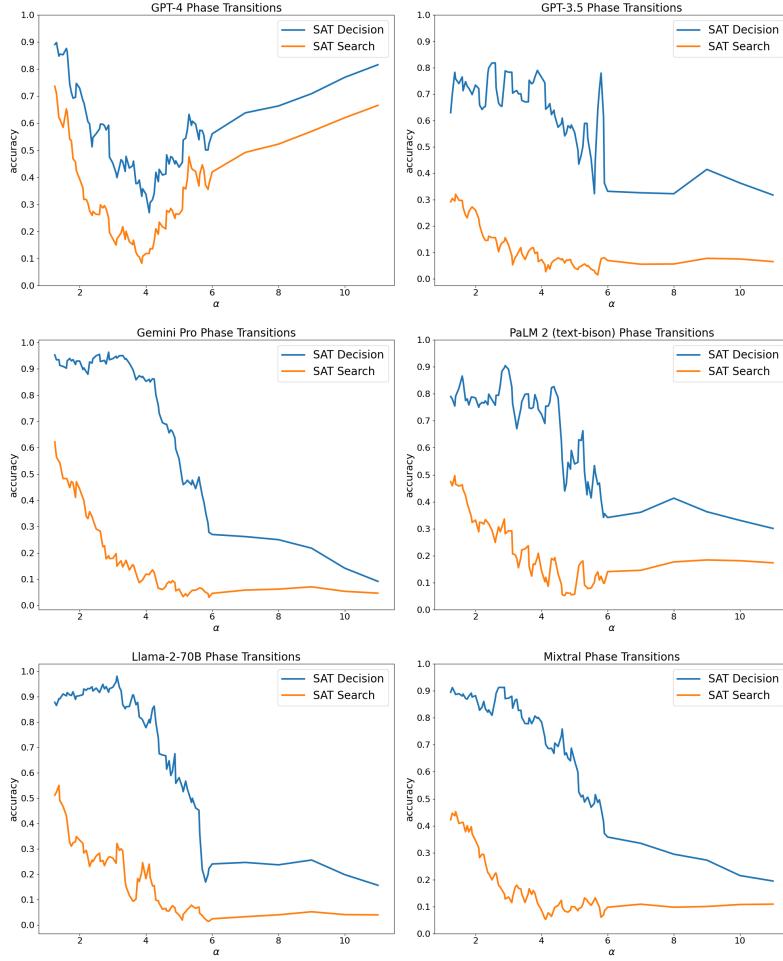
**Fig. 10 LLM-Module Framework comparison.** Figure compares SAT-Menu, SAT-CNF, and SAT-Translate performances across different LLMs. In general, input type (Menu vs. CNF) does not affect the performance. SAT-Translate outperforms the rest, showing the significance of augmenting LLMs with symbolic solvers. compared to the NP-complete nature of SAT solving. We use the 3-SAT search setting. The plot was generated using a size 4 moving window on  $\alpha$  values.



**Fig. 11 0-shot vs. 3-shot accuracy.** Figure compares 0-shot and 3-shot performance comparing all LLMs. It can be observed that, except GPT-4, in-context learning does not enhance performance for other LLMs. The setup is the search version SAT-Menu. The plot was generated using a size 4 moving window on  $\alpha$  values.



**Fig. 12 Confusion matrices for 3-SAT Decision Problem.** Figure compares the accuracy of all LLMs on the 3-SAT decision problem. It can be observed that, except GPT-4, all other LLMs struggle to correctly classify unsatisfiable instances. 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.



**Fig. 13 SAT Decision vs. SAT Search comparison.** Figure illustrates the phase transitions in solving 3-SAT problems, specifically comparing the decision and search variants. Although both variants fall under the same complexity class, empirical evidence shows that LLMs more readily solve the decision problem than the search problem. Among these models, only GPT-4 demonstrates the distinct Easy-Hard-Easy phase transition characteristic. The setup is SAT-CNF with 0-shot prompting. The plot was generated using a size 4 moving window on  $\alpha$  values.