TuringQ: Benchmarking AI Comprehension in Theory of Computation

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Abstract

 We present TuringQ, to the best of our knowl- edge, the first effort to evaluate the reasoning capabilities of large language models (LLMs) in the theory of computation. TuringQ consists of 4,006 question-answer pairs spanning under- graduate and graduate-level problems collected from a diverse set of universities. It covers three difficulty levels and six main concepts, including a valuable subset of axioms and es- sential theoretical concepts. We evaluated vari-011 ous open-source LLMs and GPT-4 using Chain of Thought prompting and human expert as- sessment. Additionally, we explored an auto- mated LLM-Judge, demonstrating its potential to compete with human precision. We show 016 that fine-tuning an LLaMA-3B model on Tur- ingQ improves its reasoning ability. TuringQ serves as both a benchmark and a fine-tuning 019 resource for enhancing LLM reasoning in this complex domain. Our comparative analysis reveals insights into LLM performance, con- tributing to advancements in AI comprehension of theoretical computer science.^{[1](#page-0-0)} **023**

⁰²⁴ 1 Introduction

 The reasoning and comprehension capabilities of large language models across complex domains are crucial due to their recent vast number of applica- tions [\(Guo et al.,](#page-5-0) [2023\)](#page-5-0). As LLMs grow in capa- bility, robust benchmarks are needed to accurately assess their performance, especially in domains re- quiring deep understanding and logical reasoning [\(Brown et al.,](#page-5-1) [2020;](#page-5-1) [Ling et al.,](#page-5-2) [2024\)](#page-5-2). While ef- forts like BIG-Bench [\(Srivastava et al.,](#page-5-3) [2022\)](#page-5-3) have introduced multi-task benchmarks across various domains, a dedicated dataset to assess LLM per- formance on theoretical concepts and problems in the theory of computation has been notably absent. Assessing comprehension in formal languages is

particularly important to understand the depth of **039** LLMs' reasoning abilities. This can be a signifi- **040** cant step toward developing LLMs into effective **041** [p](#page-5-4)roblem solvers in complex domains [\(Bender and](#page-5-4) **042** [Koller,](#page-5-4) [2020\)](#page-5-4). **043**

TuringQ provides a robust platform to rigorously **044** assess and compare the reasoning capabilities of **045** different LLMs on complex theoretical domains, **046** driving advancements in enhancing their skills for **047** tackling intricate computational concepts and con- **048** tributing to the development of more capable and **049** [r](#page-6-0)eliable AI systems [\(Radford et al.,](#page-5-5) [2019;](#page-5-5) [Yang](#page-6-0) **050** [et al.,](#page-6-0) [2023\)](#page-6-0). Moreover, a strong grasp of theory **051** of computation principles is crucial for LLMs as **052** these foundational concepts underpin modern com- **053** puting systems. Enhancing LLM comprehension **054** in this domain can unlock their potential for reason- **055** ing about computational problems, analyzing algo- **056** rithms, and potentially contributing to the develop- **057** ment of new computational models and methodolo- **058** gies [\(Sipser,](#page-5-6) [2006\)](#page-5-6). Figure [1](#page-1-0) presents a complete **059** visual overview of our work. Our contributions are **060** threefold: 061

- 1. TuringQ Dataset: We introduce a new **062** resource of 4,006 theory of computation **063** question-answer pairs from universities world- **064** wide. This dataset spans undergraduate and 065 graduate-level concepts across three difficulty **066** levels and seven main areas, including a sub- **067** set focused on theoretical essentials. It serves **068** as a comprehensive tool for evaluating and **069** fine-tuning LLMs in this domain. **070**
- 2. LLM-based Evaluation: We explore the fea- **071** sibility of leveraging LLMs themselves as **072** evaluators for TuringQ [\(Zheng et al.,](#page-6-1) [2024\)](#page-6-1). **073** By defining an Autograde-TuringQ prompt us- **074** ing Llama-3-8b, we investigate the potential **075** for automating the evaluation process, thereby **076** reducing the time and cost associated with **077** manual grading. 078

¹The dataset, code, and fine-tuned model will be made publicly available upon publication.

Figure 1: TuringQ Dataset and its Evaluation Framework. This diagram presents the TuringQ dataset, a comprehensive resource for theory of computation, and illustrates the automated assessment of LLMs using Llama3- 8b. It showcases sample questions, LLM responses, and their evaluation by the AI evaluator. The fine-tuned Llama3-8b-ft-TuringQ model demonstrates improved performance, yet encounters certain challenges in addressing TuringQ questions.

079 3. Llama3-8b-ft-TuringQ Model: We fine- tuned a large language model on the Tur- ingQ dataset, creating Llama3-8b-ft-TuringQ, a model specialized for theory of computation reasoning. Through comprehensive evalua- tion using custom metrics, we provide a com- parative analysis of LLM performance across different TuringQ categories, shedding light on their ability to tackle complex queries rela-tive to human performance.

⁰⁸⁹ 2 Related Works

 Evaluating Reasoning Capabilities of LLMs Large Language Models have shown remarkable progress, but evaluating their mathematical and computer science reasoning capabilities is still an evolving field [\(Frieder et al.,](#page-5-7) [2023;](#page-5-7) [Li et al.,](#page-5-8) [2024;](#page-5-8) [Ahn et al.,](#page-5-9) [2024\)](#page-5-9). While various datasets have been introduced to assess mathematical reasoning abili- ties [\(Ahn et al.,](#page-5-9) [2024\)](#page-5-9), and approaches like graph- based verification have been proposed to enhance reasoning [\(Cao,](#page-5-10) [2024\)](#page-5-10), the theory of computation domain awaits similar advancements.

101 Automated LLM Evaluation Automated evalu-**102** ation of large language models is an active area

of research. Various techniques, such as self- **103** consistency, truth-checking against external data, **104** and adversarial probing, have been proposed to en- **105** [a](#page-5-11)ble LLMs to evaluate their own outputs [\(Huang](#page-5-11) **106** [et al.,](#page-5-11) [2024\)](#page-5-11). Parallel studies have explored using **107** LLMs to calibrate and augment human raters for **108** evaluating text generation outputs [\(Zhang et al.,](#page-6-2) **109** [2024\)](#page-6-2). The combination of LLM evaluations with **110** human grading for written assessments has also **111** been investigated, providing a novel perspective on **112** human-AI collaboration [\(Ren et al.,](#page-5-12) [2024\)](#page-5-12). How- **113** ever, the trustworthiness of LLMs for evaluation **114** has been questioned, leading to proposals for scal- **115** able meta-evaluation of LLMs as evaluators via **116** agent debate [\(Chern et al.,](#page-5-13) [2024\)](#page-5-13). Additionally, re- **117** search has focused on aligning LLM-assisted eval- **118** uation of LLM outputs with human preferences **119** [\(Shankar et al.,](#page-5-14) [2024\)](#page-5-14). These works contribute to **120** the understanding and enhancement of automated **121** LLM evaluators. **122**

3 The TuringQ Dataset **¹²³**

TuringQ is a comprehensive dataset comprising **124** 4,006 question-answer pairs covering undergradu- **125** ate and graduate-level theory of computation prob- **126**

(a) Category Distribution of TuringQ

(b) Difficulty Distribution of TuringQ

Figure 2: Category and Difficulty level Distribution of TuringQ

 lems. The questions are categorized into three diffi- culty levels and seven main conceptual areas: Regu- lar Languages, Theoretical Concepts, Context-Free Languages, Computability Theory, Countability Concepts, Complexity Theory, and Fundamental Concepts, as detailed in Table [9.](#page-11-0) The difficulty lev- els were determined by domain experts, ensuring an even distribution across categories and a clear distinction between difficulty levels and conceptual categories. The distribution of the dataset based on category and difficulty level is illustrated in Fig- ure [2.](#page-2-0) Examples of dataset entries are provided in **139** Table [8.](#page-10-0)

140 3.1 Data Collection

 We curated a collection of questions from publicly available exam sets and homework solutions from 29 top-tier universities to ensure a high-quality dataset in the Theory of Computation domain. The primary dataset consists of 2,155 carefully selected university exam and homework questions, ensuring fair distribution across various categories. Addi- tionally, 61 question-answer pairs from reputable non-university resources were incorporated. To complement the academic questions, we developed a secondary set focusing on fundamental concepts, theorems, lemmas, and essential knowledge. Do- main experts identified these topics, and the Claude 3 Sonnet model [\(Anthropic,](#page-5-15) [2024\)](#page-5-15) was utilized to generate 1,790 question-answer pairs covering the core principles of Theory of Computation.

¹⁵⁷ 4 Experiments

 For further evaluation and analysis, we employ a di- verse set of language models: Llama-3-8B-Instruct [\(Meta,](#page-5-16) [2024\)](#page-5-16), Llama-2-7b-chat-hf [\(Touvron et al.,](#page-5-17) [2023\)](#page-5-17), Mistral-7B [\(Jiang et al.,](#page-5-18) [2023\)](#page-5-18), Gemma-7b- it [\(Team et al.,](#page-5-19) [2024\)](#page-5-19), and GPT-4-32k [\(OpenAI,](#page-5-20) [2023\)](#page-5-20). To assess these models, we curated a strat-ified sample of 500 questions from the TuringQ

dataset, maintaining the original distribution across **165** difficulty levels and categories. This approach en- **166** sures a representative subset for our comparative **167** analysis. **168**

4.1 AI-Driven Assessment 169

We used Llama-3-8b to generate responses using 170 [d](#page-5-21)irect and Chain of Thought (CoT) prompts [\(Wei](#page-5-21) **171** [et al.,](#page-5-21) [2023\)](#page-5-21). To evaluate LLMs as assessors, we **172** developed the 'AutoGrade-TQ' prompt, guiding **173** models to score answers on a 1-4 scale. Three inhouse domain experts provided ground-truth evalu- **175** ations with substantial inter-rater agreement (Fleiss' **176** Kappa $\kappa = 0.742$). Majority votes were derived 177 from their scores. Models evaluated both CoT **178** and simple answers. Analysis suggests LLMs can **179** be effective evaluators, with Llama3-8b achieving **180** 77.8% binary accuracy. Key findings include: **181**

CoT answers generally received higher scores, **182** improving performance in open-source models. **183** GPT-4 showed the lowest alignment with human **184** evaluators. GPT-4 led in 4-level accuracy (49%), **185** while Llama3-8b led in 2-level accuracy (77.8%) . Llama3-8b and human evaluators' average scores **187** for CoT answers were nearly identical. Full prompt **188** details and statistics are presented in Tables [2](#page-8-0) and **189** [7.](#page-9-0) **190**

4.2 Model Specialization 191

We fine-tuned the Llama3-8b model, resulting in **192** Llama3-8b-ft-TuringQ, using our extensive dataset **193** of detailed answers to enhance its performance on **194** specific tasks. Our approach combined Quantized **195** Low-Rank Adaptation (QLoRA) [\(Dettmers et al.,](#page-5-22) **196** [2023\)](#page-5-22), a Parameter-efficient Fine-tuning (PEFT) **197** technique [\(Xu et al.,](#page-5-23) [2023\)](#page-5-23), and Supervised Fine- **198** Tuning (SFT)^{[2](#page-2-1)}. We utilized three datasets derived 199 from TuringQ for fine-tuning: a training set (3,006 **200** instances), a validation set (500 instances), and a **201**

²https://huggingface.co/docs/trl/en/sft_trainer

 test set (500 instances), generated using stratified sampling based on difficulty level and category for balanced representation. Our fine-tuning process incorporated advanced techniques like quantization and low-rank adaptation to optimize performance within computational constraints. Despite limita- tions, we achieved high-quality results, and further fine-tuning could yield better performance. Setup and hyperparameters are detailed in Appendix [A.1.](#page-7-0)

²¹¹ 5 Results

212 5.1 Performance Evaluation

 We evaluated seven LLMs, including our fine-tuned model "Llama3-8b-ft-TuringQ", using the TuringQ test set. Assessment utilized a Chain-of-Thought prompt and an AutoGrader prompt for automatic evaluation. We measured performance using score and binary accuracy metrics. The score metric quantifies response quality, while binary accuracy classifies answers as valid or invalid based on the score, providing a more comprehensive assess- ment of answer correctness. As shown in Table [1,](#page-3-0) Llama3-8b-ft-TuringQ increased binary accu- racy by 2.2%, a significant improvement given the computational resources used. This enhancement primarily resulted from an increase in responses with a score of 3. While performances across mod- els were similar, GPT-4 only slightly outperformed others despite its superior capabilities, highlight- ing the challenges LLMs face with TuringQ ques- tions. Figure [4](#page-7-1) shows the score distribution for each model.

233 5.2 Category-Specific Performance Analysis

 Analysis of the seven categories in the TuringQ dataset revealed consistent model performance across categories without drastic differences. Con- trary to expectations, the "theoretical concepts" category did not yield the highest scores, poten- tially due to its more descriptive manner compared to other categories. The best performance was observed in the context-free languages category. GPT-4 exhibited exceptional performance in the "Countability" concepts category, achieving 90.9% accuracy—23.2% higher than the average binary accuracy of open-source models (Table [5\)](#page-8-1). The fine-tuned model outperformed Llama3-8b in ev- ery category except theoretical concepts, where it showed a 5% decrease. In context-free languages, it demonstrated a substantial 22% increase com-pared to Llama3-8b (Figure [3\)](#page-7-2).

Model	Mean Score	Binary Accuracy		
$GPT-4$	3.276	82.40%		
$Llama3-8b-ft-$	2.984	76.00%		
TuringQ				
Llama3-8b	3.030	73.80%		
Gemma-7B	3.022	72.20%		
$LLaMA-2-7B$	3.020	70.80%		
Mistral-7B	2.986	70.40%		
Gemma-2B	2.872	65.20%		

Table 1: Comparative Performance Metrics of Language Models on the TuringQ Test Set

5.3 Impact of Difficulty Levels on Model **251** Performance **252**

The TuringQ dataset's difficulty levels were vali- **253** dated by domain experts, acknowledging the inher- **254** ent subjectivity of difficulty assessments. Interest- **255** ingly, our findings contradict conventional human **256** expectations regarding question difficulty. Ques- **257** tions labeled as Level 3 and Level 2 achieved higher **258** average scores (3.17) than Level 1 questions (2.95) **259** and Axiom-level questions (2.90). Binary accuracy **260** metrics further corroborate these findings, with the **261** highest accuracies observed in Level 3 and Level **262** 2 questions (Tables [4](#page-8-2) and [6\)](#page-9-1). This unexpected per- **263** formance pattern across difficulty levels suggests a **264** potential misalignment between human-perceived **265** difficulty and the capabilities of language models **266** in this domain. **267**

6 Conclusion **²⁶⁸**

We presented TuringQ to evaluate the reasoning **269** capabilities of large language models (LLMs) in **270** the theory of computation covering three difficulty **271** levels and six main concepts, including key ax- **272** ioms and theoretical concepts. We evaluated vari- **273** ous open-source LLMs and GPT-4 using Chain of **274** Thought prompting and human expert assessment, **275** and explored an automated LLM-Judge, demon- **276** strating its potential to compete with human pre- **277** cision. Fine-tuning an LLaMA-3B model on Tur- **278** ingQ improved its reasoning ability. This effort pro- **279** vides a valuable benchmark for evaluating LLM **280** understanding and could also be used as an ed- **281** ucational resource. Assessing comprehension in **282** formal languages was crucial for understanding the **283** depth of LLMs' reasoning abilities, representing **284** a significant step toward developing LLMs into **285** effective problem solvers in complex domains. **286**

7 Ethics Statement

 The TuringQ dataset comprises publicly available exams and homework questions from renowned universities worldwide, obtained from the internet. Each source is duly labeled in the dataset's meta- data, and no question has been extracted without mentioning the original source. After data collec- tion, we reviewed and enhanced some answers to maintain the dataset's high quality and ensure its value as a resource. This enhancement process did not involve any bias or alteration of the original content or answers.

 For the theoretical concepts, we utilized the Claude 3 sonnet model to generate answers for the specified theorems and lemmas. We believe this approach could benefit the TuringQ dataset. Subsequently, we checked and edited the model- generated answers to ensure the absence of bias, hallucinations, or errors in our work.

 Regarding non-university sources, we made ef- forts to gather solutions from diverse, reliable sources, including computer science portals and books. As the theory of computation and theoreti- cal computer science is an advancing and complex field, we have included answers that are accurate based on our current knowledge, particularly con- cerning P and NP, and open problems. We ac- knowledge that as our understanding progresses, some open questions in our dataset may require updates to their answers. However, to the best of our present knowledge, this dataset is up-to-date.

8 Limitations

 The present study encountered several limitations that future research should address. Firstly, com- putational resource constraints hindered our ability to utilize larger language models with 70 billion or more parameters. Instead, we focused on smaller yet powerful models that were more feasible for our research scope. These resource constraints also impacted the fine-tuning process, limiting the Llama3-8b-ft-TuringQ model to only three epochs of fine-tuning, which may have curtailed its po- tential performance. Consequently, future studies should explore extended training periods and alter- native fine-tuning approaches using the TuringQ dataset to fully leverage its capabilities.

 Evaluating descriptive questions posed a signif- icant challenge. While we developed two metrics for evaluating descriptive questions, incorporating more extensive human evaluation would be beneficial. Although this approach is more resource- **337** intensive and time-consuming, it could provide **338** valuable insights into model performance. Ad- **339** ditionally, the development and implementation **340** of new, more comprehensive evaluation metrics **341** would be beneficial for assessing model capabili- **342** ties. **343**

Our dataset effectively captures the essential **344** categories and fundamentals of theory of compu- **345** tation. However, it lacks coverage of more ap- **346** plied tasks, such as code generation. Future re- **347** search could investigate how fine-tuned, special- **348** ized models impact performance in related domains **349** like code generation, reasoning, and mathematical **350** problem-solving. It would be particularly interest- **351** ing to explore the extent to which domain-specific **352** fine-tuning may affect a model's general capabil- **353** ities. Further study into the broader implications **354** and potential trade-offs of such fine-tuning on large **355** language models is encouraged. **356**

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A Appendix

A.1 Fine-tuning Setup and Hyperparameters

 Our fine-tuning approach for the Llama3-8b model combined Quantized Low-Rank Adapta- tion (QLoRA), a Parameter-efficient Fine-tuning (PEFT) method, with Supervised Fine-Tuning (SFT) using the SFTTrainer from *HuggingFace's* [3](#page-7-3) *trl library*³. QLoRA, as a PEFT technique, al- lows for task-specific tuning without modifying all model parameters, while SFT provides a frame- work for supervised learning on our specific task. LoRA (Low-Rank Adaptation) freezes the LLM's weights and injects trainable rank-decomposition matrices [\(Hu et al.,](#page-5-24) [2021\)](#page-5-24). QLoRA extends this by incorporating quantization techniques, further reducing memory usage while maintaining or im- proving model performance. We configured the PEFT settings with the following hyperparameters:

- Alpha: 64
- Dropout rate: 0.05
- Optimizer: 'paged_adamw_8bit'
- Learning rate: 5e-6
- Learning rate scheduler: Linear
- Number of epochs: 3 (due to computational limitations)
- Batch size: 4 (for both training and evalua-tion)
- Gradient accumulation steps: 2

 Evaluation was performed at every step, with re- sults logged for detailed performance tracking. We employed quantization via the *BitsAndBytes* method^{[4](#page-7-4)}, setting the compute data type to bfloat16 and loading the model in 4-bit with a quantization type of "nf4". This configuration enabled double quantization, potentially improving the efficiency of our model training. Our approach, combining QLoRA, SFT, and quantization techniques, allowed us to achieve high-quality results despite computa-tional constraints.

Figure 3: Bar chart showing the difference in binary accuracy (%) between Llama3-8b-ft-TuringQ and the Llama3-8b across various TuringQ categories. Categories C1 (Countability Concepts), C2 (Computability Theory), C3 (Context-Free Languages), C4 (Fundamental Concepts), and C5 (Complexity Theory) demonstrate positive accuracy gains for Llama3-8b-ft-TuringQ compared to Llama3-8b, indicating performance improvements after fine-tuning. C6 (Regular Languages) exhibits no change in accuracy and C7 (Theoretical Concepts) has a minor decrease in performance.

Figure 4: Score Distribution Across Models on the Test Split of the TuringQ Dataset

<https://huggingface.co/docs/trl/en/index>

<https://huggingface.co/docs/bitsandbytes/main/en/index>

	Average	MSE	Variance	Correlation	2-Class Acc	4-Class Acc	
$Llama-2-7b$	3.494	1.758	1.4979	0.1169	0.6800	0.3440	
$Llama-2-7b-CoT$	3.456	1.656	1.4928	0.0478	0.7040	0.3520	
Llama-3-8b	2.858	1.746	1.7301	0.1772	0.6400	0.3180	
Llama-3-8b-CoT	3.032	1.268	1.2676	0.3408	0.7780	0.3520	
Gemma-2h	3.2969	2.068	1.9737	0.1400	0.6784	0.3753	
Gemma-2b-CoT	3.4854	2.006	1.8295	0.1463	0.7050	0.4121	
Gemma-7b	3.1674	1.678	1.6520	0.0479	0.6801	0.2733	
Gemma-7b-CoT	3.3162	1.524	1.4479	0.0355	0.7084	0.3203	
Mistral-7 _b	3.454	1.538	1.3171	0.3474	0.7260	0.4520	
Mistral-7b-CoT	3.374	1.686	1.5823	0.2632	0.7120	0.4620	
$GPT-4$	2.69	1.390	1.3036	0.5103	0.7000	0.4880	
$GPT-4-CoT$	2.366	2.106	1.6354	0.3906	0.6080	0.3980	
Human	2.984						
Human-CoT	3.052						

Table 2: Statistical Measures of LLM Performance as Evaluators on the TuringQ Test Set

Category	llama3-8b	Llama3-8b-ft-TuringQ Gemma-2b		Gemma-7b	$llama2-7b$	Mistral-7b	GPT4
Complexity Theory	3.1	3.1	3.0	3.2	3.1	3.2	3.4
Computability Theory	3.1	3.3	3.1	3.3	3.2	3.3	3.4
Context-Free Languages	2.8	3.3	3.2	3.3	3.4	3.1	3.4
Countability Concepts	2.9	3.2	2.8	2.9	3.2	2.8	3.6
Fundamental Concepts	3.1	3.1	3.0	3.1	3.3	2.9	3.2
Regular Languages	3.1	3.0	3.0	3.2	3.2	3.1	3.4
Theoretical Concepts	3.0	2.8	2.7	2.9	2.8	2.9	3.2

Table 3: Comparative Analysis of Mean Scores Across Models by Category

Table 4: Comparative Analysis of Mean Scores Across Models by Difficulty Level

Category	llama3-8b	Llama3-8b-ft-TuringQ	Gemma-2b	Gemma-7b	$llama2-7b$	Mistral-7b	GPT4
Complexity Theory	81.2%	83.3%	75.0%	83.3%	81.2%	81.2%	85.4%
Computability Theory	74.5%	88.2%	76.5%	78.4%	76.5%	80.4%	84.3%
Context-Free Languages	66.7%	88.9%	74.1%	74.1%	81.5%	74.1%	77.8%
Countability Concepts	66.7%	78.8%	60.6%	63.6%	75.8%	60.6%	90.9%
Fundamental Concepts	72.1%	78.7%	68.9%	73.8%	82.0%	65.6%	77.0%
Regular Languages	75.4%	75.4%	73.7%	71.9%	75.4%	70.2%	84.2%
Theoretical Concepts	74.0%	69.1%	57.0%	69.1%	61.0%	68.2%	81.6%

Table 5: Comparative Analysis of Mean Binary Accuracy Across Models by Category

Table 6: Comparative Analysis of Mean Binary Accuracy Across Models by Difficulty Level

Table 7: Prompts Employed for Automated Grading and Answer Generation via Chain of Thought Reasoning

Table 8: Sample Instances from the TuringQ Dataset

Table 9: Detailed Analysis and Interpretation of the TuringQ Dataset Categories