# MEDAGENTSBENCH: Benchmarking Thinking Models and Agent Frameworks for Complex Medical Reasoning

Xiangru Tang<sup>\*\*</sup>, Daniel Shao<sup>\*</sup>, Jiwoong Sohn<sup>\*\*</sup>, Jiapeng Chen<sup>\*</sup>, Jiayi Zhang<sup>\*</sup>, Jinyu Xiang<sup>\*</sup>, Fang Wu<sup>\*</sup>, Yilun Zhao<sup>\*</sup>, Chenglin Wu<sup>\*</sup>, Wenqi Shi<sup>\*</sup>, Arman Cohan<sup>\*</sup>, Mark Gerstein<sup>\*</sup>

Yale University

Stanford University

UT Southwestern Medical Center

xiangru.tang@yale.edu

## **Abstract**

Large Language Models (LLMs) have shown impressive performance on existing medical question-answering benchmarks. This high performance makes it increasingly difficult to meaningfully evaluate and differentiate advanced methods. We present MEDAGENTS-BENCH, a benchmark that focuses on challenging medical questions requiring multi-step clinical reasoning, diagnosis formulation, and treatment planning—scenarios where current models still struggle despite their strong performance on standard tests. Drawing from seven established medical datasets, our benchmark addresses three key limitations in existing evaluations: (1) the prevalence of straightforward questions where even base models achieve high performance, (2) inconsistent sampling and evaluation protocols across studies, and (3) lack of systematic analysis of the interplay between performance, cost, and inference time. Through experiments with various base models and reasoning methods, we demonstrate that the latest thinking models, DEEPSEEK R1 and OPENAI 03, exhibit exceptional performance in complex medical reasoning tasks. Additionally, advanced search-based agent methods offer promising performance-to-cost ratios compared to traditional approaches. Our analysis reveals substantial performance gaps between model families on complex questions and identifies optimal model selections for different computational constraints. Our benchmark and evaluation framework are publicly available at https://github.com/gersteinlab/ medagents-benchmark.

# 1 Introduction

LLMs have demonstrated remarkable capabilities in medical natural language processing tasks, from answering clinical questions to assisting in diagnostic processes (Singhal et al., 2025; Jin et al., 2022; Chen et al., 2023a,b; Zhou et al., 2023; Gao

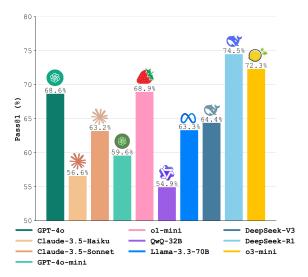


Figure 1: Performance analysis of large language models on medical tasks. Overall Pass@1 accuracy comparison across models in zero-shot setting. The score is an average of seven test sets' results (MedQA, PubMedQA, MedMCQA, MedBullets, MMLU, MMLU-Pro, MedExQA, and MedXpertQA).

et al., 2024). However, as shown in Figure 1, even OPENAI 03, GPT-40 and CLAUDE 3.5 SONNET struggle with complex medical scenarios that require deep domain expertise and multi-step reasoning (Xu et al., 2024; Fan et al., 2025; Shi et al., 2024).

To enhance LLMs' medical reasoning capabilities, researchers have proposed various approaches. As summarized in Table 1, these methods range from general-purpose techniques like CHAIN-OF-THOUGHT (COT) and SELF-CONSISTENCY (SC) (Wei et al., 2022; Wang et al., 2022) to domain-specific frameworks such as MEDPROMPT (Chen et al., 2024b). While these traditional approaches provide modest improvements, recent evidence suggests that agent-based methods, or "agent workflows," demonstrate superior performance. Methods like MEDAGENTS (Tang et al., 2023) and MDAGENTS (Kim et al., 2024a) leverage multiagent collaboration frameworks to achieve more robust medical reasoning. However, with the ad-

<sup>\*</sup> Equally contribution.

Method Description

Chain-of-Thought (Wei et al., 2022) Self-Consistency (Wang et al., 2022) MedPrompt (Chen et al., 2024b) Multi-Persona (Wang et al., 2023) Self-Refine (Madaan et al., 2024) MedAgents (Tang et al., 2023) MDAgents (Kim et al., 2024a)

AFlow (Zhang et al., 2024)

SPO (Xiang et al., 2025)

Elicits reasoning in large language models
Improves chain of thought reasoning through sampling diverse reasoning paths
Multi-round prompting with ensemble voting for medical question answering
Task-solving agent through multi-persona self-collaboration
Iterative refinement with self-feedback

Collaborative multi-agent framework for zero-shot medical decision making
Dynamic multi-agent collaboration framework for medical reasoning
Automating agentic workflow generation
Self-supervised prompt optimization

Table 1: **Methods Overview.** The reasoning approaches spanning four categories: baseline prompting methods, advanced prompting techniques, agent-based frameworks, and search-based agent methods.

vent of advanced thinking models like OPENAI O3-MINI and DEEPSEEK R1, as well as the development of search-based agent frameworks, it remains an open question how these models perform in medical reasoning tasks.

Several critical challenges in the evaluation of medical reasoning capabilities create a significant gap in our ability to assess advanced LLMs and agent frameworks. (a) As shown in Table 2, existing medical reasoning datasets, while extensive, contain a substantial proportion of straightforward questions derived from standardized examinations. On these simpler questions, even base LLMs achieve high performance (see Table 3, "FULL" columns), obscuring meaningful evaluation of advances in reasoning methods. (b) The inconsistent sampling practices across different studies—where researchers arbitrarily extract approximately 300 questions from datasets containing thousands of examples (Tang et al., 2023; Kim et al., 2024a)—further inhibit reliable comparisons between approaches. (c) Moreover, current benchmarks fail to systematically capture the critical interplay between performance, computational costs, and inference time—factors that significantly impact real-world deployment decisions.

This landscape motivates our work on MEDA-GENTSBENCH, a benchmark specifically designed to evaluate complex medical reasoning capabilities where standard benchmarks fall short. Unlike existing benchmarks that either focus on general medical knowledge or suffer from ceiling effects, MEDAGENTS BENCH employs a rigorous pipeline that: (1) draws from seven diverse established medical datasets (MedQA, PubMedQA, MedMCQA, MedBullets, MMLU, MMLU-Pro, MedExQA, and MedXpertQA); (2) applies adversarial filtering to identify truly challenging questions where models currently struggle; (3) conducts thorough contamination analysis to ensure validity; and (4) incorporates human annotations from medical professionals to verify reasoning depth requirements. Our

comprehensive experiments yield several key insights: (a) thinking models like DEEPSEEK R1 and OPENAI O3 substantially outperform traditional approaches, achieving 15-25% higher accuracy on complex medical reasoning tasks; (b) among traditional and agent-based approaches, advanced search-based agent methods like AFLOW offer the best performance-to-cost ratio, achieving results that approach thinking models while requiring fewer computational resources; and (c) opensource models can achieve competitive results at significantly lower operational costs.

#### 2 Related Work

The evolution of medical reasoning has progressed with numerous specialized datasets. Popular benchmarks like MedQA (Jin et al., 2021), PubMedQA (Jin et al., 2019), and MedMCQA (Pal et al., 2022) established the foundation with standardized multiple-choice questions from medical licensing exams and PubMed abstracts. The field then expanded to domain-specific resources like clinical notes (Pampari et al., 2018) and question summarization (Abacha et al., 2021). This evolution continued with integrating visual elements through datasets like pathology images (He et al., 2020), radiology questions (Soni et al., 2022; Bae et al., 2023), and dental care (Zeng et al., 2025), broadening the scope of medical reasoning beyond text-only questions. To address linguistic and regional diversity, multilingual datasets emerged (Vilares and Gómez-Rodríguez, 2019; Hertzberg and Lokrantz, 2024; Olatunji et al., 2024). Additionally, event-driven resources like COVID-QA (Möller et al., 2020) were developed to address pandemicspecific information needs. The ecosystem further matured with comprehensive collections such as MultiMedQA (Singhal et al., 2023), which combines seven distinct medical datasets.

Research in applying LLMs to medical tasks has progressed through several distinct phases. Initial efforts focused on evaluating the capabil-

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Benchmark	Size	Avg Lens	Options	Description
MedQA (Jin et al., 2021)	1273	167.1	4	Multiple choice questions from medical licensing exams
PubMedQA (Jin et al., 2019)	500	316.1	3	Questions based on PubMed abstracts
MedMCQA (Pal et al., 2022)	2816	18.7	4	Questions from AIIMS & NEET PG entrance exams
MedBullets (Chen et al., 2024a)	308	213.1	5	Questions from Medbullets online medical study platform
MedExQA (Kim et al., 2024b)	935	19.1	4	Multiple-choice questions across additional five medical specialties
MedXpertQA (Zuo et al., 2025)	2450	257.4	10	Advanced medical questions with understanding (U) and reasoning (R)
MMLU (Hendrycks et al., 2020)	1089	55.9	4	Multitask questions covering medical and other academic domains
MMLU-Pro (Wang et al., 2024)	818	57.4	3-10	Multitask questions covering medical and other academic domains
MEDAGENTSBENCH	862	147.4	3-10	HARD subset across all datasets

Table 2: **Medical Question-Answering Datasets.** Knowledge-based QA datasets are curated from medical literature, professional journals, and educational resources. Traditional benchmarks, recently emerging benchmarks, and general purpose benchmarks are shown with corresponding colors.

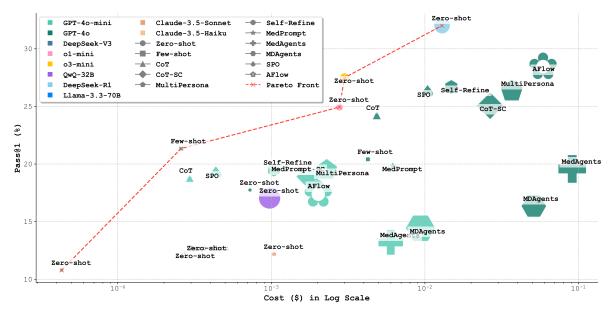


Figure 2: **Performance analysis of agents and models on MEDAGENTSBENCH.** Cost-performance trade-off analysis showing **Pass@1** accuracy versus cost per sample (in log scale), with marker sizes indicating inference time. Different markers represent various prompting methods, while colors distinguish different models. The Pareto frontier (red dashed line) indicates optimal cost-performance trade-offs.

ities of general-purpose LLMs in medical contexts, with numerous surveys and benchmarks (Thirunavukarasu et al., 2023; Liévin et al., 2024; Gilson et al., 2023) establishing baseline performance metrics. Foundation models (Singhal et al., 2023; Achiam et al., 2023) have achieved physician-level performance through careful prompt engineering. This was followed by a wave of fine-tuned or pretrained open-source models specifically for the medical domain (Han et al., 2023; Wu et al., 2024; Chen et al., 2023c). The field then advanced toward specialized reasoning methods (Liu et al., 2024; Shi et al., 2024) and retrieval-augmented generation (Jin et al., 2023; Jeong et al., 2024; Xiong et al., 2024). More recently, agent-based frameworks have shown particular promise, with MedAgents (Tang et al., 2023) and MDAgents (Kim et al., 2024a) leveraging collaborative multi-agent systems for complex medical decision-making. These developments collectively represent a shift toward more sophisticated reasoning capabilities in medical AI, with thinking models demonstrating exceptional performance on complex medical reasoning challenges.

## 3 MEDAGENTSBENCH

MEDAGENTSBENCH is a carefully curated benchmark designed to evaluate complex medical reasoning tasks. Drawing from eight established medical datasets (MedQA (Jin et al., 2021), PubMedQA (Jin et al., 2019), MedM-CQA (Pal et al., 2022), MedBullets (Chen et al., 2024a), MMLU (Hendrycks et al., 2020), MMLU-Pro (Wang et al., 2024), MedExQA (Kim et al., 2024b), and MedXpertQA (Zuo et al., 2025)), we systematically construct a challenging subset that focuses on more complex reasoning scenarios. A detailed description can be found in Appendix A.

As shown in Table 3, these source datasets vary

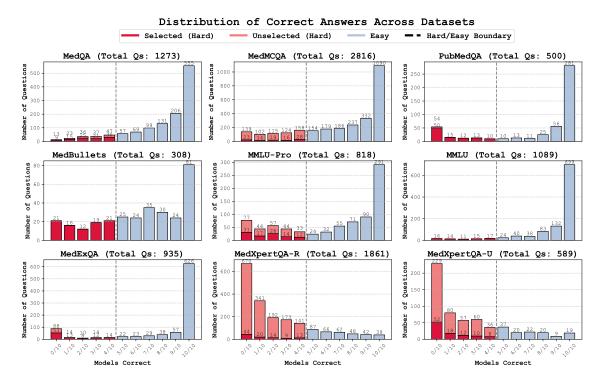


Figure 3: Distribution of model performance across eight medical datasets (MedQA, MedMCQA, PubMedQA, MedBullets, MMLU-Pro, MMLU, MedExQA, and MedXpertQA. Each subplot shows the number of questions answered correctly by different proportions of models (x-axis: k/N, where k is the number of correct models and N is the total number of models). Questions are categorized as either hard (left of the dashed line, < 50% of models correct) or easy (right of the dashed line,  $\ge 50\%$  of models correct), with selected questions highlighted in darker shades. The total question count for each dataset is indicated in the subplot titles.

significantly in size (from 174 to 2,816 questions), average token length (18.7 to 316.1), and number of options (3 to 10), providing diverse evaluation contexts. Our hard-set selection process is based on three key criteria:

- 1. Model Performance Distribution As visualized in Figure 3, we analyze the proportion of models that correctly answer each question (k/N) ratio). Questions, where less than 50% of models provide correct answers (left of the dashed line in Figure 3), are categorized as hard candidates. This ensures our benchmark focuses on truly challenging questions that current models struggle with.
- 2. Question Diversity We carefully balanced our dataset to ensure comprehensive coverage across various medical knowledge domains. Our HARD subset includes precisely 100 questions each from MedQA, PubMedQA, MedMCQA, MMLU-Pro, and MedExQA. From MedXpertQA, we incorporated both its Reasoning (MedXpertQA-R) and Understanding (MedXpertQA-U) subsets (100 questions each), which were annotated in the original paper to distinguish between questions requiring complex clinical reasoning versus those primarily testing medical knowledge. Additionally, we

included 89 questions from MedBullets and 73 questions from MMLU. This distribution maintains proportional representation while ensuring sufficient sampling depth to evaluate model performance across diverse medical subdomains and reasoning requirements.

**3. Reasoning Depth** We prioritize questions that require multi-step reasoning, as evidenced by the performance gap between base models and agent-based approaches. As shown in Table 3, while models achieve high accuracy on the FULL set (e.g., GPT-40: 87.8% on MedQA), their performance drops significantly on our HARD subset (e.g., GPT-40: 32.0% on MedQA-HARD), confirming the increased difficulty.

In summary, we first evaluate each candidate question across multiple model architectures (as shown in Table 3) to ensure the architecture-independent difficulty. Secondly, we conduct a data contamination analysis using MELD (Memorization Affects Levenshtein Detector) (Nori et al., 2023). This analysis involves providing models with the first half of each question in our test set and measuring the similarity between their generated continuations and the original second half.

Table 3: **Performance heatmap by base models and datasets.** For each task, accuracy values are in percentages, with separate columns for FULL and HARD. **The best values** and the second-best values are highlighted.

Model	FULL	dQA   Hard	PubM FULL	<b>ledQA</b> Hard	MedN	MCQA HARD	MedI FULL	Bullets Hard		ILU Hard	MMI FULL	U-Pro Hard		E <b>xQA</b> Hard	MedX FULL	pert-R HARD	MedX FULL	pert-U Hard
GPT-40-MINI	73.4	22.0	76.2	10.0	66.0	17.0	53.6	10.1	84.3	12.3	57.5	11.0	78.4	4.0	13.9	6.0	16.6	5.0
GPT-40	87.8	32.0	<u>79.2</u>	9.0	76.6	<u>25.0</u>	70.5	19.1	91.3	24.7	69.1	21.0	84.7	18.0	22.5	7.0	23.3	6.0
DEEPSEEK-V3	79.3	16.0	73.6	12.0	74.3	19.0	61.0	13.5	89.7	15.1	64.7	12.0	83.4	7.0	18.7	6.0	23.3	9.0
O1-MINI	89.9	<u>49.0</u>	77.4	11.0	73.2	21.0	73.1	38.2	90.7	31.5	67.8	19.0	82.5	15.0	29.0	29.0	27.0	14.0
o3-mini	92.7	53.0	79.6	16.0	<u>77.1</u>	24.0	82.1	50.6	93.4	<u>35.6</u>	70.0	15.0	<u>85.2</u>	<u>18.0</u>	<u>33.9</u>	<u>25.0</u>	<u>31.9</u>	15.0
QwQ-32B	78.6	29.0	77.8	16.0	69.7	24.0	54.2	12.4	87.0	19.2	65.2	<u>28.0</u>	81.5	10.0	17.7	9.0	17.3	6.0
DEEPSEEK-R1	92.0	47.0	76.2	<u>13.0</u>	81.9	31.0	<u>79.2</u>	<u>43.8</u>	95.0	43.8	79.6	37.0	86.6	26.0	37.3	<u>25.0</u>	37.5	26.0
LLAMA-3.3-70B	76.8	14.0	77.8	13.0	71.4	20.0	61.7	16.9	85.2	12.3	61.7	10.0	79.3	7.0	20.2	9.0	22.4	9.0
CLAUDE-3.5-S	77.7	18.0	76.4	10.0	68.8	10.0	56.5	9.0	86.9	16.4	64.2	14.0	81.0	13.0	20.4	9.0	24.1	11.0
CLAUDE-3.5-H	63.4	13.0	73.8	12.0	62.9	23.0	49.4	10.1	79.7	11.0	57.5	12.0	77.3	13.0	14.6	8.0	16.5	6.0

Table 4: **Performance heatmap by methods and datasets.** All tasks are evaluated on the HARD set with accuracy in % using two base models: GPT-40-MINI and GPT-40. **The best values** and the second-best values are highlighted.

Method	MedQA	PubMedQA	MedMCQA	MedBullets	MMLU	MMLU-Pro	MedExQA	MedXpert-R	MedXpert-U   Average
	40-м   40	40-м   40	40-м   40   4	40-м   40   4	4о-м   4о	4о-м   4о	4о-м   4о	40-м   40	40-M   40   40-M   40
ZERO-SHOT	22.0   32.0	10.0 9.0	17.0   25.0	10.1   19.1	12.3 24.7	11.0   21.0	4.0 18.0	6.0 7.0	5.0   6.0   10.8   18.0
FEW-SHOT	30.0   28.0	22.0 20.0	31.0   29.0	23.6   23.6	28.8   27.4	10.0   9.0	<b>25.0</b>   <u>24.0</u>	<u>16.0</u>   14.0	8.0   11.0   21.6   20.7
CoT	21.0   39.0	13.0 10.0	26.0   30.0	18.0   28.1	28.8 26.0	35.0   35.0	14.0 <u>24.0</u>	6.0 12.0	10.0   15.0   19.1   24.3
CoT-SC	20.0 37.0	11.0 6.0	20.0 35.0	16.9 30.3	28.8 30.1	34.0 <b>43.0</b>	19.0   22.0	10.0 10.0	13.0   14.0   19.2   25.3
MULTIPERSONA	29.0 45.0	13.0 15.0	21.0   25.0	15.7   29.2	26.0 37.0	36.0 <u>42.0</u>	17.0 21.0	7.0 10.0	12.0   16.0   19.6   26.7
SELF-REFINE	32.0 41.0	12.0 13.0	24.0 34.0	15.7   28.1	27.4 34.2	31.0   34.0	16.0 22.0	7.0 <b>17.0</b>	12.0   <b>19.0</b>   19.7   <u>26.9</u>
MEDPROMPT	29.0   34.0	14.0 11.0	30.0   26.0	13.5   22.5	20.5 26.0	34.0   22.0	18.0   16.0	6.0 14.0	13.0   9.0   19.8   20.1
MEDAGENTS	24.0   43.0	12.0 15.0	22.0   30.0	15.7   27.0	24.7   28.8	3.0   8.0	12.0   19.0	4.0   3.0	5.0   6.0   13.6   20.0
MDAGENTS	22.0   36.0	23.0 11.0	16.0   22.0	14.6 21.3	17.8 24.7	9.0   8.0	10.0   13.0	8.0 4.0	9.0   5.0   14.4   16.1
SPO	19.0   31.0	<u>25.0</u> <b>31.0</b>	20.0 30.0	22.5   29.2	19.2 32.9	32.0   36.0	14.0   19.0	11.0 15.0	11.0 16.0 19.3 26.7
AFLOW	30.0 <b>48.0</b>	15.0 18.0	25.0   31.0	15.7 34.8	24.7 <b>38.4</b>	29.0   37.0	7.0 22.0	7.0 13.0	7.0 <u>18.0</u> 17.8 <b>28.9</b>

As shown in Figure 4, the HARD subset selected for our MEDAGENTSBENCH benchmark consistently demonstrates lower similarity scores (20-40%) compared to the original datasets, suggesting our filtering process effectively selects questions that test genuine reasoning rather than memorization. Complete details of our MELD methodology and its limitations are discussed in Section 5.1. Finally, four medical professionals (M.D. students) review the final question set to verify clinical relevance and reasoning complexity. The resulting MEDAGENTSBENCH benchmark contains 862 questions with an average token length of 147.4.

#### 4 Experiments

We conduct comprehensive evaluation of both base models and agentic reasoning methods across our MEDAGENTSBENCH benchmark. Our experiments follow a standardized protocol to ensure fair comparison, with consistent prompting strategies and evaluation metrics across all models and methods.

### 4.1 Experimental Setup

For base model comparison, we evaluate both closed-source models (GPT-40, GPT-40-MINI,

CLAUDE-3.5-SONNET, CLAUDE-3.5-HAIKU, O1-MINI, and O3-MINI) and open-source alternatives (DEEPSEEK-V3, DEEPSEEK-R1, LLAMA-3.3-70B, and QWQ-32B).

Additionally, we evaluate 11 distinct agentic reasoning approaches spanning three categories. The first category includes baseline prompting methods such as ZERO-SHOT, FEW-SHOT, CHAIN-OF-THOUGHT, and SELF-CONSISTENCY. The second encompasses advanced prompting techniques: MULTI-PERSONA, SELF-REFINE, and MEDPROMPT. The third category covers agent-based frameworks, including medical-specific collaboration frameworks (MEDAGENTS and MDAGENTS, which we reimplemented to ensure accurate parsing of multiple-choice responses) and search-based agent methods (SPO and AFLOW) with search strategies consistent with the original setting..

Our data contamination analysis (Figure 4) revealed that OpenAI models demonstrate consistently lower memorization metrics across all datasets compared to other model families. This finding guided our decision to use GPT-40 and GPT-40-MINI as primary models for agentic reasoning to minimize performance advantages stem-

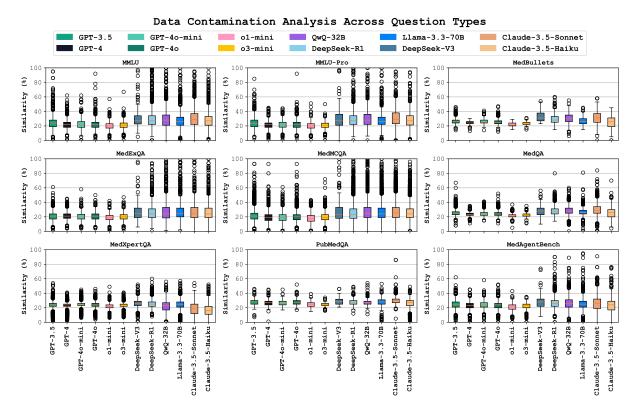


Figure 4: **Data contamination analysis across medical question-answering datasets using MELD.** The boxplots display similarity percentages between model-generated text and original question text, with higher values potentially indicating memorization of training data. Lower similarity scores suggest minimal data contamination, while higher values may indicate potential contamination in model training data.

ming from potential training data contamination.

Standardized evaluation All experiments utilize identical prompt templates and evaluation protocols to ensure a fair comparison. We implement a standardized two-round inference protocol per query for agent-based methods requiring multiple inference rounds (e.g., MEDAGENTS). Multi-agent approaches (e.g., MULTI-PERSONA) consistently employ three distinct agent roles for all evaluations. This standardization mitigates confounding factors that might result from implementation variations, allowing us to more accurately attribute performance differences to the methods themselves rather than differences in their implementations.

#### 4.2 Cost Estimation

To analyze cost-performance trade-offs, we followed a standardized evaluation protocol. Understanding these trade-offs is particularly important given the significant computational resources required by advanced thinking models, where their enhanced reasoning capabilities often come with substantially higher inference costs and longer processing times than traditional models. Similarly, multi-agent frameworks necessitate multi-

ple rounds of API calls for agent interactions, further increasing both computational costs and inference times. For API-based commercial models (OPENAI and CLAUDE), we calculated costs using their published pricing rates based on total token usage (input + output). Based on their platform rates, we estimated costs for open-source models run on Together AI . The total cost of experimentation was \$226.17. We measured inference time as wall-clock time per sample, including prompt construction and model inference, with agent-based methods including their complete interaction cycles.

#### 4.3 Main Results

Most models demonstrate significant difficulty with our challenging benchmark, with even powerful systems like GPT-40 achieving only 32.0% accuracy on MedQA and 18.0% on MedExQA in our HARD subset. This substantial performance drop confirms that our selection criteria effectively identifies questions requiring advanced reasoning capabilities. Amid these challenges, DEEPSEEK-R1 demonstrates remarkable performance, achieving the highest scores on five datasets

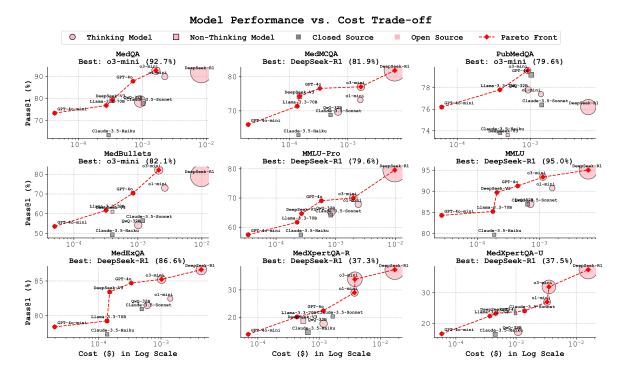


Figure 5: Cost-performance analysis across seven medical datasets, comparing open and closed-source language models. Each subplot shows Pass@1 accuracy (%) versus cost per sample (USD, log scale). Marker shapes distinguish thinking models from non-thinking models, while colors indicate open-source (blue) versus closed-source (red) models. Marker sizes represent inference time, and the red dashed line shows the Pareto frontier of optimal cost-performance trade-offs.

(MedMCQA: 31.0%, MMLU: 43.8%, MMLU-Pro: 37.0%, MedExQA: 26.0%, and MedXpertQA-U: 26.0%). Similarly, O3-MINI excels on three datasets (MedQA: 53.0% and MedBullets: 50.6%, with a tie on PubMedQA at 16.0%).

When examining reasoning methods in Table 4, we find that advanced approaches generally outperform baseline methods. Specifically, AFLOW demonstrates superior performance, achieving the highest scores on four datasets with GPT-40 (MedQA: 48.0%, MedBullets: 34.8%, MMLU: 38.4%, and MedXpertQA-U: 18.0%), which indicates the effectiveness of automated agentic workflow generation for medical reasoning. Additionally, MULTIPERSONA performs exceptionally well on MedQA (45.0% with GPT-40) and contributes to the second-best results on several other datasets, highlighting the benefits of multi-persona selfcollaboration. Traditional methods like CHAIN-OF-THOUGHT with SELF-CONSISTENCY (COT-SC) show consistent improvements over basic CoT, with average gains of 2-3% across datasets, and excel particularly on MMLU-Pro (42.0% with GPT-40). However, domain-specific methods like MED-PROMPT show mixed results—performing well on specific datasets but lacking consistency across different medical tasks.

Despite their specialized design for medical sce-

narios, agent-based methods like MEDAGENTS (best: 43.0% on MedQA with GPT-40) and MDAGENTS don't consistently outperform the latest thinking models across all datasets, and they incur significantly heavier computational overhead. This suggests that while agent frameworks provide benefits for specific tasks, the inherent reasoning capabilities of advanced base models may be more important for complex medical reasoning than the framework itself. Overall, our results demonstrate that thinking models, particularly DEEPSEEK-R1 and O3-MINI, consistently excel in complex medical reasoning tasks, while search-based agent methods like AFLOW also show promising performance in handling intricate medical queries.

## 5 Analysis

In this section, we comprehensively analyze our experimental results, focusing on two key aspects that impact the performance and reliability of LLMs in medical reasoning tasks.

#### 5.1 Data Contamination

To ensure the reliability of our benchmark evaluation, we employ memorization effects Levenshtein Detector (MELD), initially introduced by Nori et al. (2023) to analyze potential data contamination across various datasets and language models.

MELD quantifies memorization by splitting each question into two halves: the first half serves as context for the model, which must then generate the second half. It calculates the proportion of matching characters by measuring the Levenshtein distance ratio between the generated output and the original unseen portion. Higher similarity scores suggest memorization rather than genuine reasoning. Since our benchmarks are multiple-choice questions with short answers represented as index letters (e.g., A, B, C, D), including the answer index in MELD has minimal impact on the similarity score. This is because the primary determinant of memorization is whether the question itself has been seen. While seeing a question does not necessarily mean the model has seen its exact answer, it significantly increases the risk of contamination compared to a model that has not encountered the question at all. The ability to reproduce question text verbatim indicates potential exposure during training, which could give certain models an unfair advantage regardless of whether they've memorized the specific answer.

The analysis spans GPT-3.5/4, CLAUDE-3.5, and various open-source LLMs, providing comprehensive coverage of different model architectures and training approaches. MELD exhibits high precision but unknown recall, meaning that while a detected match strongly indicates memorization, the absence of a match does not guarantee that the data was not seen during training. For instance, Nori et al. (2023) report that GPT-4 reproduces SQuAD 2.0 questions with 99% character overlap in 17% of cases, highlighting significant memorization.

Figure 4 reveals distinct memorization patterns between commercial and open-source models. OpenAI models demonstrated consistently lower similarity scores (median 20-25%) across medical datasets, suggesting minimal verbatim memorization. In contrast, several open-source models (DEEPSEEK-R1, QwQ-32B, and LLAMA-3.3-70B) exhibited substantially higher scores, particularly on MedExQA (median 25-30%, with outliers exceeding 80% similarity).

Concerningly, some open-source models reproduced question texts with over 95% character-level accuracy on certain benchmarks, with MMLU and MMLU-Pro showing vulnerability in the 60-90% similarity range. There were clear instances of training data contamination, challenging the valid-

ity of fair comparison. HARD set selected from MEDAGENTSBENCH demonstrated significantly lower MELD scores across all models, confirming its utility for more reliable performance assessment. Meanwhile, a manual review of high-similarity cases in MedMCQA and MedExQA revealed that while some shared text consisted of standard medical terminology, this likely contributed to the high similarity in these specialist QA datasets rather than direct data contamination.

#### 5.2 Cost-Performance Trade-off

Our evaluation examines both model architecture efficiency and reasoning method effectiveness through a cost-performance lens. We analyze these dimensions separately using two complementary visualizations.

## 5.2.1 Base Model Cost-Efficiency

As shown in Figure 5, we compare ten base models across the performance-cost spectrum, categorizing them as open-source (blue) or closed-source (red), and as thinking models (circles) or non-thinking models (squares). This analysis reveals several important patterns:

The Pareto frontier (red dashed line) identifies models that deliver optimal performance for their cost—any model below this line represents a suboptimal investment, while models along the line represent the most efficient options available. DEEPSEEK-R1 and O3-MINI consistently appear as Pareto-optimal solutions across multiple datasets, indicating their exceptional efficiency in medical reasoning tasks.

Domain-specific patterns emerge across different medical benchmarks. For example, MedQA demonstrates steep performance improvements with increased computational investment (jumping from ~20% to over 50% accuracy with higher-cost models), while PubMedQA shows more modest gains, suggesting diminishing returns from larger models in certain domains.

Thinking models (circles) consistently outperform non-thinking counterparts (squares) at comparable cost points, with performance differentials of 5-10% in complex tasks like MedBullets. This suggests that structured reasoning capabilities justify their computational overhead, particularly for challenging diagnostic scenarios.

Open-source models demonstrate surprisingly competitive performance despite their lower costs. DEEPSEEK-R1 achieves comparable or superior

performance to many closed-source alternatives while requiring 10x more computational costs, most notably in MedMCQA (81.9% accuracy) and MMLU-Pro (79.6% accuracy).

# 5.2.2 Reasoning Method Efficiency

Figure 3 extends our analysis to compare various reasoning methods applied to base models, revealing additional insights about cost-effective approaches to medical reasoning:

Search-based agent methods like AFLOW achieve exceptional efficiency on the Pareto frontier, delivering performance comparable to much more expensive base models. This suggests that architectural improvements in reasoning strategies can offset raw model size and parameter count.

Traditional reasoning methods like CoT-SC demonstrate consistent improvements over basic CoT, particularly on datasets like MMLU-Pro, where they achieve up to 43.0% accuracy with GPT-40.

Advanced prompting techniques occupy different positions relative to the Pareto frontier, with MULTIPERSONA showing exceptional efficiency for MedQA (45.0% with GPT-40) but less consistent performance across other datasets.

Specialized medical frameworks like MEDA-GENTS show mixed efficiency profiles—while they excel at specific tasks (43.0% on MedQA with GPT-40), they don't consistently outperform simpler approaches across all datasets, suggesting that general reasoning capabilities may sometimes be more important than domain-specific frameworks.

The overall Pareto frontier reveals a hierarchy of efficiency, where certain combinations of models and methods (e.g., DEEPSEEK-R1 with basic prompting or O3-MINI with minimal augmentation) deliver optimal performance per dollar spent, making them particularly valuable for resource-constrained deployment scenarios.

These complementary analyses demonstrate that both model architecture and reasoning method significantly impact the cost-efficiency of medical AI systems. When selecting approaches for medical reasoning tasks, practitioners should consider both the base model's capabilities and the reasoning framework applied, evaluating them within the context of specific medical domains and available computational resources.

#### 6 Conclusion

Through MEDAGENTSBENCH, we provide several important contributions to medical AI evaluation. First, our comprehensive experiments demonstrate that thinking models, particularly DEEPSEEK-R1 and OPENAI O3-MINI, consistently excel in complex medical reasoning tasks, outperforming traditional approaches across diverse domains. Second, advanced search-based agent methods like AFLOW show promising performance-to-cost ratios, especially on diagnostic reasoning tasks requiring multistep inference. Our cost-performance analysis reveals that open-source models can achieve competitive results at significantly lower operational costs, with DEEPSEEK-R1 emerging as a particularly effective option for resource-constrained environments.

Beyond raw performance metrics, our findings suggest important directions for future research. We observe that agent frameworks provide substantial benefits for specific medical tasks but may not consistently outperform base thinking models across all scenarios. This indicates the need for more task-specific adaptation of reasoning frameworks. Additionally, our contamination analysis highlights the importance of robust evaluation protocols in medical AI, where data contamination can significantly confound performance assessments. Future work should explore hybrid approaches combining the inherent reasoning strengths of thinking models with specialized medical knowledge frameworks, and develop more sophisticated verification mechanisms for ensuring clinical accuracy and safety.

#### Limitations

While MEDAGENTSBENCH provides a rigorous benchmark for evaluating medical reasoning capabilities, several important limitations remain:

First, our benchmark primarily focuses on medical question-answering tasks based on educational resources, which may not fully reflect the complexity and nuance of real-world clinical scenarios. A more comprehensive evaluation would require incorporating real-world clinical cases, physician-patient dialogues, and diagnostic decision-making processes.

Second, we lack systematic verification of model outputs by practicing clinicians. This raises concerns about the reliability and alignment of model-generated reasoning paths with established medical

knowledge. Future work should establish a more rigorous verification framework involving domain experts to assess answer correctness, the validity of reasoning steps, and potential hallucinations.

Finally, while our work demonstrates the effectiveness of multi-agent and ensemble approaches in medical reasoning, we have only scratched the surface of potential ensemble strategies. Sophisticated ensemble methods like step-wise verification, task-wise verification, and dynamic agent collaboration could yield even better performance. For instance, verifying intermediate reasoning steps through model consensus, utilizing heterogeneous model combinations, or implementing adaptive voting strategies based on agent expertise remain unexplored. Future research could investigate:

(1) More sophisticated voting and aggregation strategies beyond simple majority voting. (2) Adaptive ensemble methods that dynamically adjust agent weights based on task characteristics. (3) Hierarchical ensemble approaches that combine both step-wise and task-wise verification. (4) Methods for increasing response diversity through systematic prompt variation and temperature tuning. (5) Integration of expert knowledge to guide ensemble selection and verification.

While our current approach shows promising results, we lack a thorough theoretical understanding of why specific ensemble configurations outperform others in medical reasoning tasks. A more systematic study of ensemble properties - such as diversity, correlation, and calibration - could guide the development of more effective medical reasoning systems.

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## **A Detailed Description of Datasets**

This appendix provides detailed descriptions of the seven established medical datasets used in the construction of MEDAGENTSBENCH.

**MedQA** MedQA is a large-scale open-domain question answering dataset collected from professional medical board exams. Introduced by Jin et al., it covers three languages: English, simplified Chinese, and traditional Chinese. The English portion contains 1,273 questions, with an average token length of 167.1 tokens per question. Each question is accompanied by 4 multiple-choice options. Questions are sourced from the United States Medical Licensing Examination (USMLE) and similar professional medical board exams. The questions test a wide range of medical knowledge, including diagnosis, treatment, and medical concepts. MedQA is notable for its multilingual coverage and focus on professional-level medical knowledge assessment. The questions require both factual medical knowledge and clinical reasoning abilities.

**PubMedQA** PubMedQA (Jin et al., 2019) is a biomedical question answering dataset collected from PubMed abstracts, designed to test reasoning over biomedical research texts. The dataset contains 500 expert-annotated QA instances used in our benchmark, with an average token length of 316.1 tokens per question. Each question has 3 possible answers (yes/no/maybe). Each PubMedQA instance consists of a research question derived from an article title, a context from the corresponding abstract (excluding its conclusion), and an answer that summarizes whether the research supports a yes, no, or maybe conclusion. PubMedQA is unique in requiring reasoning over biomedical research texts, including understanding of quantitative research findings and statistical evidence. It tests the ability to synthesize scientific information rather than recall medical facts.

MedMCQA MedMCQA (Pal et al., 2022) is a multiple-choice question answering dataset designed to address real-world medical entrance exam questions. Our benchmark includes 2,816 questions from this dataset, with an average token length of 18.7 tokens. Each question has 4 possible answers. Questions are collected from AIIMS and NEET PG entrance exams, covering 2,400+ health-care topics and 21 medical subjects. The questions test various reasoning abilities across a wide range

of medical domains. MedMCQA stands out for its topical diversity and focus on entrance exam questions that test not just knowledge but application of medical concepts in practical scenarios.

MedBullets MedBullets (Chen et al., 2024a) comprises USMLE Step 2/3 style clinical questions collected from the Medbullets online medical study platform. The dataset contains 308 questions with an average token length of 213.1 tokens per question. Each question is accompanied by 5 multiple-choice options. Questions are designed to simulate clinical scenarios similar to those encountered in medical licensing exams. Each question is paired with a case description, answer choices, and explanations of correct and incorrect answers. MedBullets questions are specifically chosen to be challenging, focusing on realistic clinical scenarios that require integration of medical knowledge with clinical reasoning. The inclusion of expert explanations makes this dataset particularly valuable for evaluating reasoning paths.

MedExQA (Kim et al., 2024b) is a benchmark designed to evaluate LLMs' understanding of medical knowledge through explanations across multiple specialties. The dataset contains 935 questions with an average token length of 19.1 tokens per question. Each question has 4 multiplechoice options. MedExQA spans five distinct medical specialties that are underrepresented in current datasets: Audiology, Nutrition, Occupational Therapy, Physical Therapy, and Speech-Language Pathology. Each question-answer pair is accompanied by multiple explanations. MedExQA uniquely focuses on the ability of models to generate nuanced medical explanations, moving beyond classification accuracy to assess deeper understanding. It specifically addresses specialties where current LLMs demonstrate limited knowledge.

MedXpertQA MedXpertQA (Zuo et al., 2025) is a challenging benchmark designed to evaluate expert-level medical knowledge and advanced reasoning capabilities. The dataset includes 2,450 questions with an average token length of 257.4 tokens. Questions have up to 10 possible answers. MedXpertQA spans 17 medical specialties and 11 body systems, incorporating specialty board questions to improve clinical relevance. The dataset is divided into two subsets: MedXpertQA-Understanding (U) for testing basic medical knowledge comprehension and MedXpertQA-Reasoning

(R) for evaluating complex clinical reasoning. MedXpertQA is specifically designed to challenge advanced models with expert-level questions. Its reasoning-oriented subset is particularly valuable for assessing the capabilities of thinking models on complex medical decision-making tasks.

MMLU (Medical Subset) The Massive Multitask Language Understanding benchmark (Hendrycks et al., 2020) includes several subsets focused on medical knowledge, which They extract for our benchmark. They include 1,089 medical-related questions from MMLU, with an average token length of 55.9 tokens per question. Each question has 4 multiple-choice options. The medical portions of MMLU include subjects such as clinical knowledge, anatomy, college medicine, medical genetics, professional medicine, and more. The benchmark covers both basic and advanced medical concepts. MMLU tests knowledge across many difficulty levels, from elementary to advanced professional. Its standardized format makes it useful for comparing medical reasoning to other domains of knowledge.

MMLU-Pro MMLU-Pro (Wang et al., 2024) is an enhanced version of MMLU designed to be more challenging and reasoning-focused, with an expanded choice set. We include 818 medical-related questions from MMLU-Pro with an average token length of 57.4 tokens. Questions have between 3-10 multiple-choice options. MMLU-Pro eliminates trivial questions from MMLU and integrates more challenging, reasoning-focused questions that require deeper understanding of concepts. MMLU-Pro is specifically designed to address the ceiling effects observed in MMLU as models improved. Its expanded choice set and focus on reasoning rather than simple knowledge recall make it more discriminative for advanced models.