LLMs May Perform MCQA by Selecting the Least Incorrect Option

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Abstract

In the field of NLP, Large Language Models (LLMs) have markedly enhanced performance across a variety of tasks. However, the comprehensive evaluation of LLMs remains an inevitable challenge for the community. Recently, the adoption of Multiple Choice Question Answering (MCQA) as a benchmark for assessing LLMs has gained considerable traction. However, concerns regarding the robustness of this evaluative method persist. Building upon previous discussions on the issue of variability, we reveal an additional dimension of concern: LLMs may perform MCQA by selecting the least incorrect option rather than distinctly correct. This observation suggests that LLMs might regard multiple options as correct, which could undermine the reliability of MCQA as a metric for evaluating LLMs. To address this challenge, we introduce an enhanced dataset augmentation method for MCQA, termed MCQA+, to provide a more accurate reflection of the model performance, thereby highlighting the necessity for more sophisticated evaluation mechanisms in the assessment of LLM capabilities.

1 Introduction

The emergence of Large Language Models (LLMs), such as GPT-3 (Brown et al., 2020), LLaMA (Touvron et al., 2023a), and ChatGPT (OpenAI, 2022), represents a paradigm shift in the field of Natural Language Processing (NLP). These models have exhibited exceptional proficiency in mimicking human-like textual outputs, establishing their significance across various applications. However, the challenge of effectively evaluating LLMs persists (Chang et al., 2023). This difficulty arises from the intricate nature of natural language. Conventional evaluation metrics for generative tasks often fall short in accurately assessing the performance of LLMs, since most LLMs can gen-

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erate text contextually rich and coherent (Thoppilan et al., 2022), complicating the assessment of the outputs through merely quantitative evaluation based on text matching such as BLEU (Papineni et al., 2002) and ROUGE (Lin, 2004).

Multiple-Choice Question Answering (MCQA) is a fundamental format for various tasks in NLP, such as commonsense reasoning (Talmor et al., 2019; Sap et al., 2019; Zellers et al., 2018), reading comprehension (Lai et al., 2017; Huang et al., 2019) and cloze-style tasks (Zellers et al., 2019; Mostafazadeh et al., 2016). Each MCQA instance comprises a question paired with several answer options, requiring models to identify the correct response as depicted in Figure 1. As a non-subjective metric, MCQA serves as a prominent automatic evaluation method with accuracy as an evaluation metric for numerous LLMs to test for the commonsense knowledge or knowledge for specific domain (Gao et al., 2021; Touvron et al., 2023a; OpenAI et al., 2023).

Question: Where does the sun rise? Option: (A) East (B) West (C) North (D) South

Correct option: Ease	Incorrect options: West, Nort	h, South
Option Ranking	P(East Where does the sun rise?) = 0.96
Symbol Ranking	P(A Where does the sun rise?)	= 0.96

Figure 1: An MCQA example and ranking strategies.

Despite the advanced performance of LLMs on the accuracy of MCQA-format benchmarks like MMLU (Hendrycks et al., 2021), previous studies have discussed a key challenge that persists in evaluating LLMs is maintaining *invariability* in responses when confronted with different orders of answer choices for a same question (Robinson and Wingate, 2022; Wang et al., 2023; Zheng et al., 2023), which underscores an issue that the accuracy of MCQA-format tasks may not reflect the

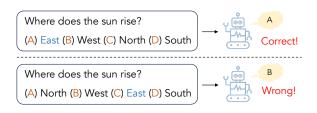


Figure 2: A case for variability issue of LLMs.

authentic capability of LLMs as an example in Figure 2. However, the above phenomenon may not be the *only* issue in the evaluation of LLMs with MCQA-format questions.

To eliminate the potential impact of variability in model responses, we begin by filtering a dataset, denoted as \mathcal{D} , to extract a subset $\mathcal{D}^{\blacklozenge}$, which contains instances where the LLMs can consistently predict the correct answer across all permutations of the answer options, thereby demonstrating invariability. Following this, we conduct a comprehensive experimental analysis using various configurations derived from the original MCQs in $\mathcal{D}^{\blacklozenge}$. Our experimental results indicate that while LLMs often select the most correct answer, they may also regard other options as correct to some extent. Consequently, evaluating LLM performance solely based on MCQA can produce ambiguous results. This newly identified issue prompts a reconsideration of the suitability of MCQA as a reliable metric for LLM evaluation and offers a possible explanation for the observed differences in LLM performance on generative versus discriminative tasks (West et al., 2024).

To address this issue, which is inherently difficult to resolve, we propose an augmentation of the MCQA dataset, termed MCQA+, which introduces variations of the original MCQs and is designed to more accurately reflect LLM capabilities. Empirical findings demonstrate that LLM performance on the MCQA+ dataset is significantly lower than on the original MCQA dataset, indicating that MCQA+ can serve as a more effective benchmark for developing robust and adaptable NLP models. This augmentation may ultimately contribute to narrowing the gap between machine learning models and human-like understanding and reasoning in NLP tasks.

In summary, our contributions are as follows:

 We identify a novel issue with MCQA-based evaluation of LLMs, beyond the variability in answer options, where LLMs may approach MCQA by selecting the option that is "least incorrect".

- This issue implies that while LLMs consistently select the correct answer for specific MCQs, they may also incorrectly identify certain other options as correct under different circumstances.
- We introduce a dataset augmentation method, expanding the original MCQA into MCQA+, which more accurately reveals LLM capacities and performance.

2 Related Work

LLMs (Brown et al., 2020; Touvron et al., 2023b; OpenAI, 2022) have led the research of NLP into a new era. Recent advancements, including supervised fine-tuning and alignment with human values (Ouyang et al., 2022; Chung et al., 2022; Bai et al., 2022), have further augmented the capabilities of LLMs, enabling them to adhere more closely to human instructions and ethical considerations. Nonetheless, challenges persist since LLMs may show variability in the model responses, especially under the scenarios of MCQA. Robinson and Wingate (2022) termed the ability to associate the answer options and corresponding symbols as multiple choice symbol binding (MCSB) and proved that the MCSB ability varied significantly by models. Additionally, Wang et al. (2023) revealed vulnerabilities in the ranking of candidate responses, which could be manipulated by altering the presentation order. Zheng et al. (2023) investigated the token selection bias in LLMs. Kadavath et al. (2022) explored the reliability of the LLM performance and calibration, focusing exclusively on a set of private models under the MCQA settings. Recently, West et al. (2024) examined the performance gap between generative and discriminative tasks in LLMs. Pezeshkpour and Hruschka (2024) proposed two calibration techniques to reduce variability in LLM responses. Previous work has focused on mitigating bias in answer options or developing techniques to ensure that LLMs exhibit consistency across different orders of options. A common thread among these studies is the belief that if LLMs can demonstrate robustness to variations in the order of answer options, their predictive reliability can be improved. However, our research identifies another limitation: even if LLMs consistently predict the correct answer across varied option orders, they may still struggle to accurately

Original MCQ Question: Where does the sun rise?	(A) East (B) West (C) North (D) South <i>correct</i>		
MCQ-derived True-or-False questions True or False: with the correct option True or False: with the incorrect options	Question: Is it true that the sun rises from the east? Question: Is it true that the sun rises from the west? Question: Is it true that the sun rises from the north? Question: Is it true that the sun rises from the south?		
MCQs with None of the above options Question: Where does the sun rise?	(A) West (B) North (C) South (D) None of the above		

Figure 3: A case of an original MCQ, True-or-false questions derived from the MCQ and the MCQ with the correct options replaced by "None of the above".

answer questions derived from the original MCQ because LLMs may perform MCQA by selecting which is the least incorrect.

3 Does Invariability Imply Reliability?

As discussed previously, prior research has demonstrated that LLMs may exhibit variability in their responses across different permutations of answer options in MCQs (Robinson and Wingate, 2022; Pezeshkpour and Hruschka, 2024). Various techniques have been explored to ensure that LLMs exhibit invariability in response to such permutations, with the assumption that invariability could serve as a proxy for model reliability in MCQ tasks. However, this raises an important question: does invariability truly equate to reliability?

3.1 Models and Datasets

In this study, we focus on evaluating several prominent generative models that have garnered significant attention within both academic and public domains. These include LLaMA models (Touvron et al., 2023b) (LLaMA 3 8B, LLaMA 2 13B¹, LLaMA 3 70B), Mixtral (Jiang et al., 2024) (Mixtral $8 \times 7B$), and ChatGPT (OpenAI, 2022) (ChatGPT-3.5, ChatGPT-4o, and ChatGPT-4o-mini). For the datasets, we sample from two widely recognized benchmarks: the first is MMLU (Hendrycks et al., 2021), a general-domain benchmark widely used in MCQA evaluation for LLMs; the second is MedMCQA (Pal et al., 2022), which is specific to the medical domain and re-

¹LLaMA 3 currently comprises models with 8B and 70B parameters

quires extensive domain-specific knowledge, presenting a significant challenge for most LLMs.

3.2 Invariability Dataset Preparation

Due to our work aiming to demonstrate certain deficiencies in using MCQs to test LLMs, and to facilitate subsequent experiments, we first conduct tests on MCQs with option permutations on subsets of MMLU and MedMCQA datasets with questions testing for knowledge instead of reasoning (like math). Then, we filter out the subsets MMLU⁴ and MedMCQA⁴ where the LLMs show invariability.

3.3 Transforming to True-or-False Format

We transform the original MCQAs in only MMLU^{\blacklozenge} and MedMCQA^{\blacklozenge} into a True-or-False (T/F) format to explore how the LLMs behave on the questions that they have predicted correctly with invariability in MCQA-format. For every MCQA instance, we generate T/F-format questions, including one with the correct option (T/F: correct) and other questions with the incorrect options (T/F: incorrect) ² as depicted in Figure 3, anticipating that the LLMs will respond accurately with "Yes" and "No" respectively.

Table 1 presents an analysis of LLM performance on T/F questions. If consistency were a reliable indicator of accuracy, we would expect LLMs to achieve near-perfect performance in this format on both the "T/F: correct" and "T/F: incorrect" datasets. In the few-shot scenario, we provide the LLMs with two examples as demonstrations, one with the answer "correct" and the other with

²"None of the above"-like options are not transformed into T/F format.

		(0-shot		w-shot
		MMLU♦	MedMCQA◆	MMLU♦	MedMCQA◆
LLaMA 3 8B	T/F: correct	93.3	92.4	95.1	93.0
LLaWIA 5 OD	T/F: incorrect	43.7	52.7	48.9	55.5
LLaMA 2 13B	T/F: correct	70.3	70.5	73.1	71.8
LLaMA 2 15D	T/F: incorrect	52.5	55.8	55.4	55.6
LLaMA 3 70B	T/F: correct	97.2	92.3	97.8	92.8
LLaWIA 5 70D	T/F: incorrect	41.7	42.3	44.1	36.8
Mixtral 8×7B	T/F: correct	90.7	83.2	91.2	82.7
	T/F: incorrect	58.8	54.7	59.2	55.5
ChatGPT-3.5	T/F: correct	87.6	76.6	87.8	75.6
Chalor 1-5.5	T/F: incorrect	68.5	69.9	68.9	71.6
ChatGPT-4o-mini	T/F: correct	93.6	89.0	94.1	88.7
ChalGP1-40-mini	T/F: incorrect	65.9	72.4	65.2	73.1
ChatGPT-40	T/F: correct	95.1	88.7	96.4	89.9
ChatGP 1-40	T/F: incorrect	73.0	80.2	70.2	80.4

Table 1: Accuracy of LLMs on the True-or-False questions derived from MCQs. ♦ means the subsets of datasets where LLMs have answered correctly across all re-ordered answer options of the MCQs.

Table 2: Accuracy of LLMs on the MCQA^{\diamond} datasets with the correct options replaced with the "None of the Above" option. \diamond denotes the subsets of datasets where LLMs have shown invariability across re-ordered answer options before the alteration of "None of the above".

	0)-shot	fe	w-shot
	MMLU♦	MedMCQA◆	MMLU♦	MedMCQA◆
LLaMA 3 8B	18.3	20.6	19.1	20.4
LLaMA 2 13B	17.2	12.3	6.7	0.0
LLaMA 3 70B	22.6	24.9	31.3	29.8
Mixtral 8×7B	24.7	31.1	40.3	30.1
ChatGPT-3.5	23.7	36.0	48.5	41.7
ChatGPT-4o-mini	43.6	42.6	50.6	51.4
ChatGPT-40	60.3	60.1	68.6	67.5

that of "incorrect". In practice, LLMs demonstrate varying levels of accuracy on the "True/False: correct" datasets, ranging from 70.3% to 96.4%. This suggests that LLMs can generally perform well on T/F questions derived from MCQs with correct options. However, a notable performance decline occurs when the T/F questions include incorrect options. For instance, LLaMA 3 70B achieves an accuracy as low as 36.8% on the "T/F: incorrect" datasets based on MedMCQA⁴. Similar trends are observed across almost all tested LLMs. This highlights a critical limitation: while LLMs tend to be consistent when handling questions with both MCQA and T/F formats with correct options, they frequently misclassify statements containing incorrect options as correct.

3.4 "None of the Above" Options

Kadavath et al. (2022) examined the potential impact of "None of the above" options on certain close-source LLMs with the entire MCQA datasets, without considering the confounding factor of variability. In this study, we extend the analysis to a broader range of LLMs, focusing exclusively on variability-free sub-datasets, that are MMLU⁴ and MedMCQA[♦], as illustrated in Figure 3. For the few-shot scenarios, demonstrations involve MCQs with the correct answer of "None of the above". As presented in Table 2, the substitution of correct options with the "None of the above" leads to a substantial decline in model performance. With the exception of scenarios involving ChatGPT-40 and ChatGPT-4o-mini, the LLMs consistently fail to select the "None of the Above" option in place of the



Figure 4: Illustration of the hypothesis: LLMs may perform MCQA by selecting the least incorrect option.

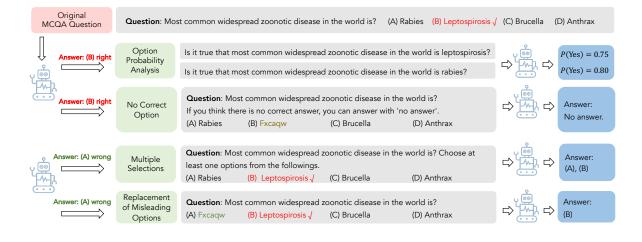


Figure 5: The validation experiments consist of (1) "Option probability analysis" (2) "No correct option" on the MCQA^{\diamond}, along with (3) "Multiple selections" and (4) "Replacement of misleading options" on the original MCQs where the LLMs made incorrect predictions. (1) assesses the confidence of LLMs when handling T/F questions with correct and incorrect answer options from the MCQA^{\diamond} datasets; (2) assesses whether LLMs can respond with "no answer" when presented with MCQs that do not contain correct options; (3) prompts the LLMs to selected all the answers options they consider correct in the MCQs where they previously made incorrect prediction. (4) replaces the incorrect options previously chosen by the model with non-semantic tokens.

correct answer, with accuracy not exceeding 48.5% across all other scenarios. Even the ChatGPT-40 model demonstrates a failure rate exceeding 31% on the MCQA^{\bullet} datasets.

3.5 Analysis

Despite the invariability in LLM performance on MCQs, modifying the MCQA datasets to include (1) T/F questions derived from incorrect options in the original MCQs, and (2) scenarios where the correct option is replaced by "None of the Above," results in a pronounced performance decline. This finding highlights a critical issue: the invariability exhibited by LLMs in handling multiple-choice questions does not necessarily signify reliability. Specifically, the models demonstrate unexpected behavior when confronted with questions involving options other than the correct answer options, raising concerns about the robustness of their decision-making processes in such contexts.

4 LLMs May Do MCQA by Selecting Which Is the Least Incorrect

Through our experiments with modified datasets only with the incorrect options in the original MCQs, we have shown that invariability in LLM responses does not necessarily equate to reliability. Based on these observations, we propose the following hypothesis:

While LLMs demonstrate invariability on specific MCQs with a consistent answer option, they may not regard this option as uniquely correct. Rather, LLMs may treat the selected option as the most accurate among the choices, without dismissing the potential partial correctness of other, incorrect options—albeit to a lesser degree than the chosen one.

which is visually illustrated in Figure 4.

If this hypothesis holds true, it suggests that LLMs may recognize some of the unselected options as partially correct. This could offer a plausible explanation for the observed model behavior in the aforementioned experiments. To further inves-

Table 3: Confidence of answer options in MCQA tasks with open-source LLMs. $C_{correct}$: mean confidence of the correct options. $C_{incorrect}$: mean confidence of the incorrect options that score with the highest confidence. R_c : relative confidence score. \blacklozenge denotes the experiments on the sub-datasets where the LLMs predict correctly with the original MCQA settings.

	LLaMA 3 8B		LLaMA 2 13B		LLaMA 3 70B		Mixtral 8×7B	
	MMLU♦	MedMCQA♦	MMLU♦	MedMCQA♦	MMLU♦	MedMCQA♦	MMLU♦	MedMCQA♦
C _{correct}	16.4	18.7	35.0	36.0	23.6	25.5	31.2	34.6
$C_{\mathit{incorrect}^*}$	16.3	18.5	32.5	30.1	20.3	21.9	29.1	33.1
R_c	99.4%	98.9%	92.9%	83.6%	86.0%	85.9%	93.3%	95.7%

Table 4: Ratio of the instances where the LLMs can generate "no answer" on the MCQs with no correct option under the few-shot settings.

	MMLU♦	MedMCQA♦
ChatGPT 4o-mini	32.8	32.6
ChatGPT 40	59.5	60.0

tigate this phenomenon, we explore the behavior of the models from the following four perspectives, as depicted in Figure 5.

4.1 Option Probability Analysis

Leveraging the MMLU[♦] and MedMCQA[♦] datasets, we investigate the confidence of LLMs by examining the distribution of token probabilities for answer option tokens, as discussed in Chen et al. (2023). To do this, we convert MCQs into T/F format as illustrated in Figure 5. The confidence scores for each answer option are derived based on the "yes" or "no" token probabilities assigned by the LLMs. For T/F questions that include the correct answer options from the original MCQs, we compute the confidence score C_{correct} using instances where the LLMs made correct predictions. This score quantifies the degree of confidence the LLMs exhibit when recognizing a claim with the correct option as accurate. Conversely, for T/F questions containing incorrect answer options from the MCQs, we compute the confidence score Cincorrect based on cases where the LLMs made incorrect predictions. This score measures how confidently the LLMs mistakenly identify a claim with an incorrect option as correct. For a specific MCQ, we consider the incorrect* option with the highest confidence in corresponding T/F questions for Cincorrect*.

$$\mathbf{C}_{correct} = \frac{1}{N} \sum_{z \cdot \mathbf{y}_{es"} > z \cdot \mathbf{n}_{0"}} \frac{e^{z \cdot \mathbf{y}_{es"}}}{\sum_{t \in V} e^{z_t}}$$

$$\mathbf{C}_{incorrect} = \frac{1}{M} \sum_{z``no`` > z``yes``} \frac{e^{z``no``}}{\sum_{t \in V} e^{z_t}}$$

where z_t is the logit for each token t in the vocabulary, and V denotes the full vocabulary set. Nand M is the number of corresponding questions.

Table 3 demonstrates the confidence of LLMs for the correct options ($C_{correct}$) and the incorrect^{*} options ($C_{incorrect^*}$), along with the relative confidence scores. The experimental results show that while LLMs consistently consider the incorrect^{*} options as less correct than the correct options, demonstrated by all relative confidence being below 100%, the incorrect^{*} options still achieve substantial confidence ranging from 83.6% to 99.4% of those for the correct options. Consequently, despite invariability, LLMs may still perceive certain incorrect options as correct, though to a lesser extent compared to the correct ones.

4.2 MCQA with No Correct Option

In our previously described scenarios for evaluating LLMs on MCQs, there has always been a correct answer among the candidate options. However, when no correct answer is present, we expect LLMs to recognize that the question is flawed. To guide the model in such cases, we prompt the LLMs with "If you think there is no correct answer, you can respond with 'no answer'," to observe whether the model generates a "no answer" response. Empirically, even large-scale open-source models such as LLaMA 3 70B struggle to effectively follow this instruction. Consequently, our analysis focuses on the ChatGPT-4 series models. Using the MCQA[◆] dataset, where the models exhibit invariability, we replace the correct options with non-semantic tokens. As shown in Table 4, with appropriately designed prompts, ChatGPT-4o successfully identifies that there is no correct answer in approximately 60% of the MCQs. However, for the remaining

Table 5: Experiments on the altered MCQA datasets with multiple selections. $Recall_{correct}$: recall of the correct options. $Recall_{misleading}$: recall of the misleading options (the incorrect options LLMs have chosen). \dagger denotes the subsets where the LLMs have generated incorrect answers on the original MCQA datasets.

	M	MLU^{\dagger}	Med	MCQA [†]
	Recall _{correct} Recall _{misleading}		Recall _{correct}	Recall _{misleading}
LLaMA 3 8B	85.1	70.1	82.3	74.2
LLaMA 2 13B	92.5	67.5	78.9	70.3
LLaMA 3 70B	94.2	72.2	84.0	80.1
Mixtral 8×7B	91.5	76.4	84.6	85.4
ChatGPT-3.5	85.1	66.7	81.3	69.7
ChatGPT-4o-mini	85.0	89.2	84.4	91.6
ChatGPT-40	89.9	90.8	83.2	92.1

40% of the questions, it still selects one option as correct, indicating that LLMs do not fully recognize all incorrect options as incorrect.

4.3 MCQA with Multiple Selections

For the MCQA datasets involved in this study, LLMs are tasked with identifying only one correct option per MCQ. We collect the instances where LLMs incorrectly predict the answers, denoted as $MMLU^{\dagger}$ and $MedMCQA^{\dagger}$. In the above instances, the incorrect options which LLMs have regarded as the correct ones mistakenly are defined as misleading options. Then, LLMs are prompted to recognize all plausible correct options among all answer options. Table 5 showcases the recall for the correct and misleading options for the instances where LLMs render multiple selections. The results reveal that the correct options are included in the selections in over 78.9% of instances, reaching up to 94.2%. This indicates that the LLMs also recognize the correct options as correct but less correct than the misleading ones.

4.4 MCQA with the Misleading Option Replacement

Apart from the multi-selection scenario, we explore the impact of replacing misleading options with arbitrary non-semantic tokens in MMLU[†] and MedMCQA[†]. Table 6 elucidates that the LLMs correctly identify the correct options in 30.9% to 58.0% of instances, highlighting the influence of misleading options on their predictions. For cases where LLMs continue to make incorrect predictions, a fundamental deficit in relevant knowledge likely underpins the LLM incapability to generate the correct answers.

Table 6: Ratio of the instances where the LLMs turn to predict correctly with the replacement of misleading options (the incorrect options LLMs have chosen).

	MMLU [†]	MedMCQA [†]
LLaMA 3 8B	42.1	30.9
LLaMA 2 13B	58.0	41.0
LLaMA 3 70B	46.3	41.1
Mixtral 8×7B	50.4	34.8
ChatGPT-3.5	53.6	44.5
ChatGPT-4o-mini	39.7	41.2
ChatGPT-40	41.1	48.6

4.5 Summary

The analyses conducted across the four experimental scenarios provide substantial support for the validity of the proposed hypothesis. This leads to a critical observation that highlights a fundamental limitation of using MCQA-based evaluations to assess the capabilities of LLMs: *In the context of MCQA*, while LLMs may select the correct answer, there remains a possibility that they also attribute correctness to other, incorrect options.

5 MCQA+ for Robust Evaluation

Dataset Preparation Experimental analyses have revealed significant limitations in using the MCQA benchmark to evaluate LLMs, highlighting that LLMs may consider options they did not select in MCQs as correct. To address this, we propose an augmentation approach based on the original MCQA dataset, informed by the empirical findings from the above experiments. Each MCQ is transformed into one of the following settings: (a) Original MCQs; (b) MCQs with re-ordered answer options; (c) True-or-False questions derived from correct answer options; (d) True-or-False questions derived from incorrect answer options; (e) MCQs

	MMLU			MedMCQA				
	MCQA	MCQA+	MCQA+hard	$MCQA+(\times 1)$	MCQA	MCQA+	MCQA+hard	$MCQA+(\times 1)$
LLaMA 3 8B	75.1	56.8	40.5	58.4	47.9	36.3	24.4	34.1
LLaMA 2 13B	72.7	46.1	21.2	45.3	43.2	38.8	16.5	40.0
LLaMA 3 70B	78.9	60.2	46.8	57.1	53.1	42.8	29.1	44.4
Mixtral 8×7B	71.2	58.6	43.7	58.5	51.4	43.5	28.7	42.7
ChatGPT-3.5	65.0	63.2	57.8	64.0	56.9	53.9	49.6	54.1
ChatGPT-4o-mini	79.0	70.9	63.0	72.4	68.3	64.4	60.2	63.8
ChatGPT-40	82.4	80.7	73.1	79.7	72.7	69.7	64.0	71.3

Table 7: Model performance on the original MCQA, MCQA+, MCQA+ hard and MCQA+ (×1) datasets.

where the correct options are replaced with "None of the above"; and (f) MCQs with no correct options, where LLMs are expected to generate "no answer" as the response. Using these settings, we propose three dataset augmentation approaches: (1) **MCQA+**: Encompasses all of the above settings; (2) **MCQA+**^{hard}: Includes only the settings (b, d, e, f), serving as a much more challenging benchmark for LLMs. (3) **MCQA+** (×1): Samples one question from the MCQA+ settings as an efficient approximation to MCQA+.

The mean accuracy across all settings is adopted as the evaluation metric for LLMs. For settings with multiple questions (e.g., (b)), accuracy_b is measured as the mean accuracy across all questions in setting (b). Table 7 illustrates the comparative performance of LLMs on the original MCQA dataset, MCQA+, MCQA+hard, and MCQA+ $(\times 1)$. Performance on the MCQA+ dataset shows a significant decline across all LLMs compared to the original MCQA dataset. For example, accuracy for LLaMA 3 8B dropped from 75.1% to 56.8% on the MMLU dataset. Performance on the MCQA+hard benchmark is even lower, likely for reasons discussed in Section 4. Even ChatGPT-40 experienced a performance decline of 9.3% from the original MCQA to MCQA+hard on the MMLU dataset.

Although MCQA+ and MCQA+^{hard} provide a more accurate reflection of LLM capabilities, they entail significantly higher computational costs compared to the original MCQA. Therefore, MCQA+ (×1), which samples from MCQA+ for each MCQ, requires no additional computational cost compared to the original MCQA. As shown in Table 7, this cost-efficient approach still effectively reveals the true capabilities of LLMs.

Discussion The MCQA+ strategy offers an efficient and refined approach to augmenting existing MCQ datasets, enabling a more accurate as-

sessment of model capability. However, ensuring consistent performance across tasks not addressed by MCQA+, such as generative tasks, remains a challenge. Based on the results of this study, we hypothesize that the observed performance decline may be linked to the training strategies of LLMs in generative tasks during pre-training and instructiontuning, that is predicting the next token based on the ranking of probability. LLMs have been only instructed to choose the best options but not to treat those options as exclusively correct. While reinforcement learning aligns the model's outputs with human preferences, it does not fully resolve the issue where incorrect options might still receive high probabilities in different contexts. This could explain the discrepancies in model performance between discriminative and generative tasks, as noted by West et al. (2024). As such, the reliability of evaluating LLMs using MCQs necessitates further scrutiny and attention.

6 Conclusion

In this study, we investigated the limitations of using MCQA as a benchmark for evaluating the performance of LLMs through a comprehensive series of experiments. Our findings suggest that LLMs may not always select the distinctly correct option, but instead opt for the least incorrect option. This behavior raises concerns about the robustness and reliability of MCQA-based evaluations. To address these issues, we proposed the MCQA+ dataset augmentation method, which provides a more refined evaluation framework by challenging LLMs to demonstrate a deeper level of understanding. Our work underscores the importance of continued efforts to develop more comprehensive evaluation methodologies for LLMs, ensuring that their true capabilities are accurately reflected, not only in discriminative tasks, such as MCQA but also in broader, more complex contexts.

Limitations

In this study, we analyzed a probable issue that LLMs may face when answering MCQs. Building on previous research on the variability of large models, we conducted experiments demonstrating that although LLMs can achieve impressive results on MCQA benchmarks, their treatment of incorrect options may be ambiguous, potentially recognizing incorrect options in other contexts. This issue may stem from negative impacts introduced by different stages of the training objectives of LLMs, such as instruction-tuning and RL-based alignment, presenting a broader challenge for the entire NLP field. Therefore, we propose a method to improve the reliability of model evaluations through diversity testing, which represents a trade-off between efficiency and accuracy, without fundamentally addressing the core challenges of evaluating LLMs based on MCQs. We aim to draw attention from the community to the potential long-term impacts of this issue and to collaboratively work towards resolving it.

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