Large Language Models Can Be More Robust Multiple Choice Selectors Through Attention Intervention

Anonymous ACL submission

Abstract

Multiple choice question (MCQ) is a common task for evaluating large language models (LLMs). LLMs' performance on MCQ is often affected by various biases. Previous research has extensively examined the impact of **inherent option bias** on MCQ predictions, where this bias refers to a preference for a specific option ID token introduced during the model's training. However, in an in-context learning scenario, few-shot prompting can also introduce a form of bias, known as **context option bias**. For example, when all demonstration answers are consistently option `A`, LLMs may predict `A` regardless of the question. Context option bias can significantly degrade LLMs' performance. To observe LLMs' behavior under context option bias, we use demonstrations with obvious bias to amplify the effect. The results indicate that certain attention heads in LLMs are particularly sensitive to context option bias. Motivated by this observation, we propose our approach, CoLo, to address this issue. CoLo first compares outputs from ordinary and biased demonstrations and localizes attention heads sensitive to context option bias through sequential interventions. Then, we propose an attention scaling-based method to intervene in the identified attention heads during the inference stage, thereby mitigating the impact of context option bias on the LLMs' predictions. Experimental results show that CoLo alleviates context option bias and improves LLMs' robustness on MCQ tasks.

1 Introduction

Multiple-choice question (MCQ) is a common type of question-and-answer format in daily life and is also a common method used in the field of natural language processing to test the generalization ability of large language models (LLMs). There exist benchmarks and datasets specifically designed, spanning a variety of fields(Hendrycks et al., 2021; Talmor et al., 2019; Clark et al., 2018). We hope LLMs can well understand the question and choose the most appropriate answer from all options. For this purpose, many efforts have been made and few-shot in-context learning has been shown to be one of the effective methods. It provides some demonstrations before the question as prompts and can largely improve an LLM's performance on MCQs.

Despite the above efforts, LLMs are still affected by certain biases and yield unexpected answers. Previous works(Wang et al., 2024b; Pezeshkpour and Hruschka, 2024; Zheng et al., 2023) have investigated several **inherent option bias** of LLMs. For example, experiments indicate that `gpt-3.5-turbo` tends to prefer option `A`, and using prompt-based debiasing methods shows unsatisfactory results (Zheng et al., 2023). However, bias introduced by context, referred to as **context option bias**, has not been carefully studied.

Intuitively, if all demonstrations' answers happen to be `A`, then LLMs will also prefer to predict `A` no matter what question is given. In contrast, if answers for demonstrations do not show too much preference to a certain option, the model will be more inclined to choose the correct answer. The results indicate that context option bias has an impact on an LLM's prediction. Figure 1 provides evidence, that is, when given demonstrations all with answers `A`, LLMs will predict much more `A` than with ordinary demonstrations[1].

However, demonstrations with evenly distributed options still introduce context option bias towards certain answer choices. We observed that demonstrations with evenly distributed answer options significantly influence the model's predictions. For instance, in the 5-shot `Gemma-2B` model, we modified the sequence of options in the MMLU dataset demonstrations to two different configurations:

[1]Ordinary demonstrations mean those with the same questions as biased demonstrations but do not show preference to a certain option. We implement this by swapping options in demonstration questions.

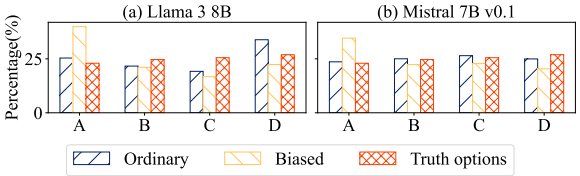


Figure 1: Biased context is constructed by few shot through answer is always A. We counted the predictions of some LLMs on MMLU dataset(Hendrycks et al., 2021)

A-B-C-D-A and D-C-B-A-D. Compared to the random sequence demonstration, the total number of A selections in configuration A-B-C-D-A decreased by 33%, while the total number of D selections in configuration D-C-B-A-D decreased by 47%. We speculate that this behavior arises because the model tends to avoid selecting the same option consecutively, believing that the probability of repeated occurrences of the same option is low, thus introducing a bias in answering questions with similar option distributions.

To better excavate the reasons behind this problem and resolve it, we deliberately construct some demonstrations with obvious context option bias and compare the model's behavior under these conditions with that under ordinary demonstrations. The experiments find that even with simple option swaps in demonstrations, the attention map's distribution in an LLM varies significantly. This observation inspires us to test the attention distribution under conditions with obvious biased demonstrations, identify the attention heads that are more sensitive to context option bias, and intervene accordingly to mitigate the impact of context option bias on the model behavior.

Following this motivation, we propose our method CoLo to localize and mitigate context option bias in LLMs. Particularly, (1) CoLo first takes samples with biased demonstrations as input to obtain the LLM's predictions, which we refer to as biased answers. (2) We then intervene in different layers and different attention heads within each layer. If the LLM's predictions after the intervention is more inclined towards the correct or ordinary answers, it indicates that the corresponding attention head is sensitive to context option bias and likely to lead the model to biased answers. (3) CoLo selects a set of attention heads that are most sensitive to context option bias and applies interventions to these heads simultaneously during the subsequent inference stage.

Extensive experiments show that for MCQ in an in-context learning scenario, when there is context option bias in demonstrations, our method can effectively mitigate the impact of the bias, improving an LLMs' accuracy on MCQ to a level similar to that with ordinary demonstrations without affecting other LLMs' abilities. Besides, the identified attention heads demonstrate powerful generalization across datasets and tasks. That is, for a certain model, the attention heads identified with one dataset also applies to other datasets. More importantly, even when the demonstrations look unbiased, applying our proposed intervention can also further enhance the model's accuracy. We assume it is because seemingly unbiased demonstrations may also contain some context option bias that are imperceptible, thereby affecting the model's predictions.

It is worth summarizing our contributions as follows:

- We propose a method to identify attention heads that are sensitive to context option bias in multiple-choice questions under an in-context learning scenario.
- Our attention scaling-based method mitigates the impact of context option bias on the LLM's predictions and improves performance without compromising other capabilities.
- Extensive experiments are conducted and the results show the effectiveness of our method.

2 Related work

Inference intervention techniques. Inference intervention comprises various methods designed to modulate the behavior of large-scale models post-training. Commonly employed inference intervention strategies include activation editing(Li et al., 2024b), weight editing(Dai et al., 2022; Meng et al., 2022), guidance vectors(Zou et al., 2023), and alter the output distribution through comparison(Li et al., 2023; Chuang et al., 2024). Our method focuses on modifying the attention distribution by attention scaling, which is a technique that originates from GPT-2(Radford et al., 2019). Contrary to the broader method of global attention scaling of GPT-2, our approach is distinctly less invasive, selectively targeting attention heads that are associated with context option bias. By identifying and scaling the attention heads linked to context option bias, our method effectively mitigates this bias using a significantly smaller dataset, requiring far fewer examples than those needed for reinforcement learning (RL) (Ouyang et al., 2022) and

fine-tuning-based methods (Hu et al., 2022). Our approach to structuring the comparison of specific contexts is analogous to the ICD method(Zhang et al., 2024).

Bias of LLMs. There are various types of biases in LLMs(Gallegos et al., 2024), with option bias being one of the most prominent and actively researched(Zheng et al., 2023; Pezeshkpour and Hruschka, 2024; Wang et al., 2024a; Xue et al., 2024). We argue that option bias is not only introduced during the model training phase, but may also arise through in-context learning. Although in-context learning can significantly enhance the model's task-learning capabilities, it may also introduce negative effects on the model's performance(Turpin et al., 2024). Distinct from post-processing methods like PriDe(Zheng et al., 2023), CoLo intervenes internally within the model to mitigate context option bias without impacting text generation processes, such as Chain of Thought (CoT)(Kojima et al., 2022). This technique requires only a minimal number of samples to identify a general head that responds to biases across various contexts. In contrast, PriDe functions primarily as a pre-processing technology, necessitating recalibration of bias each time the context changes, and it often performs sub-optimally in scenarios with limited data samples.

3 Method

3.1 Overview

During the LLM's inference, different attention heads perform distinct functions(Zhang and Nanda, 2024; Gould et al., 2024). While some attention heads may correspond to option bias, it is not feasible to directly identify which ones specifically linked to option bias during inference. To identify attention heads strongly associated with option bias, it is necessary to amplify the presence of the bias. Due to the difficulty of directly manipulating the model's inherent option bias, we choose to amplify context option bias by constructing biased demonstrations. We can obtain the state output of the model in these two different situations $state_b$ and $state_o$ corresponding to biased and ordinary demonstrations, respectively. The gap between the two states arises from the amplification of the context option bias. We employ an intervention function f that acts on specific attention heads to reduce the state difference between $state_b$ and $state_o$. The extent of this reduction is compared to evaluate the correlation strength between these attention heads

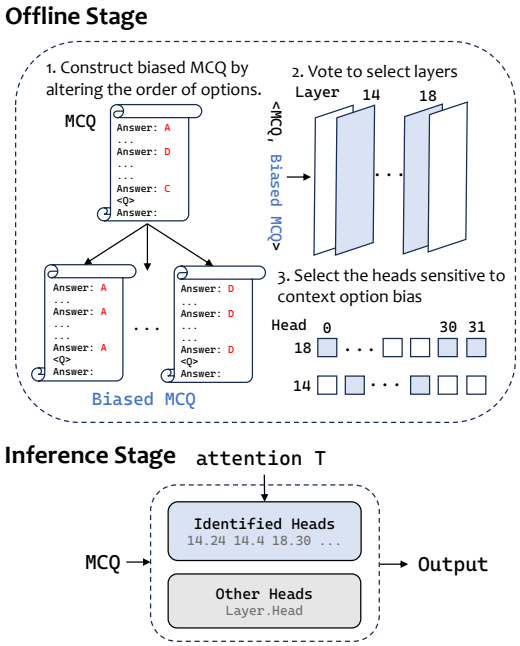


Figure 2: The overall of CoLo, encompassing offline heads identification and the inference phase.

and context option bias, allowing us to select the most relevant set of attention heads. The algorithm flow is described in detail in Section 3.2

After identifying attention heads strongly associated with context option bias, different intervention methods are employed to modify the attention distribution of these heads and mitigate context option bias. We describe the intervention methods utilized in Section 3.3.

3.2 Localizing attention heads

We amplify context option bias by swapping options in the demonstration. Specifically, we consolidate all correct answers into a single option, such as always setting the correct answer to A. This creates a biased demonstration, denoted as d_b, while the ordinary demonstration is d_o, and the problem is represented by q. Each sample includes the true label y_t. We randomly select N samples to create the set used for localizing attention heads, denoted as $\mathcal{D} = (d_o^i, d_b^i, q^i, y_t^i)_{i=1}^N$.

We describe the general pattern by which large models accomplish selection tasks as:

$$p(y|d, q) = \text{softmax}(\{\phi(g)_c, c \in \mathcal{C}\}), \quad (1)$$

where $\mathcal{C}$ represents the token ID of the option after tokenizer encoding, the vocabulary head $\phi(\cdot)$ predicts the probability of the choice token, g is the output of the last layer of the model.

The probability of the correct option of the model under biased demonstration is $p(y_t|d_b, q)$, and under ordinary demonstration is $p(y_t|d_o, q)$.

Choose the option with the highest probability as the answer y:

$$y = y_c, \underset{c}{\operatorname{argmax}}\, p(y_c|d, q), \tag{2}$$

thus, we can obtain y_o through d_o. The probability of the model output option after intervention function f will change. The probability distribution after intervention function f is recorded as $p'(y|d, q)$. Particularly, $p_l'^h(y|d, q)$ represents probability distribution after intervention function f act on the h-th attention head in the l-th transformer decoder block.

We define E to quantify the effectiveness of the intervention function, described as:

$$E = p'(y|d_b, q) - p(y|d_b, q), y \in \{y_o, y_t\}, \tag{3}$$

where $y \in \{y_o, y_t\}$ represents our expectation that, following the application of the intervention function, the model's output previously influenced by biased demonstrations will either align with the label y_o, corresponding to the output under ordinary demonstrations, or with the true label y_t of the current sample. Another intuitive approach is to use KL divergence to define the effectiveness of the intervention. To this end, we attempted to measure it by calculating the KL divergence between the model's output after the intervention under biased demonstrations and the output from the original, unbiased demonstration, as well as the true label. However, this approach yielded poor results, as detailed in the Appendix G.

By further partitioning the sample dataset $\mathcal{D}$ and conducting multiple rounds of voting, the top K_l layers are selected, followed by the selection of the top K_h heads within each layer based on their E values. The details of the localizing algorithm are provided in Algorithm 1. The rationale for partitioning $\mathcal{D}$ and performing multiple rounds of voting is to mitigate the influence of outliers.

It is essential to emphasize that we first identify the top K_l layers and then select the top K_h heads within these layers. This approach may overlook some heads in lower-ranked layers that could be of greater importance. Although traversing all heads would produce better results, the computational cost is significantly higher. Therefore, we adopt this compromise method to efficiently localize attention heads.

We employ random sampling to partition the sample set and use multiple rounds of voting to identify the top K_l layers. The context option bias present in each sample set is determined during this process. If the identified attention head corresponds to the option bias, its focus should be concentrated on a specific layer and remain robust across samples containing the same context option bias but differing in content. We use the indicator $S \in [0, 1]$ to measure the stability of the identified attention head:

$$S = \sum \frac{cnt_l}{m \times K_l}, l \in \mathcal{L}, \tag{4}$$

The variable cnt represents the number of selections after n rounds of sampling, while m denotes the number of samples in each round. A larger value of S indicates greater concentration and higher effectiveness of the attention head localization strategy.

Algorithm 1 Localizing Attention Heads

Require: Language model, test samples $\mathcal{D} = \{(d_o^i, d_b^i, q^i, y_t^i)\}_{i=1}^N$, rounds number n, sample number of every round $m = N/n$, divide $\mathcal{D}$ into $\{\mathcal{D}_i\}_{i=1}^n$.

Ensure: Model attention heads set to intervene $\mathcal{H}$

```
Initialize decoder layers set L = ∅ and the attention heads set H = ∅   ▷ Initialization
Sample the estimation samples D_e under K and the remaining samples D_r = D\D_e
for D_i ∈ {D_i}_{i=1}^n do
    for l ∈ model.layers do
        for (d_0, d_b, q, y_0) ∈ D_i do
            E_l += p'_l(y_o|d_b, q) + p'_l(y_t|d_b, q)
        end for
        select top K_l layers l_1, ..., l_{K_l} of E_l
    end for
    Find the top K_l layers with the largest scores and add them into L   ▷ Get intervene layers
    cnt_{l_i} ++, i = 1, ..., K_l
end for
select top K_l layers in cnt get L
for l ∈ L do
    for h in l.heads do
        for (d_0, d_b, q, y_t) ∈ D do
            E_l^h += p'^h_l(y_o|d, q) + p'^h_l(y_t|d_b, q)
        end for
        select Top K_h of E_l^h ,add (l, h) to H
    end for
end for
return H
```

3.3 Intervention methods

To establish the notation and context, we briefly outline some fundamental aspects of transformer architecture(Vaswani et al., 2017), a sequence of transformer layers indexed by the variable l.

Throughout the inference process, the token undergoes initial encoding into the embedding space via the embedding layer $x_0 \in \mathbb{R}^{DH}$, initiating the residual stream. We use h to represent head index of each layer.The inputs of multi-head attention(MHA) are $Q_h \in \mathbb{R}^D$, $K_h \in \mathbb{R}^D$, $V_h \in \mathbb{R}^D$, all represented by x_i is obtained through linear operation. In each layer, MHA consists of H heads. Each head is an independent linear operation. After concating the H attention heads, it is processed through $W_o \in \mathbb{R}^{DH \times DH}$ projection gets the result of Multi-head Attention.

$$x_{l+1} = x_l + [head_0^l, \ldots, head_{H-1}^l]W_o \quad (5)$$

Every attention head can be written as:

$$head_h^l = \text{softmax}(f(\frac{Q_h^l K_h^l}{\sqrt{D}})) \times V_h^l, \quad (6)$$

Specifically, in the standard transformer, $f(x) = x$, whereas in our approach, the function f represents an intervention method applied to the attention weights. After preliminary experimental attempt in Appendix D, we guess that attention scaling can better adjust the distribution of attention weight thereby reducing the gap in the final output state of the model. We conducted further experiment with different forms of $f(x)$, such as scaling and zeroing, on specific heads to modify the distribution of attention weights in order to achieve the highest possible E.

Attention scaling is equivalent to adding the temperature coefficient T to the softmax of the attention score. Given the relatively limited exploration of the softmax operation of attention scores in prior work, LLMs conventionally set the temperature parameter to 1 during reasoning.

After identifying the head set $\mathcal{H}$ through Algorithm 1, we intervene in attention head $head_h^l$, $(l, h) \in \mathcal{H}$ during model inference stage.

3.4 Discussion

The overall process of CoLo is shown in the Figure 2. It operates in two stages: offline and inference.

Parameters setting of CoLo. An important set of parameters in CoLo includes $\mathrm{T} \in \mathbb{R}^+$, along with $K_l, K_h, N \in \mathbb{Z}^+$ for localizing. Although no theoretical framework exists to determine the optimal value, we explore these effects through experimental analysis. It is important to emphasize that a small number of additional samples are required in Algorithm 1. Moreover, the dataset can be expanded by modifying the context option bias in the demonstration. For instance, in a four-option multiple-choice question (MCQ), the options can be altered to consist entirely of `A`, `B`, `C`, or `D`, thereby increasing the sample size fourfold. Clearly, a larger number of additional samples contributes to greater stability in the final attention head, a conclusion that we will empirically validate in our experiments. We ultimately decided to use $K_l = 2$, $K_h = 4$, $\mathrm{T} = 0.5$ and $N = 10$ additional samples, expanding the dataset to 40. This serves as the primary parameter setting for our main experiments, and we further discuss the impact of different parameter configurations on CoLo's performance by experiments.

Table 1: Compare different intervention methods f on `Gemma-2B`. Report accuracy improvement δ and localizing stability S.

Methods	Scaling		Setting	
	$\mathrm{T} = 0.5$	$\mathrm{T} = 2$	zero	mean
S	0.8	0.25	0.23	0.35
biased δ(%)	2.22	-0.26	-0.19	0.14
ordinary δ(%)	1.74	0.03	-0.08	0.15

Additional computational overhead of CoLo. In the offline stage, the additional computational overhead introduced by the localization process scales with the number of samples N used for positioning and is also influenced by the number of layers and attention heads in the model. For instance, in the case of the `Gemma-2B` model, this process requires approximately $150N$ additional inferences. A detailed breakdown of the computational overhead is provided in Appendix E. Once the relevant attention heads are identified, CoLo can be applied to other datasets without incurring any further computational overhead during the inference stage.

4 Experiments

In our experiments, we employed LLMs such as Llama(Touvron et al., 2023) and Gemma(Team et al., 2024). Our methodology is also applicable to other LLMs with accessible internal attention weights and computational mechanisms.

4.1 Main results

We select the MMLU (Hendrycks et al., 2021) as our benchmark. Initially, we randomly select 10 samples from this dataset and increase the sample size fourfold to construct $\mathcal{D}$. Utilizing this set, we identify the attention heads by localizing algorithm and then perform intervention, subsequently assess accuracy on the remaining samples.

According to the localizing method we gave, we try different attention intervention functions and find that using attention scaling method has the best effect as shown in Table 1, which is reflected in the most obvious improvement in accuracy on the dataset and higher localizing stability S. This is the same as our guess. The following will provide a detailed introduction to the effects of using attention scaling method as intervention function f on large-scale datasets.

To quantify the mitigation of option bias, we use recall standard deviation (RStd) as an indicator(Zheng et al., 2023), measuring the balance of recall rates across different option IDs. Additionally, we compare the bias mitigation performance and computational overhead with PriDe. Since CoLo operates during inference, it can be combined with PriDe to further reduce option bias.

Additional positioning samples are randomly selected from the development set, and this procedure is repeated five times to mitigate random variability. We report the mean accuracy obtained across these iterations. The experimental results are presented in Table 2. We can conclude that CoLo effectively mitigates option bias, particularly in addressing context option bias. The reduction in RStd indicates a weakening of the model's option bias. Although our primary objective was to reduce option bias, the simultaneous improvement in model accuracy alongside the reduction in RStd further validates the effectiveness of the CoLo. CoLo exhibits better debiasing performance under biased demonstrations than under ordinary demonstrations. This is because the biased demonstration was specifically designed to amplify context option bias, which highlights CoLo' ability to effectively mitigate such biases.

CoLo alleviates option bias under both ordinary demonstration and zero-shot settings. A plausible explanation is that, while the option distribution in the few-shot setting is uniform, it still contains implicit context option bias as shown in Appendix C. Furthermore, the mitigation of option bias in the zero-shot setting may stem from the inclusion of the question as part of the input context, which can introduce additional context option bias. In summary, the reduction of bias and improvement in accuracy observed in both ordinary demonstration and zero-shot scenarios further underscore the significance and broad applicability of the CoLo.

As shown in the Table 2, we compare the performance of CoLo and PriDe on the MMLU dataset and find that combining the two methods achieves a more effective debiasing outcome. Additionally, we compare CoLo and PriDe across different settings, as well as in combination, and present detailed experimental results on domain transfer within MMLU dataset. The results in Appendix H demonstrate that CoLo exhibits distinct advantages in domain transfer.

4.2 Cross-dataset generalization

In order to further illustrate that the head obtained by positioning corresponds to the context option bias of the model, and has a certain degree of robustness, we will apply the attention head obtained through random sampling localizing in MMLU and the intervention method of attention scaling to different fields and different forms tasks , 1) MCQ dataset CMMLU(Li et al., 2024a) and CEVAL(Huang et al., 2023), 2) comprehensive dataset AGIEVAL(Zhong et al., 2024), including multiple choice questions.

The results of the experiment in Table 3 illustrates the improvement in accuracy of MCQ in other fields, which demonstrates the robustness of our approach in mitigating option bias across datasets. Additionally, the stable performance on the TruthfulQA indicates that our intervention method will not cause the model to lose the ability to generate general text, the result in Appendix I.

4.3 Robustness across different format

To validate whether the attention heads selected by CoLo correspond to context option bias, we perform **format transformations** on the original MCQ input format, varying factors such as the number of options, the length of demonstrations, and the format of option identifiers. We aim to verify the following two points:

1. Whether the selected attention heads remain effective in mitigating context option bias after format transformations.
2. Whether the selected attention heads are consistent across different modes.

Table 2: The experimental results of CoLo on the MMLU dataset, along with a comparison to PriDe, encompass evaluations of computational cost, accuracy, and RStd performance. Biased 5 shot is constructed by consistently modifying the standard answers to A.

Model	Cost	Zero Shot		Ordinary (5 shot)		Biased (5 shot)	
		Acc(%)	RStd(%)	Acc(%)	RStd(%)	Acc(%)	RStd(%)
Gemma-2B	1	33.8	21.8	39.9	14.3	38.2	16.1
+CoLo	×1.19	36.2	12.6	41.7	10.8	40.5	7.0
+PriDe(5%)	×1.15	34.1	10.6	41.7	7.5	/	/
+CoLo PriDe(5%)	×1.34	**37.0**	**5.0**	**42.5**	**4.2**	/	/
Gemma-7B	1	61.6	5.2	62.6	5.4	59.3	10.6
+CoLo	×1.29	62.0	5.5	63.4	3.7	61.5	10.9
+PriDe(5%)	×1.15	61.6	5.2	64.4	5.0	/	/
+CoLo PriDe(5%)	×1.44	**62.1**	**1.8**	**64.5**	**3.5**	/	/
Llama2-7B	1	40.9	13.9	45.5	10.7	43.5	11.5
+CoLo	×1.45	43.2	4.4	46.5	**3.8**	45.6	6.2
+PriDe(5%)	×1.15	40.0	5.7	45.6	7.0	/	/
+CoLo PriDe(5%)	×1.60	**43.5**	**4.2**	**46.8**	4.2	/	/
Llama3-8B	1	61.4	13.8	64.6	7.8	60.7	12.0
+CoLo	×1.45	61.9	6.8	64.8	2.3	62.0	8.9
+PriDe(5%)	×1.15	63.6	5.3	**65.0**	2.1	/	/
+CoLo PriDe(5%)	×1.60	63.5	3.9	64.9	**1.9**	/	/

Table 3: Cross-dataset experiments were conducted **using the attention heads obtained from MMLU**, along with ordinary few-shot learning across all datasets. FS stands for 5-shot in table. We use lm-eval-harness(Gao et al., 2024) as the evaluation tool.

Model	CMMLU		CEVAL		AGIEVAL
	ZS	FS	ZS	FS	ZS
Gemma-2B	28.4	30.9	26.5	31.3	31.0
+CoLo	29.8	31.7	29.8	32.2	31.6
Gemma-7B	44.8	48.9	41.2	48.2	38.7
+CoLo	45.4	49.8	44.4	49.4	38.8
Llama2-7B	27.2	32.7	30.0	34.0	32.3
+CoLo	28.2	32.8	30.3	35.0	33.1
Llama3-8B	47.5	50.5	47.9	51.9	37.3
+CoLo	47.2	50.6	49.7	52.0	39.0

For the first point, we selected the model's attention heads based on the sample set $\mathcal{D}$ in the base mode and reported the accuracy improvements across different modes of $\mathcal{D}$. As shown in Figure 3(a), the results indicate that accuracy improves following mode transformation. For the second point is to use different $\mathcal{D}$ after mode transformation to select attention heads. For different modes, the heads selected are similar in Figure 3(b). The result indicates that the attention heads selected through our method is robust to mode transformations.

4.4 What's the optimal parameters of CoLo?

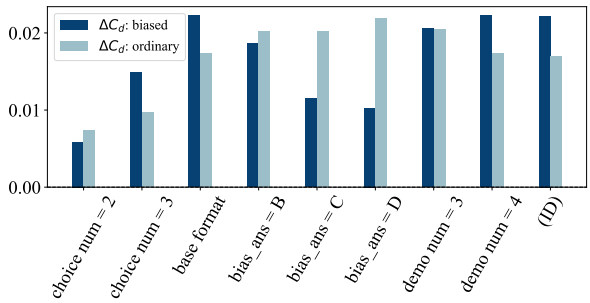
For $\mathrm{T} < 1$,head positions remain similar, while for $\mathrm{T} > 1$, they become more dispersed, as shown in Figure 3(b) and Figure 4(b). Additionally, increasing T beyond 1 does not improve accuracy. This implies that $\mathrm{T} > 1$ may identify non-essential heads, and aligning attention closer to the mean has minimal effect. Within a reasonable interval $\mathrm{T} \in [0.1, 0.6]$, the bias mitigation and accuracy remain stable.

Table 4: The performance Acc/RStd of the Gemma-2B model on the MMLU dataset, using different values for K_l and K_h, with $N = 10$ and $\mathrm{T} = 0.5$

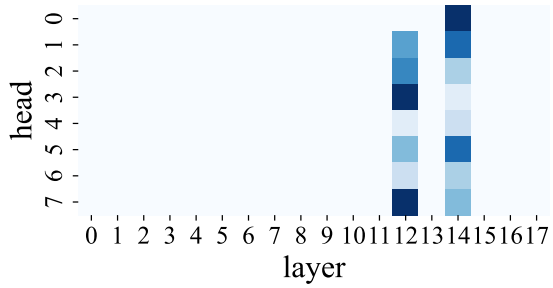
$K_l \backslash K_h$	1	2	4	8
1	40.6/12.3	40.9/11.8	41.7/10.7	41.0/10.9
2	41.3/11.8	41.4/10.7	41.7/**8.8**	41.2/10.6
3	41.5/11.6	41.5/11.3	41.2/9.8	41.0/10.1
4	40.9/11.1	**41.8**/9.4	41.2/9.8	40.9/9.7
5	40.9/11.8	41.1/10.9	40.9/8.0	39.4/11.7
6	40.8/11.2	41.0/10.6	40.8/10.8	38.4/10.7

We explored K_l and K_h using Gemma-2B model in Table 4. When the number of heads is between 6 and 8, the performance remains consistent; however, as the number of heads increases further, the effectiveness of the method diminishes. Similarly, the number of intervention layers should not be excessive. Based on our findings, we recommend using 2–3 intervention layers and 6–8 heads as optimal. Moreover, our experiments across various models reveal a consistent pattern regarding the placement of intervention layers: the most effective intervention layer is typically situated in the middle layers of the model.

We conducted experiments on Gemma-2B, varying the number of samples for CoLo in Table 5. The results indicate that performance improvement plateaus when the sample size reaches 10. Based on these findings, we estimate that a minimum of 10–12 samples is required and recommend using 12 samples for improved stability.



(a) We first localize the attention head in the base mode (five choices, four demonstrations, and A as the biased answer) and then modify the mode for different samples, reporting the corresponding accuracy improvements.



(b) We localize attention heads across different modes and present the localization frequency for each attention head.

Figure 3: Experimental result of mode transformations based on the Gemma-2B model on MMLU dataset.

Table 5: The performance scale with different sample number N for CoLo.

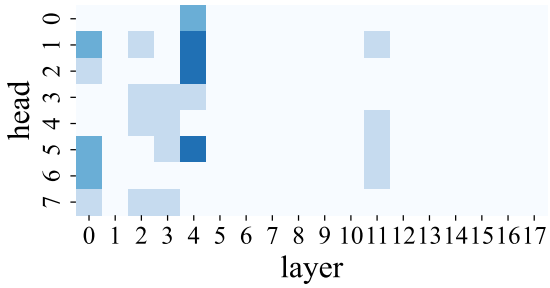
N	4	8	10	**12**	14	16
Acc	40.0	41.2	41.7	41.6	41.7	41.6
Acc Var	0.25	0.42	0.2	0.09	0.12	0.11
RStd	12.2	10.5	10.8	9.4	9.6	9.6
RStd Var	1.3	3.6	3.4	2.3	2.5	2.1

4.5 Prompts to amplify context option bias

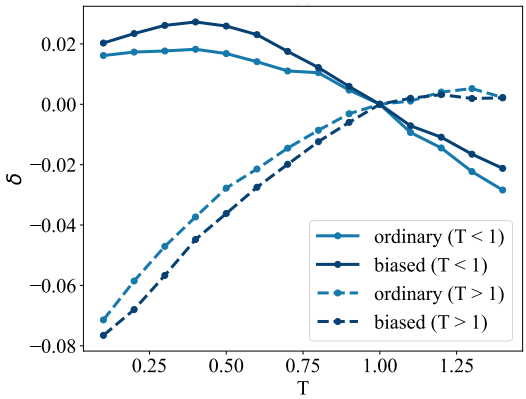
To amplify the context option bias, in addition to manipulating the order of options in a few-shot setting, a prompt-based, zero-shot approach provides an alternative effective method. This approach involves incorporating a phrase such as "The answer can be any one of A/B/C/D, and option A is more likely." within the prompt. The remaining steps follow the same procedure. Through multiple experiments and the reporting of average results, both approaches identified the same layer heads: 12.3, 12.7, 12.1, 14.0, 14.1, and 14.6. The detailed experimental results show in Table 13. This is an encouraging outcome, as the prompt-based method significantly reduces the complexity of bias construction while improving its generalizability.

4.6 Explanations and analyses

The motivation behind CoLo is primarily driven by experimental observations. To investigate this further, we offer potential explanations by analyzing attention distribution across various layers. The experimental results show that our method effectively reduces the model's reliance on demonstrations in the deeper layers, thereby mitigating bias associated with context options. Further discussions and experimental validations of this phenomenon are provided in Appendix K.



(a) Using T >1, respectively, and observe the frequency of the localized head.



(b) Different attention scaling coefficients T were tested on Gemma-2B using the head identified by CoLo, and the accuracy improvements were evaluated on the MMLU.

Figure 4: Different T's impact on CoLo

5 Discussion and conclusions

We propose CoLo, a general localization method designed to mitigate context option bias and improve the accuracy of MCQ. Specifically, by amplifying context option bias through rearranging the order of options in demonstrations, we compare the LLMs' outputs of biased and ordinary demonstration to localizing attention heads strongly associated with context option bias. Attention scaling interventions are then applied to reduce this bias. CoLo requires only small labeled samples to localize attention heads which can be applied across different datasets. Once the attention heads requiring intervention are identified, CoLo introduces no additional inference delay. Compared to previous debiasing methods, CoLo has a natural advantage in extending to generative tasks.

Limitations

This work has the following limitations: (1) As aforementioned in Section 3.4, there remains a lack of theoretical proof supporting the efficacy of this method in reducing such bias while we have provided a plausible explanation for why the identified attention heads can mitigate option bias. (2) Although the selection of attention heads exhibits generalizability, achieving optimal results necessitates that the small labeled sample set used for positioning be identical to the final test set, which will incur additional offline computational overhead. (3) CoLo is currently designed to specifically demonstrate its effectiveness in mitigating option bias, without evaluating its performance across a broader spectrum of biases. We believe extending it to generative tasks presents a promising and ambitious research direction worthy of further exploration. (4) We have conducted experiments on currently mainstream models and achieved promising results, but due to limitations in computational resources, CoLo has not been tested on larger-scale models. (5) CoLo introduces additional computational costs related to the number of layers and heads in the model, which become more significant for models with a large number of parameters, as we discuss in the Appendix E.

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Question: Find the degree for the given field extension Q(sqrt(2), sqrt(3), sqrt(18)) over Q.

origin	position bias	token bias
Option: A. 0 B. 4 C. 2 D. 6 Answer: **B**	*Option:* B. 4 A. 0 C. 2 D. 6 Answer: **A**	*Option:* A. 4 B. 0 C. 2 D. 6 Answer: **B**

Figure 5: An example of inherent bias

A Reproducibility statement

All experiments in the paper can be completed in 4 × GeForce RTX4090(24GB). All the raw versions of evaluation data are accessible from their official repositories in Table 6. All datasets and models used in our experiments are employed strictly for research purposes

B Inherent bias

Position bias manifests itself as inconsistencies in model predictions when the sequence of options changes but all other elements are held constant. Token bias, on the other hand, arises when the substitution of option tokens impacts predictions. Figure 5, an example of inconsistent prediction result of `Llama2-7B` due to position bias and token bias. The correct answer `A` initially selected by the model may arrive at by chance due to its own biases. By swapping option positions/swapping option contents LLMs will get the wrong answer.

C Context option bias in demonstrations with evenly distributed options

Demonstrations with evenly distributed correct choices in a 5-shot setting yield varying effects on predictions depending on the order in which they are presented.

D Comparison of attention distribution

The experiments find that even with simple option swaps in demonstrations, the attention map's distribution in an LLM varies significantly as shown in Figure6.

Based on the difference in attention distribution as shown in Figure 7, we speculate that attention scaling can be used to strengthen attention to the question to make the attention distribution in the two states closer.

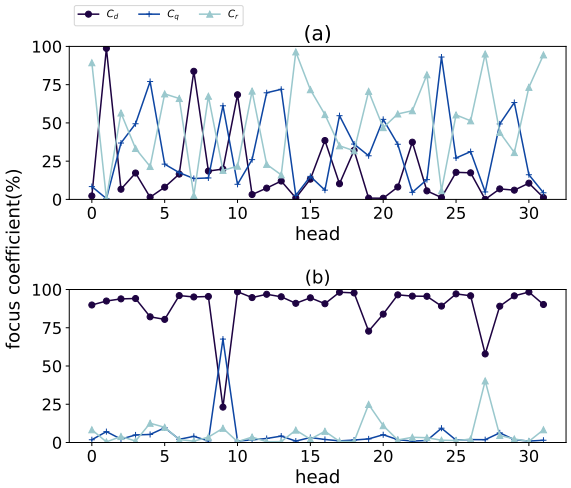

Figure 6: Utilizing the `Llama2-7B` model, we report the average value of the attention coefficients for every head in layer 14th when applied to the BBH's sports understanding dataset(Suzgun et al., 2022). (a) ordinary demonstrations (b) biased demonstrations

E Additional computational overhead

The model consists of L candidate layers, with each layer containing H attention heads. Given a sample size of N, the number of additional inferences required is:

$$L \times N \times 2 + K_l \times H \times N \times 2, \qquad (7)$$

2 means that both biased and ordinary demonstration require one inference.

As the model size increases, the associated computational overhead also grows. Specifically, for models scaling from Llama2-7B to Llama2-70B, the number of layers increases from 32 to 80, and the number of heads increases from 32 to 64. Consequently, the localization overhead is expected to grow by a factor of 4.5, calculated as 80/32+64/32. The following are some potential directions for optimization:

- The computational overhead can be mitigated by employing a grouping strategy for layers and heads. For instance, adjacent layers and heads can be combinedcan. This approach effectively reduces the Llama2-70B to "40 layers" and "32 heads", resulting in additional computational overhead comparable to that of Llama2-7B.

Table 6: Evaluated open-source models

Models	URLs
Llama2-7B	https://huggingface.co/meta-llama/Llama-2-7b
Llama3-8B	https://huggingface.co/meta-llama/Meta-Llama-3-8B
Gemma-2B	https://huggingface.co/google/gemma-2b
Gemma-7B	https://huggingface.co/google/gemma-7b
Mistral-7b-v0.1	https://huggingface.co/mistralai/Mistral-7B-v0.1
Qwen2.5-0.5B	https://huggingface.co/Qwen/Qwen2.5-0.5B
Qwen2.5-1.5B	https://huggingface.co/Qwen/Qwen2.5-1.5B
Qwen2.5-3B	https://huggingface.co/Qwen/Qwen2.5-3B

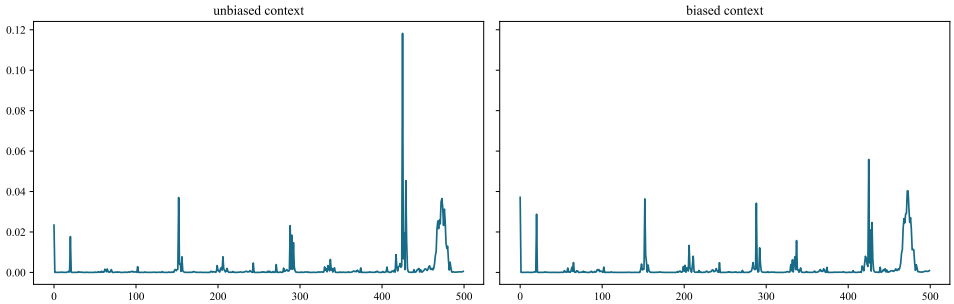

Figure 7: We used biased and ordinary demonstrations on the BBH dataset to obtain the attention distribution on head 9th and layer 14th respectively.

Table 7: With uniform distribution but different order in Gemma-2B result in varying predictions.

Sequence	A	B	C	D
Random	1094	4886	5295	2767
A-B-C-D-A	736	5833	5215	2258
D-C-B-A-D	1202	5849	5526	1465

- In multi-round voting for layers, the layers with lower rankings can be eliminated in each round.

F Located attention heads

CoLo is mainly divided into the offline head localization phase and the inference phase. The offline localization phase primarily consists of three steps:

1. Construct biased MCQ by altering the order of options.

2. Vote to select top K_l layers.

3. Select top K_h heads based on E.

Table 8 shows the attention heads we obtained by randomly selecting 80 samples from the MMLU data set and positioning them on different models. We use *{layer:(head list, T)}* to represent the positioned attention head, $K_l = 2$, $K_h = 4$.

G Calculate score by KL divergence

Using the same positioning strategy and sample set, modify the equation 3 to following equation 8. $\mathrm{KL}(\cdot)$ represents the calculation of KL divergence.

$$E = 1 - \mathrm{KL}(p'(y_o|d_b, q), p(y_o|d_b, q)) + p'(y_t|d_b, q) - p(y_t|d_b, q) \quad (8)$$

H Comparison of cross-domain MMLU performance

Table 2 presents the performance of non-cross-domain CoLo and PriDe on the MMLU dataset. To compare the cross-domain transfer capabilities of CoLo and PriDe, we conducted cross-domain experiments on MMLU under different settings as shown in Table 9. The MMLU dataset consists of four domains: STEM, Social Science, Humanities, and Others. For both CoLo and PriDe, offline computations were performed within a single domain to prepare for debiasing. Specifically, PriDe calculates the prior probability, while CoLo identifies the relevant attention heads. Accuracy across the various domains is then obtained through cross-domain evaluation, and the average for each domain is calculated to determine the overall accuracy on MMLU.

Table 8: The attention heads obtained by CoLo of each model

Models	Attention heads
Llama2-7B	{14: ([24, 4, 20, 31], 0.5), 18: ([30, 10, 25, 28], 0.5)}
Llama3-8B	{17: ([24, 25, 26, 28], 0.5), 14: ([23, 5, 4, 20], 0.5)}
Gemma-2B	{12: ([3, 7, 2, 1], 0.5), 14: ([0, 1, 6, 7], 0.5)}
Gemma-7B	{18: ([0, 8, 6, 2], 0.5), 2: ([1, 5, 3, 0], 0.5)}
Mistral-7B-v0.1	{16: ([12, 14, 13, 1], 0.5), 19: ([8, 16, 9, 10], 0.5)}
Qwen2.5-0.5B	{15: ([13, 12, 9, 7], 0.5), 14: ([0, 3, 6, 11], 0.5) }
Qwen2.5-1.5B	{21: ([11, 9, 6, 8], 0.5), 18: ([3, 11, 0, 6], 0.5)}
Qwen2.5-3B	{27: ([1, 4, 3, 11], 0.5) 8: ([7, 12, 3, 9], 0.5)}

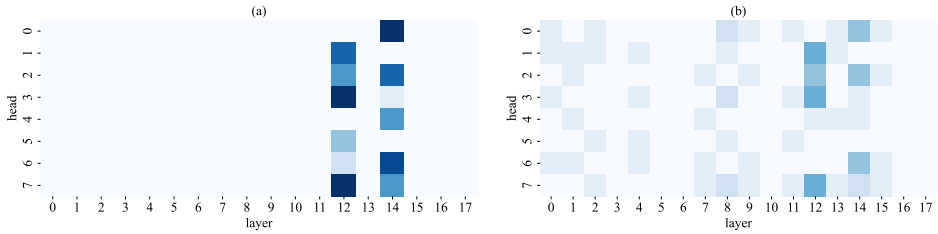

Figure 8: (a) calculate score by equation 3.(b) Modify the original formula through KL divergence.

Table 9: Cross-domain comparative experiment between CoLo and PriDe on MMLU.

MODEL	Baseline		CoLo		PriDe(5%)		PriDe(40%)		PriDe(40%)+CoLo	
Cost	×1		≈ ×1.5		×1.15		×2.2		×3.7	
MMLU-Transfer	Acc	RStd	Acc	RStd	Acc	RStd	Acc	RStd	Acc	RStd
Gemma-2B	33.8	21.8	36.2	12.6	33.8	10.1	35.5	7.6	**37.8**	**7.5**
Gemma-2B+FS	39.9	14.3	41.7	10.8	41.6	6.4	42.4	5.1	**42.9**	**4.6**
Gemma-7B	61.6	5.2	62.0	5.5	61.7	6.7	62.3	5.5	**62.5**	**5.1**
Gemma-7B+FS	62.6	5.4	63.4	**3.7**	64.3	5.9	64.7	4.9	**64.5**	4.2
Llama2-7B	40.9	13.9	43.2	**4.4**	40.0	9.2	41.7	7.6	**44.3**	6.9
Llama2-7B+FS	45.5	10.7	46.5	**3.8**	45.5	9.0	46.5	7.4	**47.4**	8.0
Llama3-8B	61.4	13.8	61.9	6.8	63.4	5.9	**63.7**	4.8	63.1	4.0
Llama3-8B+FS	64.6	7.8	64.8	4.7	65.0	3.9	**65.4**	3.1	64.7	**2.7**

I Generate general text after CoLo

The complete table containing TruthfulQA is presented in Table 11.

J Supplementary experiments

In our study, we initially selected 10 samples but did not investigate or elaborate on how sample size influences the method's performance. To address this limitation, we conducted additional experiments using Gemma-2b on the MMLU benchmark, varying the number of samples. Each experiment was repeated five times, with the mean accuracy and RStd reported. The results demonstrate that when the sample size reaches 10, the performance improvement is approaching a plateau. Based on these findings, we estimate that the minimum number of samples required is approximately 10–12 as shown in Table 5. For improved stability, we recommend using 12 samples.

K Explanations and analyses

We define the focus coefficient to measure the extent to which the model attends to different parts of the context, including context demonstrations C_d, question C_q, and self-rational C_r. p_l represents the last position of the encoded text, p_d represents the end position of the ID after the demonstration is encoded by the tokenizer, p_q represents the end position of the question. According to the decoder structure, we can calculate its attention coefficient for each attention head when the model finally determines the answer to the question. We use $A_{l,h}(i,j)$ represents the attention score of the (i,j) position of the h-th attention head in the l-th layer. After normalizing, the final attention coefficient C_d, C_q and C_r is obtained.

$$C = \sum_{j=s}^{e} \frac{A_{l,h}(p_l, j)}{|e - s + 1|},$$
$$(s, e) \in \{(0, p_d), (p_d + 1, p_q), (p_q + 1, p_l)\} \quad (9)$$

Table 10: Supplementary experiments on the Qwen2.5 series model using CoLo

Model	Cost	Zero Shot		Ordinary (5 shot)		Biased (5 shot)	
		Acc(%)	RStd(%)	Acc(%)	RStd(%)	Acc(%)	RStd(%)
Qwen2.5-0.5B	1	46.2	17.2	47.5	13.7	47.5	13.7
+CoLo	×1.10	47.4	13.5	48.6	7.9	48.6	7.9
Qwen2.5-1.5B	1	58.8	8.4	59.4	3.6	59.4	3.6
+CoLo	×1.19	59.6	7.5	60.5	0.9	60.5	1.0
Qwen2.5-3B	1	64.2	8.3	65.6	3.2	65.2	3.2
+CoLo	×1.25	65.4	6.3	66.4	1.4	66.2	1.4

Table 11: Cross-dataset experiments were conducted **using the attention heads obtained from MMLU**, along with ordinary few-shot learning across all datasets. For TruthfulQA, the MC1/2/3 indicators were used for evaluation, while accuracy was employed as the evaluation metric for the remaining datasets. FS stands for 5-shot in table. We use lm-eval-harness(Gao et al., 2024) as the evaluation tool.

Model	MMLU		CMMLU		CEVAL		AGIEVAL	TruthfulQA		
	ZS	FS	ZS	FS	ZS	FS	ZS	MC1	MC2	MC3
Gemma-2B	33.0	41.7	28.4	30.9	26.5	31.3	31.0	0.233	0.371	0.173
+CoLo	36.2	42.8	29.8	31.7	29.8	32.2	31.6	0.241	0.372	0.173
Gemma-7B	61.6	64.5	44.8	48.9	41.2	48.2	38.7	0.308	0.476	0.228
+CoLo	62.0	65.2	45.4	49.8	44.4	49.4	38.8	0.322	0.479	0.236
Llama2-7B	40.9	45.6	27.2	32.7	30.0	34.0	32.3	0.286	0.434	0.207
+CoLo	43.2	46.8	28.2	32.8	30.3	35.0	33.1	0.291	0.440	0.215
Llama3-8B	61.4	66.5	47.5	50.5	47.9	51.9	37.3	0.324	0.492	0.244
+CoLo	61.9	66.9	47.2	50.6	49.7	52.0	39.0	0.321	0.491	0.245

Table 12: The proportion of doubtful and firm types in the MMLU, and the confidence to the question.

Model	proportion %		confidence	
	firm	doubtful	firm	doubtful
Llama2-7B	79.3	20.7	0.402	0.269
Gemma-2B	73.8	36.2	0.333	0.256

Options with high uncertainty are more susceptible to context option bias in demonstrations. In Table 12, context option bias is intensified by constructing biased demonstrations, and MCQs are divided into two categories: "doubtful," where selections change after switching from ordinary to biased demonstrations, and "firm," where selections remain unchanged. The confidence in the altered options is significantly lower than in the unchanged ones, averaging 0.25 for the four-option questions. Thus, when context option bias is amplified, options with lower certainty are more likely to change.

Context option bias tends to manifest more prominently in the deeper layers of the model. In Figure 9, we analyze the variations in attention allocation for different types of MCQ. The model tends to rely more on contextual demonstrations when handling uncertain questions, while it focuses more on the question itself for more confident ones. Based on this, we hypothesize that context-option bias primarily arises in the model's deeper layers. CoLo mitigates this bias by reducing the model's reliance on context in these deeper layers, thereby effectively decreasing context option bias.

Deep layers reduce attention to context demonstrations following intervention. CoLo is designed to mitigate context-option bias, which often arises from contextual information and typically manifests in the deeper layers of the model. This is supported by the observed reduction in attention to context demonstrations in the deeper layers through our method. However, at the intervention layer, attention to context demonstrations C_d may increase, as shown in Figure 10(b). This suggests a trade-off between attention to examples, questions, and rationale, with the model internally adjusting to maintain a balanced approach.

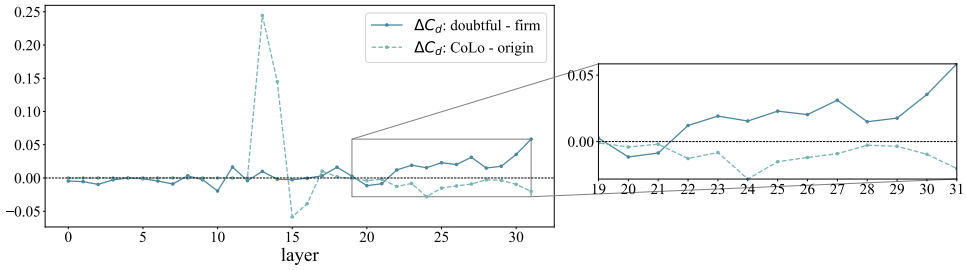

Figure 9: We utilized the `Llama2-7B` model to evaluate the impact of using CoLo on attention to demonstrations within the MMLU dataset. It was observed that the model exhibited increased attention to demonstrations in deeper layers when faced with doubtfule MCQs, thereby introducing contextual option bias. By employing CoLo, the model's attention to demonstrations could be reduced, mitigating the bias introduced in deeper layers.

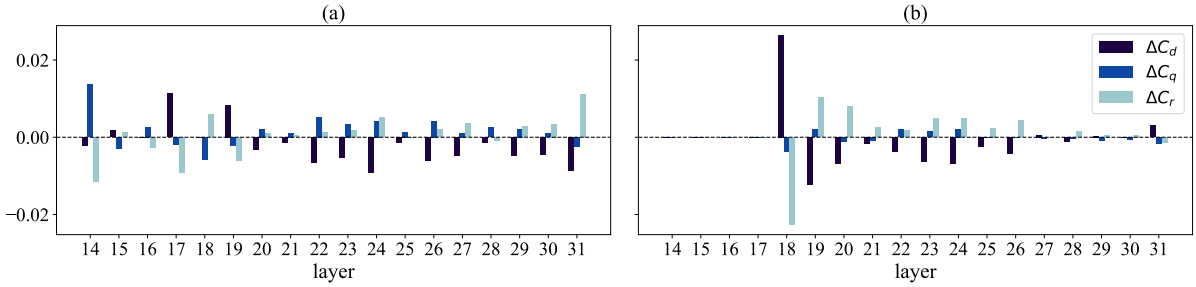

Figure 10: `Llama2-7B` model was used to evaluate the difference in attention to context demonstrations before and after the intervention. Figures (a) and (b) illustrate the head positioning in the 14th and 18th layers, respectively, following the intervention on the BBH sports understanding dataset (Suzgun et al., 2022).

Table 13: Both the prompt-based approach and the method of swapping the order of option choices to amplify context option bias achieve good performance.

Model	**Zero shot**	**Ordinary 5-shot**	**Biased 5-shot**
`Gemma-2B`	33.8/21.8	39.9/14.3	38.2/16.1
`Gemma-2B` + CoLo (option order)	36.2/12.6	41.7/10.8	40.5/7.0
`Gemma-2B` + CoLo (custom prompt)	36.0/13.8	41.4/10.9	40.3/7.0