# A Study on the Calibration of In-context Learning

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#### **Abstract**

Modern auto-regressive language models are trained to minimize log loss on broad data by predicting the next token so they are expected to get calibrated answers when framing a problem as next-token prediction task. We study this for in-context learning (ICL), a widely used way to adapt frozen large language models (LLMs) via crafting prompts, and investigate the trade-offs between performance and calibration on a wide range of natural language understanding and reasoning tasks. We conduct extensive experiments to show that such tradeoffs may get worse as we increase model size, incorporate more ICL examples, and fine-tune models using instruction, dialog, or reinforcement learning from human feedback (RLHF) on carefully curated datasets. Furthermore, we find that common recalibration techniques that are widely effective such as temperature scaling provide limited gains in calibration errors, suggesting that new methods may be required for settings where models are expected to be reliable.

## 1 Introduction

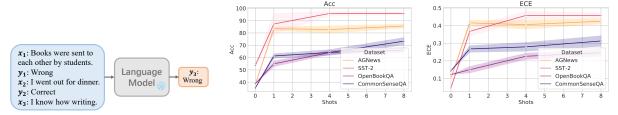
Language models (LMs) that encompass transformer-based architectures (Brown et al., 2020; Chowdhery et al., 2023; OpenAI, 2023) can generate coherent and contextually relevant texts for various use cases. Despite their impressive performance, these models occasionally produce erroneous or overconfident outputs, leading to concerns about their calibration (Dawid, 1982; DeGroot and Fienberg, 1983) which measures how faithful a model's prediction uncertainty is. Such a problem is pressing as users adapt them using a recent paradigm called in-context learning (Brown et al., 2020) to construct performant predictors, especially for applications in safety-critical domains (Bhatt et al., 2021; Kadavath et al., 2022; Pan et al., 2023).

We provide an in-depth evaluation and analysis

of how well these models are calibrated - that is, the alignment between the model's confidence in its predictions and the actual correctness of those predictions. This token-level calibration assessment will enable us to measure the discrepancy between the model's perceived and actual performance through a Bayesian uncertainty lens, providing a valuable metric for assessing the model's accuracy and reliability.

We find that LMs including GPT-2 (Radford et al., 2019) and LLaMA (Touvron et al., 2023a) are poorly calibrated and there exists a calibrationaccuracy trade-off (Fig.1), i.e. as we increase the amount of in-context samples, the prediction accuracy and calibration error both increase. Crucially, this calibration degradation worsens as the model size increases or when fine-tuning occurs using specialized data, such as curated instructions (Dubois et al., 2023), dialogues (Zheng et al., 2023), or human preference data (Ziegler et al., 2019). Though previous work (Braverman et al., 2020) shows the entropy of each generation step is drifting and can be recalibrated via scaling techniques (Platt et al., 1999) such as temperature scaling (Guo et al., 2017), we show that the miscalibration issue in ICL can not be easily addressed using such wellestablished recalibration approaches that rely on additional validation data.

Moreover, we study the trade-off in reasoning tasks that involve the generation of explanations (Camburu et al., 2018; Nye et al., 2021; Wei et al., 2022) before the answer, showing that the model can produce confidently wrong answers (using confidence histograms and reliability plots) when prompted with explanations on Strategy QA (Geva et al., 2021), Commonsense QA (Talmor et al., 2018), OpenBook QA (Mihaylov et al., 2018), World Tree (Jansen et al., 2018). We carefully design our human assessment to observe that, with the increase in model sizes and the quantity of ICL examples, there is a corresponding rise in the pro-



- (a) Demonstration of In-context Learning
- (b) The accuracy and calibration of LLaMA-30B

Figure 1: The accuracy-calibration trade-off of in-context learning. (a) ICL concerns taking task-specific examples as the prompt to adapt a frozen LLM to predict the answer. (b) Classification accuracy and expected calibration error of ICL. As the number of ICL samples increases, the prediction accuracy improves (Left); at the same time, the calibration gets worse (Right).

portion of confidently predicted examples among those incorrectly forecasted. Moreover, we find that a high proportion of wrong predictions are of high confidence and showcase those typical confidently wrong examples of LLMs.

In-context learning has been expected to learn models by gradient descent in their forward pass (Von Oswald et al., 2023), which might hopefully yield calibrated predictions (Błasiok et al., 2023) if the models are getting close to local optimality with respect to test loss through meta-optimization. However, the fact that choosing ICL samples from the validation set does not naturally lead to calibrated predictions shows that ICL learns in a fairly different way than SGD. We design controlled experiments to illustrate task learning properties of ICL, showing that when examples in the prompt demonstrate consistent task properties, the learning performance, and calibration would be improved.

## 2 Related Work

Uncertainty quantification in NLP. Uncertainty quantification in NLP, which often adopts the Bayesian principle to sophisticated methods tailored for neural networks, aims to enhance the reliability of model predictions. This may involve non-trivial designs as directly interpreting language model predictions via probabilities (Kadavath et al., 2022) and linguistic expressions (Lin et al., 2022; Mielke et al., 2022; Zhou et al., 2023) may inadvertently lead to over-reliance on the model's uncertainties (Si et al., 2023), thus complicating the establishment of trustworthy common ground between humans and models (Buçinca et al., 2021). Notable recent advancements include employing model confidence as a critical factor in various applications like dialogue generation (Mielke et al., 2022), cascading prediction (Schuster et al., 2021), open-domain QA (Fisch et al., 2020; Angelopoulos et al., 2022), summarization (Laban et al., 2022), language modeling (Schuster et al., 2022), image captioning (Petryk et al., 2023).

Calibration of LLMs. Calibration is a safety property to measure the faithfulness of machine learning models' uncertainty, especially for errorprone tasks using LLMs. Previous works find that pre-training (Desai and Durrett, 2020) and explanation (Zhang et al., 2020; González et al., 2021) improves calibration. Models can be very poorly calibrated when we prompt LMs (Jiang et al., 2021), while calibration can also depend on model size (Kadavath et al., 2022). (Braverman et al., 2020) assesses the long-term dependencies in a language model's generations compared to those of the underlying language and finds that entropy drifts as models such as GPT-2 generate text. The intricacy of explanations on complementary team performance poses additional challenges due to the overreliance on explanations of users regardless of their correctness (Bansal et al., 2021). (Mielke et al., 2022) gives a framework for linguistic calibration, a concept that emphasizes the alignment of a model's expressed confidence or doubt with the actual accuracy of its responses. The process involves annotating generations with <DK>, <LO>, <HI> for confidence levels, then training the confidencecontrolled model by appending the control token <DK/LO/HI> at the start of the output, followed by training a calibrator to predict these confidence levels, and finally predicting confidence when generating new examples. (Tian et al., 2023) finds that asking LLMs for their probabilities can be better than using conditional probabilities in a traditional way. (Shih et al., 2023) proposes a simple amortized inference trick for temperature-scaled sampling from LMs and diffusion models. To enhance the estimation of uncertainty in language models, (Kuhn et al., 2023) developed a method that aggregates log probabilities across semantically equivalent outputs. This approach utilizes bidirectional entailment through a model to identify outputs that are semantically similar, thereby refining the uncertainty estimation process. (Cole et al., 2023) identifies the calibration challenge in ambiguous QA and distinguishes uncertainty about the answer (epistemic uncertainty) from uncertainty about the meaning of the question (denotational uncertainty), proposing sampling and self-verification methods. (Kamath et al., 2020) trains a calibrator to identify inputs on which the QA model errs and abstains when it predicts an error is likely. (Zhao et al., 2023) proposes the Pareto optimal learning assessed risk score for calibration and error correction but requires additional training. (Kalai and Vempala, 2023) shows the trade-off between calibration and hallucination but they didn't study it in an ICL setting and how the predicted answer's accuracy would impact those two safety aspects.

# 3 Background

**Setting.** Given a pre-trained language model  $\mathcal{P}_{\theta}(w_t|w_{< t})$ , we seek to adapt it using the prompt  $w_0 = [x_1, y_1, x_2, y_2, \dots, x_{n-1}, y_{n-1}, x_n]$  to generate a predicted answer  $y_n = \mathcal{P}_{\theta}(w_0)$ . In the context of reasoning, a popular approach is to hand-craft some explanations/rationales/chain-of-thoughts e in the prompt  $w_0 = [x_1, e_1, y_1, x_2, e_2, y_2, \dots, x_{n-1}, e_{n-1}, y_{n-1}, x_n]$  to generate explanation  $e_n$  and answer  $y_n$ , for the  $e_n$ 

test sample: 
$$\overbrace{w_1, w_2, \dots, w_k}^{e_n}, y_n = \mathcal{P}_{\theta}(w_0).$$

We extract token-level answer probabilities of LLMs,  $^1$  e.g. for binary classification tasks, we filter and extract probabilities P("Yes") and P("No"), based on which we calculate the following statistics for studying the confidence and calibration of LMs: Confidence and feature norm. We record the maximum probability of the answer token as its confidence  $\text{Conf} = \mathcal{P}_{\theta}(y_n|w_{< n})$  and the feature norm  $z_n$  as the hidden states of the answer token from the output of the last layer of the model.

**Entropy rate.** We denote the entropy of a token  $w_t$  at position t as  $H(w_t|w_{< t}) =$ 

 $-\mathbb{E}_{w_t \sim \mathcal{P}_{\theta}(\cdot|w_{< t})}[\log \mathcal{P}_{\theta}(w_t|w_{< t})]$ . We typically measure it based on the answer token via setting  $w_t = y_n$ . Note that auto-regressive LLMs are trained via maximizing the negative log-likelihood objective  $\mathcal{L} = -\mathbb{E}_t[\log \mathcal{P}_{\theta}\left(w_t|w_{< t}\right)]$  on massive corpora.

Empirical estimate of the expected calibration error (ECE) In the realm of probabilistic classifiers, calibration is a crucial concept. A classifier, denoted as  $\mathcal{P}_{\theta}$  with parameters  $\theta$  and operating over C classes, is said to be "canonically calibrated" when, for every probability distribution p over the C classes and for every label y, the probability that the label is y given the classifier's prediction is p matches the component of p corresponding to y. This is mathematically represented as:

$$\forall p \in \Delta^{C-1}, \forall y \in Y : P(Y = y \mid \mathcal{P}_{\theta}(X) = p) = p_y.$$
(1)

Here,  $\Delta^{C-1}$  symbolizes the (C-1)-dimensional simplex, which encompasses all potential probability distributions over the C classes.

A simpler calibration criterion is the "top-label calibration." In this case, a classifier is deemed calibrated if, for every top predicted probability  $p^*$ , the probability that the true label belongs to the class with the highest predicted probability, given that this maximum predicted probability is  $p^*$ , equals  $p^*$ . Formally:

$$\forall p^* \in [0,1] : P(Y \in \arg \max p \mid \max \mathcal{P}_{\theta}(X) = p^*) = p^*.$$
(2)

To gauge the calibration of a model, we adopt Expected Calibration Error (ECE) defined as:

$$\mathbb{E}\left[|p^* - \mathbb{E}\left[Y \in \arg\max\mathcal{P}_{\theta}(X) \mid \max\mathcal{P}_{\theta}(X) = p^*\right]\right]\right]. \tag{3}$$

In real-world applications, this quantity cannot be computed without quantization. So, the ECE is approximated by segmenting predicted confidences into M distinct bins,  $B_1, \ldots, B_M$ . The approximation is then computed as:

$$\widehat{\text{ECE}} = \sum_{m=1}^{M} \frac{|B_m|}{n} \left| \operatorname{acc} (B_m) - \operatorname{conf} (B_m) \right|.$$

Here,  $acc(B_m)$  is the accuracy within bin  $B_m$ , and  $conf(B_m)$  is the average confidence of predictions in bin  $B_m$ . The total number of samples is represented by n, and the dataset consists of n

<sup>&</sup>lt;sup>1</sup>We also normalize the probability  $\mathcal{P}_{\theta}\left(y_{n} \mid w_{< n}\right) \in \Delta^{K}$  for classification problems with K choices

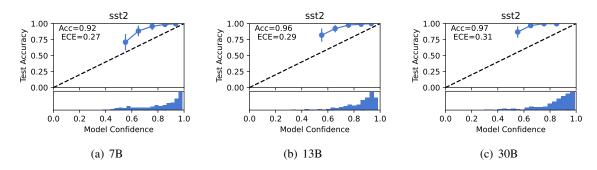


Figure 2: Reliability plots of LLaMA models.

Table 1: Accuracy and Calibration of LLaMA-30B model with three sizes across four text classification datasets and four reasoning datasets

	LLaMA-30B										
Dataset	0-shot		1-shot		4-shot		8-shot				
	Acc	ECE	Acc	ECE	Acc	ECE	Acc	ECE			
	Text Classification										
AGNews	0.383	0.10	0.835	0.416	0.828	0.406	0.856	0.425			
TREC	0.651	0.392	0.70	0.442	0.76	0.492	0.777	0.542			
СВ	0.50	0.143	0.696	0.409	0.821	0.383	0.798	0.359			
SST-2	0.537	0.047	0.873	0.367	0.958	0.458	0.958	0.458			
DBPdia	0.363	0.287	0.792	0.669	0.83	0.69	0.782	0.646			
	Reasoning with Scratchpad										
Strategy QA	0.452	0.039	0.617	0.047	0.679	0.045	0.678	0.088			
Commonsense QA	0.354	0.143	0.613	0.268	0.642	0.279	0.733	0.313			
World Tree	0.53	0.253	0.594	0.276	0.655	0.31	0.24	0.230			
OpenBook QA	0.388	0.122	0.55	0.15	0.641	0.226	0.66	0.246			

independent and identically distributed samples,  $\{(x_i, y_i)\}_{i=1}^n$ . In our work, we use this estimator to approximate the ECE.

# 4 Experimental Results

## 4.1 Experimental Settings

**Models.** We study decoder-only autoregressive LMs involving GPT-2, LLaMA (Touvron et al., 2023a), and their variants fine-tuned with instruction, dialog, or RLHF like Alpaca (Dubois et al., 2023), Vicuna (Zheng et al., 2023), and LLaMA2-Chat (Touvron et al., 2023b).

Datasets and tasks. We used both traditional NLU tasks such as AGNews (Zhang et al., 2015), TREC (Voorhees and Tice, 2000), CB (Schick and Schütze, 2021), SST-2 (Socher et al., 2013), DBPedia (Zhang et al., 2015), as well as reasoning question answering tasks like Strategy QA (Geva et al., 2021), Commonsense QA (Talmor et al., 2018), OpenBook QA (Mihaylov et al., 2018), World Tree

(Jansen et al., 2018). Notably, the reasoning task performance can be greatly improved in general via prompting methods like scratchpad (Nye et al., 2021; Wei et al., 2022) that enables models to generate natural language explanations before predicting an answer.

In-context learning settings. We prompt the model via sampling k examples from the training set for each test example in the k-shot setting. Each experiment is repeated 10 times to reduce variance and we report the mean results. We use M=10 bins for calculating calibration errors.

#### 4.2 Numerical Results

The performance of LLaMA. We seek to characterize the calibration-accuracy trade-off in both simple and realistic settings (Tab. 1). We record the performance and calibration errors in both miscalibrated and recalibrated settings. Moreover, we take a close look at the prompting approaches that explicitly include explanations in reasoning tasks

such as scratchpad (Nye et al., 2021) or chain-of-thought (Wei et al., 2022), showing that the calibration degrades after generating a long context for reasoning and explaining the final answer.

The effect of temperature scaling. We experiment with three strategies in applying temperature scaling methods (Guo et al., 2017) to fix miscalibration:

- 1. We learn one temperature for each *n*-shot ICL, i.e., we learn different temperatures for different shot numbers in ICL;
- 2. Learn a temperature from the training split (zero-shot) and apply it to all test samples with different shot numbers:
- 3. For each experiment, we fix the prompt and learn the temperature for the fixed prompt. That is, for every possible ICL prompt, we learn a corresponding temperature for calibration

Looking into Fig. 6, none of the above strategies achieves satisfactory calibration performance, which is in contrast to the well-studied supervised learning setting where scaling the confidence scores (via temperature scaling) can effectively reduce calibration errors (Guo et al., 2017). The fact that applying a post-processing calibration method, such as temperature scaling, as used in most previous work, cannot directly resolve the miscalibration issue suggests that ICL might have substantially different properties compared to making predictions via classical supervised learning models, thus future investigations are needed to address such miscalibration issues.

The effect of finetuning. We show that vicuna and alpaca are both more accurate but less calibrated than their LLaMA counterpart backbones, the margin is especially large for reasoning tasks and vicuna. Thus we compare those models' accuracy and ECE in Fig. 3, showing that finetuning might significantly degrade calibration, corroborating the evidence shown in (OpenAI, 2023), albeit it can improve the reasoning accuracy dramatically. Our results provide evidence that though finetuned on carefully curated datasets can greatly improve question-answering performance, especially for hard tasks like reasoning problems, attention may need to be paid when assessing the calibration of those models' predictions.

The accuracy is high for 0-shot ICL but has not increased much as we include more in-context examples. We also note that the pattern of zero-shot performance is totally different for two fine-tuned models, i.e. vicuna, and alpaca.

The effect of prompt repetition. In our study investigating the impact of various prompt strategies, we employ three distinct approaches: Repeatcontext: In this strategy, we construct the prompt as  $w_0 = [x_1, x_1, ..., x_1, y_1]$ , where we repetitively include only the context  $x_1$  a total of n times, excluding the label  $y_1$  from repetition. **Repeatprompt**: Here, we shape the prompt as  $w_0 =$  $[x_1, y_1, ..., x_1, y_1]$ , repeating both the context  $x_1$ and the label  $y_1$  n times within the prompt. **Normal**: In this strategy, we construct the prompt as  $w_0 =$  $[x_1, y_1, x_2, y_2, ..., x_{n-1}, y_{n-1}, x_n, y_n]$ , where distinct context-label pairs are systematically chosen to form the prompt. The results presented in Table 3 unveil essential insights: (1) The inclusion of labels within the prompt contributes to a reduction in uncertainty and facilitates more effective reasoning. Conversely, merely repeating the context without incorporating labels fails to yield improved performance. (2) Notably, the diversity inherent in the prompt's construction significantly impacts performance, particularly concerning larger language models.

#### 4.3 Qualitative Results

# Reliability diagram and confidence histogram.

A reliability diagram is a graphical tool used to evaluate the calibration of probabilistic predictions of a model across multiple classes; it compares the predicted probabilities of each class against the actual outcomes, with a perfectly calibrated model having its values lie on the diagonal y = x line. A confidence histogram, on the other hand, displays the distribution of the model's prediction confidences across all classes, showing how often the model predicts certain probabilities.

We showcase that in SST-2 (4-shot), showing that both ACC and ECE of LLaMA increase as the model size increases (Fig. 2). We can observe that confidence scores tend to concentrate on values above 0.8 as we enlarge model sizes.

#### 4.4 Ablation Studies

For case studies, we research how miscalibration can impact the selective classification of LLMs, where models are supposed to abstain from uncer-

Table 2: **Norm of representation, entropy, and confidence** of LLaMA-30B model across three text classification datasets.

Dataset	LLaMA-30B											
Dataset	Norm				Entropy				Confidence			
	0-shot	1-shot	4-shot	8-shot	0-shot	1-shot	4-shot	8-shot	0-shot	1-shot	4-shot	8-shot
AGNews	78.8	92.3	92.1	92.2	3.920	0.650	0.595	0.444	0.214	0.821	0.819	0.865
СВ	88.4	91.7	89.2	87.9	3.857	1.266	0.935	0.823	0.193	0.566	0.629	0.577
DBPdia	77.9	89.5	91.0	90.1	4.105	1.438	0.848	0.718	0.078	0.578	0.705	0.671

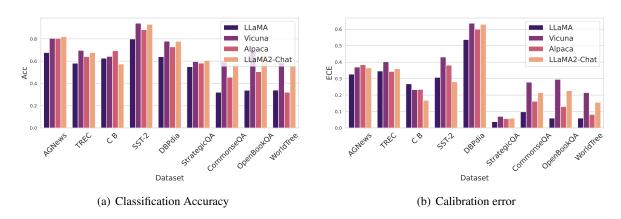


Figure 3: Accuracy and calibration errors of LLaMA and its finetuned variants.

tain predictions in high-stakes settings.

**Ablation with model sizes.** As we enlarge the sizes of models, they will become more confident and accurate (Fig. 2). As a result, the entropy decreases and ECE increases, showing that token-level calibration might have an inverse scaling relationship with model sizes.

A closer look at the hidden state and confidence score. To better understand the miscalibration issue of ICL, we conduct fined-grained experiments to take a closer look at ICL properties: we measure the norm of the representation vectors<sup>2</sup> for different number of shots in ICL, to better understand how the representation vectors are changing when increasing the number of shots in ICL. Meanwhile, we also measure the confidence and entropy of the prediction for  $y_n$ , and the results are summarized in Table 2. When switching from 0-shot to 1-shot, all three measurements (representation norm, entropy, and confidecent) drastically change. Meanwhile, more ICL samples lead to smaller entropy and higher confidence in most cases.

Confidence and wrongly classified reasoning examples. To take a closer look at the failure modes of LMs, we randomly sample 100 reasoning exam-

ples of LLaMA and plot the distribution of wrongly predicted samples and the confidence scores via thresholding. Similar to previous observations, as model sizes and the number of ICL examples scale up, LMs would generate more confident samples (Fig. 4 (c, d)). Note, that we observe "inverse scaling" behaviors where models with larger sizes are more error-prone and tend to generate more confidently wrong samples (Fig. 5).

Examples of hallucinated explanations for highly confident predictions. Next, we showcase in Table 4 that models generate both wrong explanations and incorrect predictions with high confidence. We also observe that most of the wrong predictions are highly confident. We manually examine the correctness of explanations on commonsense QA, and found its high correlations with predicted answer accuracy, which is the opposite of token-level explainability that tends to get worse when the accuracy improves.

# 5 Discussion and Concluding Remarks

In our investigation of the token-level calibration of in-context learning in contemporary Large Language Models (LLMs), we have delineated the intricate balance between ICL performance and calibration. Our findings underscore the importance of

<sup>&</sup>lt;sup>2</sup>The representation vector refers to the intermediate output before the linear prediction layer.

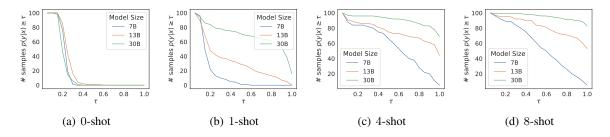


Figure 4: **Illustration of confidence distribution:** The number of samples whose confidence is greater than a threshold on Commonsense QA.

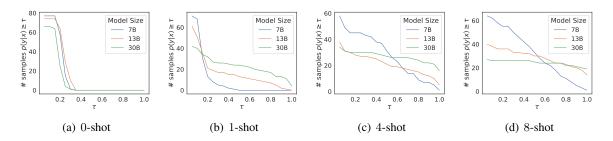


Figure 5: The number of **wrongly classified** examples whose confidence is above a threshold with different numbers of shots on Commonsense QA.

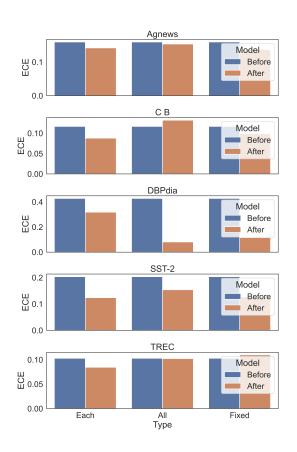


Figure 6: The comparison of calibration errors **before** and after applying different recalibration strategies.

being circumspect in model deployment, as maximizing ICL performance does not invariably translate to improved calibration. As LMs continue to evolve and gain more capabilities such as having long enough context windows that can include the whole training set as in-context examples for some downstream tasks, our result can be pedagogical when users would like to examine their uncertainty through prediction probabilities. Moreover, the work suggests the following future directions:

Understanding the internal mechanism of ICL for calibration. In this work, we observe that existing scaling recalibration methods cannot fully resolve the miscalibration issues of ICL, so better understanding and mitigation strategies are needed. A potential approach can be leveraging transparency tools and studying whether predictable errors exist during text generation.

Calibration beyond classification regimes. Our findings indicate that in multi-choice or multi-class classification tasks, even though the calibration of answer tokens may deteriorate in high-performance settings, there may be a positive correlation between accuracy and the correctness of explanations in reasoning tasks. This suggests potential avenues for future research such as exploring strategies such as the use of hedging words to express uncertainty and examining their relationship with predictive performance.

Table 3: Accuracy and Calibration of LLaMA-7B model and GPT-2 with different prompt repetition strategies.

Model	Strategy	1-shot		4-shot		8-shot		AVG ACC	AVG ECE
	2,	Acc	ECE	Acc	ECE	Acc	ECE		
	Repeat-context	78.200	0.281	78.370	0.283	77.470	0.274	78.013	0.279
LLaMA-7B	Repeat-Prompt	78.200	0.281	89.470	0.395	90.330	0.403	86.000	0.360
	Normal	78.200	0.281	95.200	0.452	96.130	0.462	89.843	0.398
GPT-2	Repeat-context	65.970	0.287	55.300	0.230	54.330	0.230	58.533	0.249
	Repeat-Prompt	65.970	0.287	62.500	0.147	57.970	0.176	62.147	0.204
	Normal	65.970	0.287	63.030	0.212	56.270	0.220	61.757	0.240

Table 4: Qualitative Results of LLaMA on Commonsense and OpenBook

Dataset	Case	Reasoning	$\hat{y}$	p					
	Question: What would you do if you have curiosity but are blind and paralyzed?								
	Options: A) hear news, B) analyse, C) go somewhere, D) examine thing, E) see favorite show								
	Ground Truth: B								
	7B	If you have curiosity but are blind and paralyzed, you would	С	0.5046					
		go somewhere to see things. You cannot hear news, analyse,							
Commonsense		go somewhere, examine thing or see favorite show.							
Commonsense	13B	If you are blind and paralyzed, you can't see anything. So, you	A	0.8684					
		can't go somewhere. You can't examine thing. You can't see							
		favorite show. You can't analyse. So, you can hear news.							
	30B	If you are blind and paralyzed, you cannot see your favorite	С	0.9720					
		show. You cannot hear news as you are blind. You cannot							
		examine thing as you are paralyzed. You can go somewhere to							
		see things.							
	Question: What would you do if you have curiosity but are blind and paralyzed?								
Open Book	Options: A) hear news, B) analyse, C) go somewhere, D) examine thing, E) see favorite show								
	Ground Truth: B								
	7B	A girl and her mom have the same hair length.	D	0.6365					
	13B	A girl and her mom have the same date of birth.	A	0.9782					
	30B	A girl and her mom have the same genes.	A	0.9831					

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