# A Study on the Calibration of In-context Learning

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## Abstract

Accurate uncertainty quantification is crucial for the safe deployment of machine learning models, and prior research has demonstrated improvements in the calibration of modern language models (LMs). We study in-context learning (ICL), a prevalent method for adapting static LMs through tailored prompts, and examine the balance between performance and calibration across a broad spectrum of natural language understanding and reasoning tasks. Through comprehensive experiments, we observe that, with an increasing number of ICL examples, models initially exhibit increased miscalibration before achieving better calibration and miscalibration tends to arise in low-shot settings. Moreover, we find that methods aimed at improving usability, such as fine-tuning and chain-of-thought (CoT) prompting, can lead to miscalibration and unreliable natural language explanations. Furthermore, we explore recalibration techniques and find that a scaling-binning calibrator can reduce calibration errors consistently.

## 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 when 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; 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 enables us to measure the discrepancy between the model's perceived and actual performance to assess its accuracy and reliability through a Bayesian uncertainty lens.

We find that LM such as LLaMA (Touvron et al., 2023a) is poorly calibrated in performant settings and there exists a calibration-accuracy trade-off (Fig.1) for low-shot settings ($k < 4$): as we increase the amount of in-context samples, both prediction accuracy and calibration error increase. Such a trade-off can be improved using more ICL examples ($k = 8$) and larger models. Crucially, this calibration degradation worsens when fine-tuning occurs using specialized data to improve usability, such as curated instructions (Dubois et al., 2023), dialogues (Zheng et al., 2023), or human preference data (Ziegler et al., 2019). Though previous common practice suggests recalibrating models' logits via temperature scaling (Guo et al., 2017), we show that in contrast to classic regimes, the miscalibration issue in ICL can not be easily addressed using such well-established scaling approaches (Platt et al., 1999). Thus we propose to use scaling-binning (Kumar et al., 2019), which fits a scaling function, bins its outputs, and then outputs the average of the function values in that bin, to reduce the expected calibration error below 0.1.

Furthermore, we study the trade-off in reasoning tasks that involve 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 evaluation and observe that, with the increase



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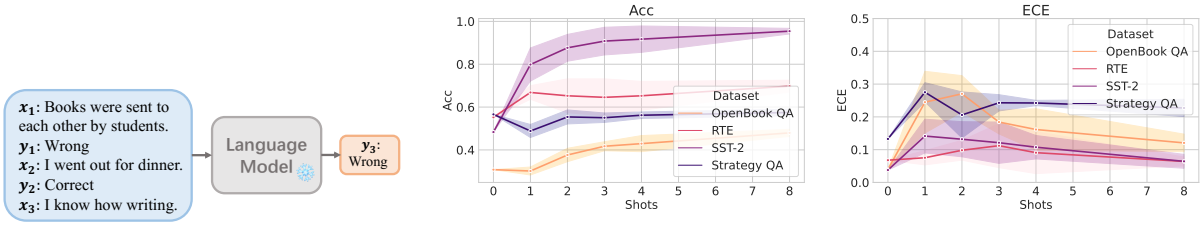



(a) Demonstration of In-context Learning

(b) The accuracy and calibration of LLaMA-7B

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 first worsens ($k < 3$) and then becomes better (**Right**).

in model sizes and the quantity of ICL examples, there is a corresponding rise in the proportion 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 LMs.

Moreover, we find that choosing ICL samples from the validation set does not naturally lead to calibrated predictions, showing that ICL learns in a fairly different way than stochastic gradient descent, a common prototype previous works hypothesize (Von Oswald et al., 2023). Motivated by this difficulty, we design controlled experiments to illustrate that when examples in the prompt are sampled from the same task instead of repeating a given example in various ways, the learning performance would be improved.

## 2 Related Work

**Calibration of language models.** Calibration is a safety property to measure the faithfulness of machine learning models' uncertainty, especially for error-prone tasks using LMs. 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 when GPT-2 generates 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 confidence-controlled 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 LMs for their probabilities can be better than using conditional probabilities in a traditional way. LHTS (Shih et al., 2023) is a simple amortized inference trick for temperature-scaled sampling from LMs and diffusion models. To aggregate log probabilities across semantically equivalent outputs, Kuhn et al. (2023) utilize 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) show the trade-off between calibration and hallucination but they didn't study it in a realistic setting and how the predicted answer's accuracy would impact those two safety aspects.

**In-context learning.** Large models such as GPT-3 (Brown et al., 2020) have demonstrated the potential of in-context learning, a method where the model infers the task at hand from the context provided in the input, without requiring explicit retraining or fine-tuning for each new task. Some recent works attempt to understand ICL through meta-learning (Von Oswald et al., 2023), Bayesian inference (Xie et al., 2021), mechanistic interpretability (Olsson et al., 2022), algorithm selection (Bai et al., 2023), synthetic data and simple function classes (Garg et al., 2022; Akyürek et al., 2022; Raventós et al., 2023). Notably, unlike previous works (Zhao et al., 2021; Han et al., 2023; Fei et al., 2023; Zhou et al., 2023a) that focus on improving task accuracy using the same "*calibration*" terminology, we study the uncertainty of ICL and measure its trade-off with accuracy.

## 3 Background

**Setting.** Given a pre-trained language model $\mathcal{P}_\theta(w_t|w_{<t})$, we seek to adapt it using the prompt $w_0 = [x_1, y_1, x_2, y_2, \ldots, x_{n-1}, y_{n-1}, x_n]$ 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 $w_0 = [x_1, e_1, y_1, x_2, e_2, y_2, \ldots, x_{n-1}, e_{n-1}, y_{n-1}, x_n]$ to generate explanation $e_n$ and answer $y_n$, for the test sample: $\overbrace{w_1, w_2, \ldots, w_k}^{e_n}, y_n = \mathcal{P}_\theta(w_0)$.

We extract answer token probabilities of LMs, e.g. for binary classification tasks, we filter and extract probabilities $P(\text{"Yes"})$ and $P(\text{"No"})$, 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 intermediate hidden state before the linear prediction layer.

**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 LMs are trained via maximizing the negative log-likelihood objective $\mathcal{L} = -\mathbb{E}_t[\log \mathcal{P}_\theta(w_t|w_{<t})]$ 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" (Kull and Flach, 2015) 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, $\forall p \in \Delta^{C-1}, \forall y \in Y$ :

$$P\left(Y = y \mid \mathcal{P}_\theta(X) = p\right) = p_y. \quad (1)$$

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 "confidence 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: $\forall p^* \in [0, 1]$,

$$P\left(Y = c(X) \mid \max \mathcal{P}_\theta(X) = p^*\right) = p^*, \quad (2)$$

where $c(X) = \arg\max p$ and ties are broken arbitrarily. To gauge the calibration of a model, we adopt Expected Calibration Error (ECE (Guo et al., 2017)) defined as:

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

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:

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

Here, $\text{acc}\left(B_m\right)$ is the accuracy within bin $B_m$, and $\text{conf}\left(B_m\right)$ is the average confidence of predictions in bin $B_m$. The total number of samples is represented by $n$, and the dataset consists of $n$ independent and identically distributed samples, $\{(x_i, y_i)\}_{i=1}^n$. In our work, we use this estimator to approximate the ECE.

## 4 Experiments

We briefly summarize our results and findings before explaining the experimental settings.

| Dataset | LLaMA-30B | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 0-shot | | 1-shot | | 2-shot | | 3-shot | | 4-shot | | 8-shot | |
| | ECE | Acc | ECE | Acc | ECE | Acc | ECE | Acc | ECE | Acc | ECE | Acc |
| | Text Classification | | | | | | | | | | | |
| AGNews | 0.261 | 0.37 | 0.043 | 0.830 | 0.049 | 0.817 | 0.067 | 0.810 | 0.049 | 0.821 | 0.047 | 0.855 |
| RTE | 0.023 | 0.672 | 0.051 | 0.742 | 0.060 | 0.747 | 0.050 | 0.738 | 0.048 | 0.748 | 0.058 | 0.752 |
| CB | 0.069 | 0.500 | 0.312 | 0.696 | 0.216 | 0.789 | 0.217 | 0.834 | 0.192 | 0.814 | 0.181 | 0.796 |
| SST-2 | 0.083 | 0.607 | 0.163 | 0.930 | 0.139 | 0.940 | 0.126 | 0.961 | 0.112 | 0.964 | 0.080 | 0.964 |
| | Reasoning with Scratchpad | | | | | | | | | | | |
| Strategy QA | 0.204 | 0.450 | 0.154 | 0.619 | 0.174 | 0.654 | 0.172 | 0.660 | 0.161 | 0.672 | 0.152 | 0.665 |
| Commonsense QA | 0.048 | 0.356 | 0.232 | 0.589 | 0.290 | 0.608 | 0.253 | 0.675 | 0.283 | 0.644 | 0.289 | 0.653 |
| World Tree | 0.112 | 0.534 | 0.211 | 0.570 | 0.251 | 0.621 | 0.185 | 0.680 | 0.206 | 0.646 | - | - |
| OpenBook QA | 0.036 | 0.386 | 0.231 | 0.561 | 0.255 | 0.604 | 0.207 | 0.644 | 0.206 | 0.648 | 0.191 | 0.662 |

Table 1: **Accuracy and Calibration** of LLaMA-30B model with across four text classification datasets and four reasoning datasets. Results are excluded when the data exceeds the context length limit.

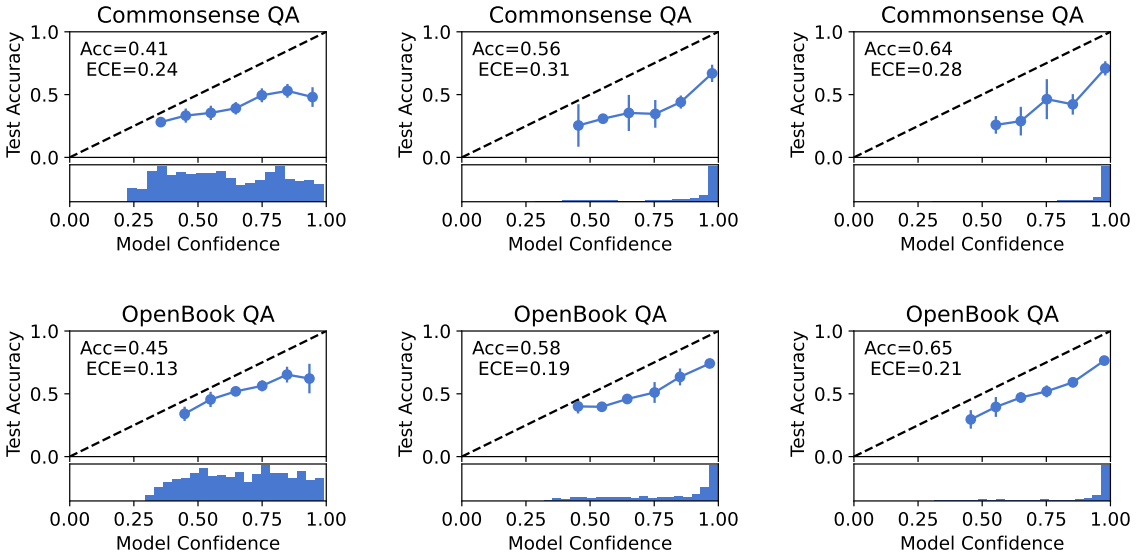



Figure 2: **Reliability plots and confidence histograms** of LLaMA models on 4-shot learning tasks. Results of different sizes 7B (left), 13B (middle), and 30B (right) are plotted.

- For the base LMs we considered, they are calibrated when prompting with a sufficient amount of ICL examples to get non-trivial performance.

- As we increase the number of ICL examples, models tend to be first more miscalibrated and then calibrated. In low-shot settings ($k < 4$), models can be mis-calibrated, in part due to poor data (aleatoric) uncertainty.

- Interventions that improve usability such as fine-tuning, and chain-of-thought (CoT) prompting would lead to miscalibration. The generated explanations from CoT can improve predictive results but may not be reliable by human evaluation.

### 4.1 Experimental Settings

**Models.** We study decoder-only autoregressive LMs involving LLaMA (Touvron et al., 2023a), ranging from 7B to 30B, and its 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.** For $k$-shot learning, we prompt the model via sampling $k$ examples from the training set for each test example. 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

**Model performance and calibration.** We record the performance and calibration errors for $k$-shot learning ($k = 0, 1, 2, 3, 4, 8$), characterizing the calibration-accuracy trade-off in both classic and realistic settings (Tab. 1). Our findings are two-fold: as more in-context examples are included, we observe a concurrent rise in both accuracy and calibration error across most low-shot situations. Especially, when $k = 0$ increases to $k = 1$, there is a marked boost in both accuracy and calibration error, demonstrating the importance of in-context examples in learning performance while one single example may not be able to reduce aleatoric uncertainty. In particular, for reasoning tasks, we explore prompting approaches that explicitly include explanations in reasoning tasks, i.e. scratchpad (Nye et al., 2021) or chain-of-thought (Wei et al., 2022), showing that calibration significantly degrades after generating a long context for reasoning and explaining the final answer. We also note that having more ICL examples does not necessarily lead to better calibration though the predictive performance can generally improve (e.g., $k = 8$ for CB in Tab.1). This may stem from the intrinsic limitations of transformers in effectively modeling long-term dependencies.

**Post-hoc recalibraiton.** We conducted experiments with three strategies (Algorithm 1) to address miscalibration using temperature scaling (Guo et al., 2017) and scaling-binning (Kumar et al., 2019) with learnable parameter $w$:

1. (0-**shot**) Learning $w$ from the training split and applying it to all test samples with different shot numbers.

2. ($k$-**shot**) Learning $w$ for each $k$-shot ICL; in other words, different temperatures are learned for different shot numbers in ICL.

3. (**Fix** $w$) Fixing the prompt for each experiment and learning $w$ corresponding to the fixed prompt. In other words, $w$ is learned for calibration for every possible ICL prompt.

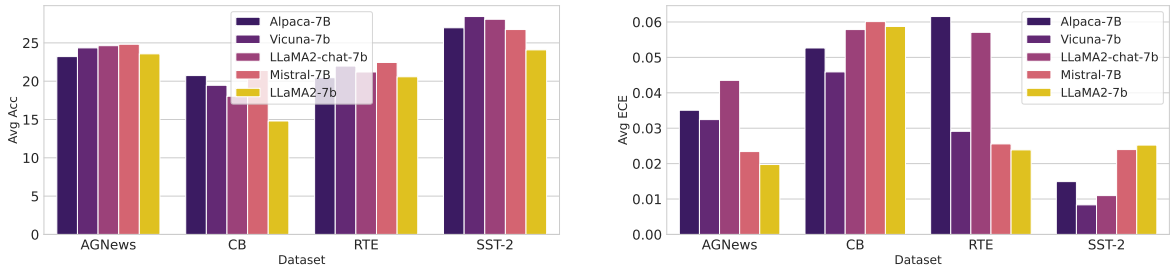
In Appendix Alg. 1, we introduce the recalibration algorithm employing temperature scaling. Additionally, we utilize the scaling-binning calibrator (Kumar et al., 2019), which fits a calibration function $w \in \mathcal{W}$ to the recalibration dataset: $\arg\min_w \sum_{(x_i,y_i)} \ell(w \cdot \mathcal{P}_\theta(x_i), y_i)$, where $\ell$ is log-loss. Subsequently, the input space is partitioned into bins, ensuring an equal number of inputs in each bin (defaulting to 10 bins). Within each bin, the average of the $w$ values is computed and outputted for recalibration.

Upon examination of Table 3 and Table 4, it is evident that none of the aforementioned strategies utilizing temperature scaling achieves satisfactory calibration performance. This finding contrasts with the well-established success of scaling confidence scores in the supervised learning setting, where it effectively reduces calibration errors (Guo et al., 2017). The fact that applying a post-processing calibration method, such as temperature scaling, cannot directly resolve the miscalibration issue suggests that ICL might have different properties compared to predictions from classical supervised learning models. On the other hand, the scaling-binning method demonstrates superior performance in our experiments, which successfully reduces calibration errors below 0.1.

**The effect of fine-tuning.** We show that vicuna, alpaca, and LLaMA2-Chat are all more accurate but less calibrated than their LLaMA counterpart backbones (Fig. 3), the margin is especially large for reasoning tasks and vicuna. Our finding indicates that fine-tuning might significantly degrade calibration, corroborating the evidence reported in GPT-4 (OpenAI, 2023), albeit it can greatly improve the reasoning accuracy. Our results provide evidence that though fine-tuning 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. Moreover, we include results of Mistral-7B (Jiang et al., 2023), a sparse Mixture of Experts (MoEs) architecture with sliding window attention. As a base model, it shows similar performance and calibration compared with LLaMA2-7B, indicating that our conclusion still holds for the model

| | 1-shot | | 2-shot | | 4-shot | | 8-shot | | Avg Acc | Avg ECE |
|---|---|---|---|---|---|---|---|---|---|---|
| | ACC | ECE | ACC | ECE | ACC | ECE | ACC | ECE | | |
| Vanilla | **0.740** | **0.098** | **0.877** | **0.132** | **0.917** | **0.108** | **0.954** | **0.064** | **0.872** | **0.100** |
| Repeat prompt | 0.740 | 0.098 | 0.693 | 0.155 | 0.801 | 0.117 | 0.820 | 0.111 | 0.764 | 0.120 |
| Repeat context | 0.740 | 0.098 | 0.668 | 0.208 | 0.657 | 0.220 | 0.607 | 0.219 | 0.668 | 0.186 |

Table 2: **Acc** and **ECE** of LLaMA-7B model on SST-2 with different prompt repetition strategies.




(a) Classification accuracy

(b) Calibration error

Figure 3: Accuracy and calibration errors of base models LLaMA and Mistral, as well as fine-tuned variants. Reported Acc and ECE results are averaged across experiments conducted with $\{0, 1, 2, 4, 8\}$ shots.

| Dataset | Strategy | 0-shot | 1-shot | 2-shot | 3-shot | 4-shot | 8-shot | Avg |
|---|---|---|---|---|---|---|---|---|
| SST-2 | None | 0.043 | 0.223 | 0.119 | 0.101 | 0.060 | 0.049 | 0.099 |
| | 0-shot | 0.043 | 0.216 | **0.082** | 0.074 | 0.047 | 0.057 | 0.087 |
| | $k$-shot | **0.034** | 0.197 | 0.101 | 0.079 | **0.041** | **0.038** | 0.139 |
| | Fix $w$ | 0.035 | **0.176** | 0.086 | **0.073** | 0.047 | 0.043 | **0.077** |
| CB | None | 0.125 | 0.316 | 0.177 | 0.202 | 0.221 | 0.210 | 0.203 |
| | 0-shot | **0.015** | 0.252 | 0.162 | 0.217 | 0.217 | 0.199 | 0.209 |
| | $k$-shot | **0.015** | 0.357 | 0.187 | 0.188 | 0.212 | 0.216 | 0.214 |
| | Fix $w$ | **0.015** | **0.217** | **0.159** | **0.173** | **0.182** | 0.210 | **0.190** |
| RTE | None | 0.108 | 0.110 | 0.142 | 0.122 | 0.128 | 0.120 | 0.122 |
| | 0-shot | 0.107 | 0.112 | 0.143 | 0.114 | 0.125 | 0.116 | 0.119 |
| | $k$-shot | 0.108 | 0.115 | 0.136 | 0.112 | 0.126 | 0.125 | 0.120 |
| | Fix $w$ | **0.101** | **0.082** | **0.097** | **0.068** | **0.076** | **0.097** | **0.088** |
| AGNews | None | 0.089 | 0.057 | 0.071 | 0.121 | 0.085 | 0.123 | 0.090 |
| | 0-shot | **0.067** | 0.087 | 0.098 | 0.160 | 0.107 | 0.130 | 0.114 |
| | $k$-shot | 0.083 | 0.074 | **0.059** | 0.109 | **0.073** | 0.082 | **0.079** |
| | Fix $w$ | 0.080 | 0.074 | 0.080 | **0.091** | **0.073** | **0.080** | 0.080 |

Table 3: **ECE for different calibration strategies using temperature scaling (Guo et al., 2017)** of base models LLaMA-2-7B across various shot settings.

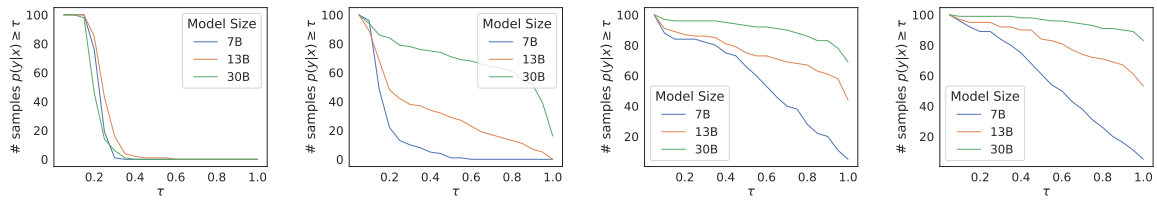
| Dataset | Strategy | 0-shot | 1-shot | 2-shot | 3-shot | 4-shot | 8-shot | Avg |
|---|---|---|---|---|---|---|---|---|
| SST-2 | None | 0.043 | 0.223 | 0.119 | 0.101 | 0.060 | 0.049 | 0.099 |
| | 0-shot | **0.015** | 0.062 | 0.055 | 0.060 | 0.062 | 0.057 | 0.052 |
| | $k$-shot | 0.022 | 0.007 | **0.008** | **0.013** | **0.004** | **0.008** | **0.010** |
| | Fix $w$ | 0.021 | **0.004** | **0.008** | **0.010** | 0.005 | 0.009 | **0.010** |
| CB | None | 0.125 | 0.316 | 0.177 | 0.202 | 0.221 | 0.210 | 0.203 |
| | 0-shot | 0.122 | 0.130 | 0.121 | **0.086** | **0.083** | 0.119 | 0.110 |
| | $k$-shot | **0.119** | 0.109 | 0.100 | 0.109 | 0.101 | **0.049** | **0.094** |
| | Fix $w$ | 0.119 | **0.088** | **0.085** | 0.110 | 0.121 | 0.069 | 0.099 |
| RTE | None | 0.108 | 0.110 | 0.142 | 0.122 | 0.128 | 0.120 | 0.122 |
| | 0-shot | 0.078 | **0.083** | 0.090 | 0.100 | **0.102** | 0.115 | **0.093** |
| | $k$-shot | 0.089 | 0.084 | **0.089** | **0.095** | 0.101 | **0.112** | 0.096 |
| | Fix $w$ | **0.077** | 0.086 | 0.092 | 0.100 | 0.108 | 0.117 | 0.099 |
| AGNews | None | 0.089 | 0.057 | 0.071 | 0.121 | 0.085 | 0.123 | 0.090 |
| | 0-shot | 0.007 | 0.013 | **0.011** | 0.014 | 0.013 | 0.014 | 0.013 |
| | $k$-shot | **0.001** | **0.009** | 0.015 | 0.018 | **0.005** | **0.005** | **0.009** |
| | Fix $w$ | 0.015 | 0.019 | 0.019 | **0.005** | 0.008 | 0.017 | 0.013 |

Table 4: **ECE for different calibration strategies using scaling-binning (Kumar et al., 2019) calibrator** of base models LLaMA-2-7B across various shot settings.

pre-trained with significantly different data and architecture. Comprehensive results and variance across different configurations are elaborated in Appendix Table 11.

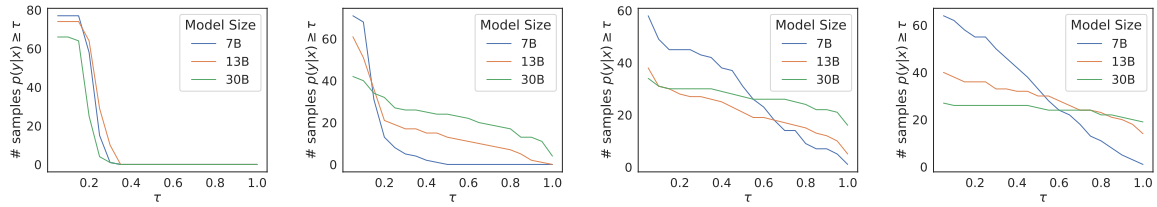
**The effect of prompt formats.** In our study, we explore the effects of different prompt strategies using three distinct methods. We consider predicting the label $y_n$ of test example $x_n$. First, the *Repeat-context* approach involves constructing prompts as $w_0 = [x_1, x_1, ..., x_1, y_1, x_n]$, where the context $x_1$ is repeated n-1 times, but the label $y_1$ is not included in the repetition. Next, the *Repeat-prompt* strategy shapes the prompt as $w_0 = [x_1, y_1, ..., x_1, y_1, x_n]$, where both the context $x_1$ and the label $y_1$ are repeated n-1 times. Finally, the *Normal* involves constructing the prompt as $w_0 = [x_1, y_1, x_2, y_2, ..., x_{n-1}, y_{n-1}, x_n]$, systematically incorporating distinct context-label pairs.

The findings, as detailed in Tab. 2, reveal certain insights: firstly, integrating labels within prompts significantly decreases uncertainty and enhances learning performance. The reason may be that it aids the model in understanding the label space, which leads to better classification outcomes. In contrast, simply repeating the context without labels does not lead to better outcomes. Secondly, the diversity of ICL examples in the prompt greatly affects performance, a potential explanation is it promotes better task learning (Pan, 2023). Those observations corroborate that ICL is performant




(a) 0-shot (b) 1-shot (c) 4-shot (d) 8-shot

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




(a) 0-shot (b) 1-shot (c) 4-shot (d) 8-shot

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

when the number of ICL examples is large and they demonstrate consistent task properties. Importantly, the trade-off persists for different controlled scenarios, i.e. as we increase the number of ICL examples, models tend to be first more miscalibrated and then calibrated.

### 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.

Recall that we found significant miscalibration for reasoning with CoT settings, therefore we closely examine the poorly calibrated reasoning cases using the above plots (Fig. 2 and Fig. 6). Our results on 4-shot settings show that for the reasoning problems (Strategy QA, Commonsense QA, OpenBook QA, World Tree) we consider, models are consistently over-confident with ECEs above 0.15. Larger models are better both in both ACC and ECE but for OpenBook QA, calibration worsens as the model size increases. Moreover, it's observed that confidence scores tend to concentrate on high values as we enlarge the model size. Especially in Commonsense QA and OpenBook QA, the confidence level of nearly all predictions of 13B and 30B models predominantly exceeds 0.8.

### 4.4 Ablation Studies

For case studies, we research how miscalibration can impact the selective classification of LMs, where models are supposed to abstain from uncertain predictions in high-stakes settings.

**Ablation with model sizes.** As we enlarge the size of models, they become more confident (as measured by the confidence histogram) and accurate (Fig. 2). Moreover, the ECE first increases and then decreases. In some settings like SST-2 and OpenBookQA, calibration errors may have a negative correlation with model sizes (Appendix Tab.9).

**Examine the hidden state and confidence score.** To better understand the miscalibration issue of ICL, we conduct fined-grained experiments to examine ICL properties: we measure the norm of the representation vectors[1] for different numbers of shots in ICL. Meanwhile, we also measure the confidence and entropy of the prediction for $y_n$,

[1]The representation vector refers to the intermediate representation before the linear prediction layer.

| Dataset | LLaMA-30B | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 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 |
| CB | 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 |

Table 5: **Norm of representation, entropy, and confidence** of LLaMA-30B across three text classification datasets.

| Dataset | Case | Reasoning | $\hat{y}$ | $p$ |
|---|---|---|---|---|
| Commonsense | 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 go somewhere to see things. You cannot hear news, analyse, go somewhere, examine thing or see favorite show. | C | 0.5046 |
| | 13B | If you are blind and paralyzed, you can't see anything. So, you can't go somewhere. You can't examine thing. You can't see favorite show. You can't analyse. So, you can hear news. | A | 0.8684 |
| | 30B | If you are blind and paralyzed, you cannot see your favorite show. You cannot hear news as you are blind. You cannot examine thing as you are paralyzed. You can go somewhere to see things. | C | 0.9720 |
| Open Book | 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 | 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 |

Table 6: Qualitative Results of LLaMA on Commonsense and OpenBook

and the results are summarized in Tab. 5. When switching from 0-shot to 1-shot, all three measurements (representation norm, entropy, and confidence) drastically change; on the other hand, when $k$ increases ($1 \rightarrow 4 \rightarrow 8$), the change of measures would become smoother. Our discovery shows that adding in-context examples can substantially impact model behaviors while the model behaves relatively similarly for various shots once the task is specified ($k \neq 0$). Meanwhile, more ICL samples lead to smaller entropy and higher confidence in most cases. Considering the alterations in feature representation, which can manifest in either an augmentation of the representation's norm or a shift in direction, quantifying changes in feature direction poses challenges. Thus, we have chosen to examine changes in the norm as a surrogate measure, suggesting that as the number of ICL samples increases, there is a systematic alteration in the model's features.

**Confidence and wrongly classified reasoning examples.** To inspect the failure modes of LMs, we randomly sample 100 reasoning examples 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)). We observe behaviors where models with larger sizes may be more error-prone and tend to generate more confidently wrong explanatory samples (Fig. 5).

**Examples of hallucinated explanations for highly confident predictions.** Next, we showcase in Tab. 6 that models generate both wrong explanations and incorrect predictions with high confidence. We also observe that most of the wrong predictions are highly confident, thus 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. For additional qualitative examination of LLaMA's performance on Strategy QA and WorldTree, please refer to Table 12.

## 5 Discussion and Concluding Remarks

In our investigation of the token-level calibration of in-context learning in contemporary language models, we illustrate the intricate trade-off between ICL performance and calibration. Our findings underscore the importance of being circumspect in model deployment, as maximizing ICL performance does not invariably translate to improved calibration for low-shot and reasoning settings. 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:

**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 in exploring strategies such as the use of hedging words to express uncertainty and examining their relationship with predictive performance.

**Implications in assessing beliefs of LMs.** Previous works show that the expected calibration error would decrease monotonically as the number of ICL examples increases (Kadavath et al., 2022) when querying LMs for answer probabilities. However, we find that zero-shot performance might be weak for models less than 30B, and in low-shot settings, calibration errors can sometimes be even worse than zero-shot. This implies that a close examination and careful control of epistemic uncertainty and aleatoric uncertainty can be needed before deriving conclusions in truthfulness (Liu et al., 2023; Azaria and Mitchell, 2023) for low-shot settings.

**Limitations**. We acknowledge the need to expand our evaluation, which is primarily focused on QA and classification tasks, beyond existing open-sourced language models and datasets. Moreover, we didn't consider nuances such as inherent disagreement about labels (Baan et al., 2022) and adaptive calibration error measures (Nixon et al., 2019) that might be important in certain use cases: it's worth noting that situations may arise where multiple labels share the highest predicted probability. In such instances, the definition (Eq. (2)) doesn't automatically become false; instead, we opt for the first maximal probability. These cases are less likely to occur in most of our experimental setups, where a substantial margin consistently exists between different labels.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## A Extended 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., 2023b) 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).

## B Additional Experimental Details

We provide prompts we adopt for experiments in Tab.7. Additional reliability plots are shown in Fig. 6. Moreover, we provide extra results that extend those in the main text. Our implementation is open-sourced at `https://github.com/hlzhang109/icl-calibration`. The greatest accuracy and ECE values are highlighted in **bold** and red, respectively. Extremely poor performance due to length truncation is omitted.

**Model performance and calibration.** We present experimental results considering different model sizes for text classification and reasoning in Tables 8 and 9, respectively. With the increase in model sizes, we observed overall improvements in model performance across most datasets. However, the calibration error (ECE) did not decrease immediately: for low-shot settings where $k < 4$, models tend to have an ECE larger than 0.1. On the other hand, ECE can decrease given more ICL examples ($k = 8$) if context length is adequate. Overall, zero-shot ICL can lead to good calibration results though the predictive performance is substantially weaker. Interestingly, for some benchmarks like SST-2 and OpenBook QA, the ECE of the 30B model even surpassed that of the 7B model. Moreover, the ECE curves of the 7B and 13B models exhibited similar patterns to the 30B results as the number of ICL samples increased, as shown in the main Tab. (1).

**The effect of fine-tuning.** We provide full results of all finetuned LLMs in Table 11, complementing Fig. (3). We reach a similar conclusion as we explain in the main text: with an increasing number of ICL examples, accuracy generally improves but ECE first increases then decreases and miscalibration is widespread; an MoE model can also have the same accuracy-calibration trade-off; fine-tuning substantially improves accuracy but hurts calibration by a large margin.

**Results reliability.** Furthermore, as prompting is susceptible to various forms of biases and noises (Zhao et al., 2021; Han et al., 2023; Fei et al., 2023; Zhou et al., 2023a), to provide a comprehensive understanding of the experimental outcomes, we delve into the variance across all experimental repetitions. Table 10 provides a detailed analysis of the variance metrics, affirming the stability and reliability of our experimental findings.

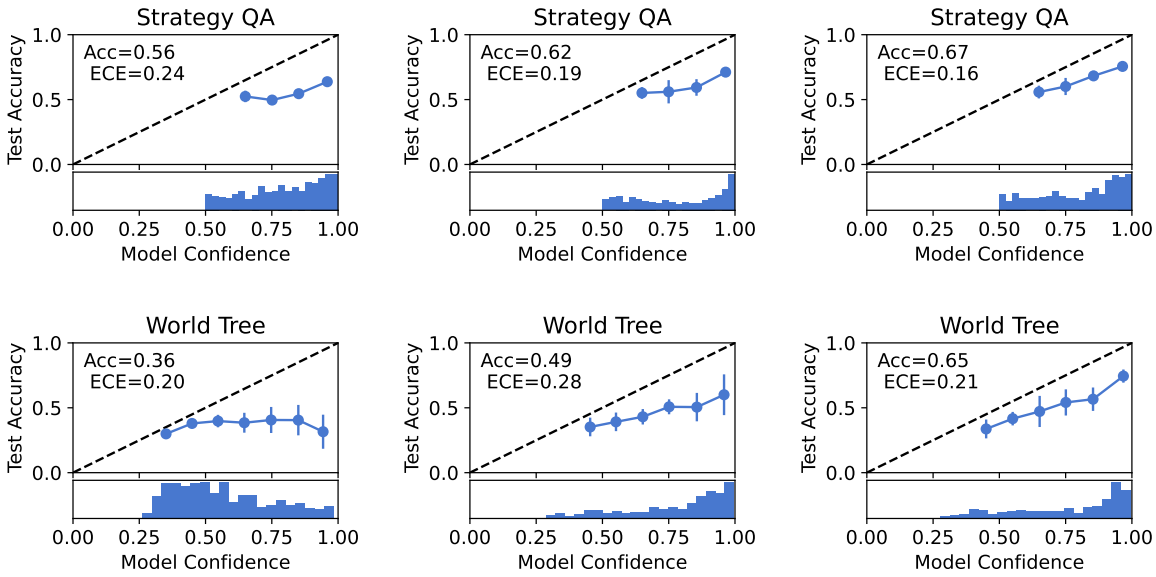


Figure 6: Reliability plots and confidence histograms of LLaMA models on 4-shot reasoning tasks. Results of different sizes 7B (left), 13B (middle), and 30B (right) are plotted.

**Algorithm 1:** Pseudocode for temperature scaling

**Data:** $\mathcal{P}_\theta(\mathbf{w})$: Original output of the classification model, $\mathcal{D}$: Training dataset, $\tau$: Temperature parameter, $k$: we use $k$-shot experimental settings, where during test the ICL prompts will consist of $k$ (sample, label) pairs.

**Result:** Adjusted probabilities after temperature scaling;

`// Training process`

`// 0-shot:` $(\mathbf{w}_i, y_i)$ `is every training samples and corresponding label.`

`//` $k$`-shot:` $\mathbf{w}_i = \{x_1, y_1, ..., x_k, y_k, x_i\}$ `uses` $k$ `prompt pairs.`

`// Fix` $w$`: the prompt in` $\mathbf{w}_i = \{x_1, y_1, ..., x_k, y_k, x_i\}$ `will be used for all training instances and used during inference.`

**for** *each training sample* $(\mathbf{w}_i, y_i) \in \mathcal{D}$ **do**

  Compute the original output: $z_i = \mathcal{P}_\theta(\mathbf{w}_i; \theta)$;

  Compute the cross-entropy loss: $L_i = \text{CrossEntropy}(z_i, y_i)$;

**end**

Compute the gradient of the loss to the temperature parameter: $\nabla_\tau \mathcal{L} = \frac{1}{|\mathcal{D}|} \sum_{i=1}^{|\mathcal{D}|} \nabla_\tau L_i$;

Update the temperature parameter using gradient descent: $\tau \leftarrow \tau - \eta \nabla_\tau \mathcal{L}$;

`// Test time`

**for** *each test sample* $\mathbf{x}_j$ **do**

  Compute the original output with prompt: $z_j = \mathcal{P}_\theta(\mathbf{x}_j; \theta)$;

  Compute the adjusted output: $\hat{z}_j = \frac{z_j}{\tau}$;

  Compute the softmax probabilities: $\hat{p}_j = \text{Softmax}(\hat{z}_j)$;

**end**

| Dataset | Prompt | Label |
|---|---|---|
| SST-2 | Review: it may not be a great piece of filmmaking, but its power comes from its soul's - eye view of how well-meaning patronizing masked a social injustice, at least as represented by this case .<br>Sentiment: Positive<br><br>Review: smith's point is simple and obvious – people's homes are extensions of themselves, and particularly eccentric people have particularly eccentric living spaces – but his subjects are charmers .<br>Sentiment: | Negative, Positive |
| CB | A: No, not really. I spend a lot of time with our income tax, though. especially, this year and last year. Um, I have been married for just a few years, so I've had to really switch around from the EZ form to the, uh, B: Schedule A. A: Right. B: Well, yeah. A: All the deductions and all that. B: Did you notice that when they passed the new simplified tax act, it seemed like it made everything harder?<br>question: when they passed the new simplified tax act it seemed like it made everything harder. true, false, or neither?<br>answer: true<br><br>There was a group of curious onlookers... Marie felt her legs give way beneath her, she sat down on the edge of the pavement, feet in the gutter, doubled-up, sick and winded as if someone had punched her in the stomach. She lifted up her head and looked again. She had watched scenes like this so often in detective films and police series on television that she could hardly believe that this was real life.<br>question: this was real life. true, false, or neither?<br>answer: | True, False, Neither |
| RTE | The main institutionalised forms of recognition for those who have made a significant contribution in the fields of physics, chemistry, medicine, literature, as well as for those working for peace (and more recently in the area of economics), are the Nobel prizes.<br>question: Nobel Peace Prize candidates have been chosen. True or False?<br>answer: False<br><br>Egypt on Thursday strongly criticized Israeli new Foreign Minister Avigdor Lieberman for his remarks that he refused to recognize the peace efforts initiated in 2007 in the U.S. city of Annapolis to restore the peace talks with the Palestinians, reported the state MENA news agency. Liebermanś remarks is "regrettable," Egyptian Foreign Ministry spokesman Hossam Zaki was quoted as saying, adding "his remarks are the first blow to the peace efforts to come from the Israeli new government."<br>question: Hossam Zaki is the new Foreign Minister of Israel. True or False?<br>answer: | True, False |
| Strategy QA | Question: Can spiders help eggplant farmers control parasites? Choose the answer from True and False.<br>Answer: The potato tuber moth is a parasite that targets the plant family Solanaceae, including eggplant Selenops radiatus is a spider genus in South Africa that effectively controls the potato tuber moth So, the answer is: True<br><br>Question: Is the voice of Genie from Disney's Aladdin still alive? Choose the answer from True and False.<br>Answer: | True, False |
| Commonsense QA | "Question: Dan was a farmer with just one heifer. But that was okay, he only kept her for milk, and he didn't think he'd find good farmland in a place as cold as where?<br>A arizona<br>B farm yard<br>C michigan<br>D german field<br>E dairy farm<br>Answer: Michigan is a state in the us where it precipitates throughout the year and areas, where it precipitates throughout the year, are generally cold. So the farmer thought he'd not find a good farmland in a place as cold as michigan. Enslaving heifers or other animals for their milk is wrong as they want to live free. All the places in the other options may not be cold. So, the answer is: C<br><br>Question: From where does a snowflake form?<br>A cloud<br>B snow storm<br>C billow<br>D air<br>E snowstorm<br>Answer:" | A, B, C, D, E |

Table 7: **Prompts used for text classification and reasoning tasks**, with a single training example showcased per task for illustrative purposes. The right column displays corresponding labels. The prompting formats and labels for WorldTree and OpenBookQA are the same as those of the CommonsenseQA dataset.

| Metric | Dataset | Model Size | 0-shot | 1-shot | 2-shot | 3-shot | 4-shot | 8-shot |
|---|---|---|---|---|---|---|---|---|
| ECE | AGNews | 7B | 0.067 | 0.105 | 0.225 | 0.158 | 0.086 | 0.075 |
| | | 13B | 0.093 | 0.084 | 0.069 | 0.121 | 0.103 | 0.045 |
| | | 30B | 0.261 | 0.043 | 0.049 | 0.067 | 0.049 | 0.047 |
| | CB | 7B | 0.133 | 0.218 | 0.172 | 0.197 | 0.202 | 0.215 |
| | | 13B | 0.029 | 0.257 | 0.282 | 0.221 | 0.263 | 0.216 |
| | | 30B | 0.069 | 0.312 | 0.216 | 0.217 | 0.192 | 0.181 |
| | RTE | 7B | 0.068 | 0.075 | 0.098 | 0.112 | 0.091 | 0.064 |
| | | 13B | 0.042 | 0.104 | 0.048 | 0.048 | 0.049 | 0.050 |
| | | 30B | 0.023 | 0.051 | 0.060 | 0.050 | 0.048 | 0.058 |
| | SST-2 | 7B | 0.038 | 0.142 | 0.132 | 0.121 | 0.108 | 0.064 |
| | | 13B | 0.051 | 0.134 | 0.108 | 0.084 | 0.073 | 0.053 |
| | | 30B | 0.083 | 0.163 | 0.139 | 0.126 | 0.112 | 0.080 |
| ACC | AGNews | 7B | 0.447 | 0.629 | 0.563 | 0.630 | 0.777 | **0.833** |
| | | 13B | 0.490 | 0.812 | 0.773 | 0.720 | 0.775 | **0.847** |
| | | 30B | 0.370 | 0.830 | 0.817 | 0.810 | 0.821 | **0.855** |
| | CB | 7B | 0.482 | 0.596 | 0.675 | 0.696 | 0.691 | **0.729** |
| | | 13B | 0.554 | 0.627 | 0.659 | 0.691 | 0.611 | **0.709** |
| | | 30B | 0.500 | 0.696 | 0.789 | **0.834** | 0.814 | 0.796 |
| | RTE | 7B | 0.552 | 0.668 | 0.653 | 0.646 | 0.653 | **0.698** |
| | | 13B | 0.679 | 0.673 | 0.708 | 0.723 | 0.723 | **0.746** |
| | | 30B | 0.672 | 0.742 | 0.747 | 0.738 | 0.748 | **0.752** |
| | SST-2 | 7B | 0.483 | 0.799 | 0.877 | 0.908 | 0.917 | **0.954** |
| | | 13B | 0.483 | 0.918 | 0.943 | 0.955 | 0.962 | **0.969** |
| | | 30B | 0.607 | 0.930 | 0.940 | 0.961 | **0.964** | **0.964** |

Table 8: Accuracy and Calibration of LLaMA model with three sizes across four text classification datasets.

| Metric | Dataset | Model Size | 0-shot | 1-shot | 2-shot | 3-shot | 4-shot | 8-shot |
|---|---|---|---|---|---|---|---|---|
| ECE | Commonsense QA | 7B | 0.070 | 0.155 | 0.237 | 0.227 | 0.238 | - |
| | | 13B | 0.066 | 0.161 | 0.282 | 0.292 | 0.310 | - |
| | | 30B | 0.048 | 0.232 | 0.290 | 0.253 | 0.283 | - |
| | OpenBook QA | 7B | 0.040 | 0.241 | 0.270 | 0.184 | 0.130 | 0.121 |
| | | 13B | 0.031 | 0.132 | 0.217 | 0.209 | 0.191 | 0.175 |
| | | 30B | 0.048 | 0.232 | 0.290 | 0.253 | 0.283 | - |
| | Strategy QA | 7B | 0.133 | 0.275 | 0.206 | 0.243 | 0.242 | 0.227 |
| | | 13B | 0.051 | 0.154 | 0.170 | 0.192 | 0.188 | 0.190 |
| | | 30B | 0.204 | 0.154 | 0.174 | 0.172 | 0.161 | 0.193 |
| | World Tree | 13B | 0.065 | 0.113 | 0.226 | 0.250 | 0.284 | - |
| | | 30B | 0.112 | 0.211 | 0.251 | 0.185 | 0.206 | - |
| | | 7B | 0.074 | 0.124 | 0.198 | 0.179 | 0.203 | - |
| ACC | Commonsense QA | 7B | 0.224 | 0.292 | 0.388 | **0.421** | 0.406 | - |
| | | 13B | 0.320 | 0.478 | 0.549 | **0.574** | 0.562 | - |
| | | 30B | 0.356 | 0.589 | 0.608 | **0.675** | 0.644 | - |
| | OpenBook QA | 7B | 0.308 | 0.298 | 0.376 | 0.417 | 0.454 | **0.480** |
| | | 13B | 0.362 | 0.454 | 0.509 | 0.551 | 0.580 | **0.611** |
| | | 30B | 0.386 | 0.561 | 0.604 | 0.644 | 0.648 | **0.662** |
| | Strategy QA | 7B | 0.566 | 0.488 | 0.554 | 0.550 | 0.562 | **0.575** |
| | | 13B | 0.554 | 0.598 | **0.621** | 0.595 | 0.618 | 0.612 |
| | | 30B | 0.450 | 0.619 | 0.654 | 0.660 | **0.672** | 0.662 |
| | World Tree | 7B | 0.302 | 0.298 | 0.326 | **0.384** | 0.362 | - |
| | | 13B | 0.444 | 0.437 | 0.495 | **0.519** | 0.492 | - |
| | | 30B | 0.534 | 0.570 | 0.621 | **0.680** | 0.646 | - |

Table 9: Accuracy and Calibration of LLaMA models across three sizes on four reasoning datasets.

| Dataset | Metric | 0-shot | 1-shot | 2-shot | 3-shot | 4-shot | 8-shot |
|---|---|---|---|---|---|---|---|
| CB | ACC | $0.500_{\pm 0.000}$ | $0.696_{\pm 0.304}$ | $0.789_{\pm 0.138}$ | $\mathbf{0.834_{\pm 0.068}}$ | $0.814_{\pm 0.068}$ | $0.796_{\pm 0.110}$ |
| | ECE | $0.143_{\pm 0.000}$ | $0.409_{\pm 0.041}$ | $0.216_{\pm 0.061}$ | $0.217_{\pm 0.057}$ | $0.376_{\pm 0.053}$ | $0.359_{\pm 0.071}$ |
| RTE | ACC | $0.672_{\pm 0.000}$ | $0.742_{\pm 0.018}$ | $0.747_{\pm 0.032}$ | $0.738_{\pm 0.044}$ | $0.748_{\pm 0.043}$ | $\mathbf{0.752_{\pm 0.039}}$ |
| | ECE | $0.023_{\pm 0.000}$ | $0.051_{\pm 0.020}$ | $0.060_{\pm 0.021}$ | $0.050_{\pm 0.023}$ | $0.048_{\pm 0.017}$ | $0.058_{\pm 0.022}$ |
| SST-2 | ACC | $0.607_{\pm 0.000}$ | $0.930_{\pm 0.025}$ | $0.940_{\pm 0.066}$ | $0.961_{\pm 0.017}$ | $\mathbf{0.964_{\pm 0.012}}$ | $\mathbf{0.964_{\pm 0.011}}$ |
| | ECE | $0.106_{\pm 0.000}$ | $0.339_{\pm 0.026}$ | $0.139_{\pm 0.058}$ | $0.126_{\pm 0.053}$ | $0.310_{\pm 0.022}$ | $0.287_{\pm 0.014}$ |
| AGnews | ACC | $0.370_{\pm 0.000}$ | $0.830_{\pm 0.015}$ | $0.817_{\pm 0.017}$ | $0.810_{\pm 0.056}$ | $0.821_{\pm 0.029}$ | $\mathbf{0.855_{\pm 0.017}}$ |
| | ECE | $0.261_{\pm 0.000}$ | $0.043_{\pm 0.009}$ | $0.049_{\pm 0.016}$ | $0.067_{\pm 0.029}$ | $0.049_{\pm 0.017}$ | $0.047_{\pm 0.018}$ |
| OpenBook QA | ACC | $0.386_{\pm 0.000}$ | $0.561_{\pm 0.028}$ | $0.604_{\pm 0.027}$ | $0.644_{\pm 0.016}$ | $0.648_{\pm 0.018}$ | $\mathbf{0.662_{\pm 0.031}}$ |
| | ECE | $0.036_{\pm 0.000}$ | $0.231_{\pm 0.049}$ | $0.255_{\pm 0.050}$ | $0.207_{\pm 0.041}$ | $0.206_{\pm 0.019}$ | $0.191_{\pm 0.022}$ |
| CommonSense QA | ACC | $0.356_{\pm 0.000}$ | $0.586_{\pm 0.028}$ | $0.608_{\pm 0.013}$ | $\mathbf{0.675_{\pm 0.027}}$ | $0.644_{\pm 0.034}$ | $0.653_{\pm 0.090}$ |
| | ECE | $0.048_{\pm 0.000}$ | $0.232_{\pm 0.102}$ | $0.290_{\pm 0.022}$ | $0.253_{\pm 0.028}$ | $0.283_{\pm 0.045}$ | $0.289_{\pm 0.140}$ |
| Strategy QA | ACC | $0.450_{\pm 0.000}$ | $0.619_{\pm 0.030}$ | $0.654_{\pm 0.033}$ | $0.660_{\pm 0.022}$ | $\mathbf{0.672_{\pm 0.015}}$ | - |
| | ECE | $0.204_{\pm 0.000}$ | $0.154_{\pm 0.029}$ | $0.174_{\pm 0.070}$ | $0.172_{\pm 0.025}$ | $0.161_{\pm 0.008}$ | - |
| World Tree | ACC | $0.554_{\pm 0.000}$ | $0.570_{\pm 0.056}$ | $0.621_{\pm 0.109}$ | $\mathbf{0.680_{\pm 0.072}}$ | $0.504_{\pm 0.074}$ | - |
| | ECE | $0.112_{\pm 0.000}$ | $0.211_{\pm 0.042}$ | $0.251_{\pm 0.101}$ | $0.185_{\pm 0.048}$ | $0.144_{\pm 0.051}$ | - |

Table 10: The full results (mean and standard deviation) for various experimental configurations extending Table. 1.

| Dataset | Metric | 0-shot | 1-shot | 2-shot | 3-shot | 4-shot | 8-shot |
|---|---|---|---|---|---|---|---|
| CB | | | | | | | |
| Alpaca-7B | ACC | $0.552_{\pm 0.000}$ | $0.668_{\pm 0.032}$ | $0.653_{\pm 0.079}$ | $0.646_{\pm 0.086}$ | $0.653_{\pm 0.067}$ | $\mathbf{0.698_{\pm 0.028}}$ |
| | ECE | $0.016_{\pm 0.000}$ | $0.119_{\pm 0.018}$ | $0.123_{\pm 0.044}$ | $0.122_{\pm 0.031}$ | $0.115_{\pm 0.017}$ | $0.127_{\pm 0.020}$ |
| LLama2-Chat-7B | ACC | $0.375_{\pm 0.000}$ | $0.566_{\pm 0.129}$ | $0.643_{\pm 0.107}$ | $0.670_{\pm 0.126}$ | $\mathbf{0.677_{\pm 0.113}}$ | $\mathbf{0.677_{\pm 0.111}}$ |
| | ECE | $0.287_{\pm 0.000}$ | $0.223_{\pm 0.078}$ | $0.170_{\pm 0.062}$ | $0.153_{\pm 0.054}$ | $0.154_{\pm 0.054}$ | $0.170_{\pm 0.054}$ |
| LLama2-7B | ACC | $0.339_{\pm 0.000}$ | $0.464_{\pm 0.193}$ | $0.511_{\pm 0.163}$ | $0.538_{\pm 0.113}$ | $0.534_{\pm 0.109}$ | $\mathbf{0.575_{\pm 0.059}}$ |
| | ECE | $0.125_{\pm 0.000}$ | $0.222_{\pm 0.190}$ | $0.174_{\pm 0.029}$ | $0.206_{\pm 0.066}$ | $0.226_{\pm 0.071}$ | $0.222_{\pm 0.058}$ |
| Mistral-7B-v0.1 | ACC | $0.500_{\pm 0.000}$ | $0.643_{\pm 0.264}$ | $0.725_{\pm 0.198}$ | $\mathbf{0.827_{\pm 0.067}}$ | $0.793_{\pm 0.063}$ | $0.793_{\pm 0.121}$ |
| | ECE | $0.063_{\pm 0.000}$ | $0.330_{\pm 0.118}$ | $0.228_{\pm 0.094}$ | $0.244_{\pm 0.036}$ | $0.193_{\pm 0.048}$ | $0.144_{\pm 0.028}$ |
| vicuna-7b-v1.5 | ACC | $0.571_{\pm 0.000}$ | $0.668_{\pm 0.049}$ | $0.663_{\pm 0.052}$ | $0.668_{\pm 0.058}$ | $\mathbf{0.675_{\pm 0.061}}$ | $0.648_{\pm 0.073}$ |
| | ECE | $0.051_{\pm 0.000}$ | $0.176_{\pm 0.034}$ | $0.172_{\pm 0.047}$ | $0.169_{\pm 0.054}$ | $0.170_{\pm 0.047}$ | $0.181_{\pm 0.052}$ |
| AGNews | | | | | | | |
| Alpaca-7B | ACC | $0.810_{\pm 0.000}$ | $0.793_{\pm 0.041}$ | $0.710_{\pm 0.110}$ | $0.715_{\pm 0.111}$ | $0.782_{\pm 0.079}$ | $\mathbf{0.832_{\pm 0.029}}$ |
| | ECE | $0.043_{\pm 0.000}$ | $0.123_{\pm 0.033}$ | $0.190_{\pm 0.095}$ | $0.167_{\pm 0.093}$ | $0.112_{\pm 0.057}$ | $0.065_{\pm 0.019}$ |
| LLama2-Chat-7B | ACC | $0.793_{\pm 0.000}$ | $0.809_{\pm 0.031}$ | $0.823_{\pm 0.046}$ | $0.829_{\pm 0.035}$ | $0.829_{\pm 0.028}$ | $\mathbf{0.843_{\pm 0.019}}$ |
| | ECE | $0.164_{\pm 0.000}$ | $0.162_{\pm 0.030}$ | $0.143_{\pm 0.039}$ | $0.138_{\pm 0.033}$ | $0.138_{\pm 0.024}$ | $0.127_{\pm 0.013}$ |
| LLama2-7B | ACC | $0.573_{\pm 0.000}$ | $0.832_{\pm 0.022}$ | $0.789_{\pm 0.112}$ | $0.801_{\pm 0.108}$ | $0.849_{\pm 0.057}$ | $\mathbf{0.868_{\pm 0.009}}$ |
| | ECE | $0.102_{\pm 0.000}$ | $0.037_{\pm 0.012}$ | $0.074_{\pm 0.083}$ | $0.078_{\pm 0.082}$ | $0.052_{\pm 0.024}$ | $0.053_{\pm 0.011}$ |
| Mistral-7B-v0.1 | ACC | $0.780_{\pm 0.000}$ | $0.847_{\pm 0.017}$ | $0.842_{\pm 0.028}$ | $0.820_{\pm 0.056}$ | $0.808_{\pm 0.085}$ | $\mathbf{0.867_{\pm 0.004}}$ |
| | ECE | $0.193_{\pm 0.000}$ | $0.059_{\pm 0.012}$ | $0.044_{\pm 0.010}$ | $0.052_{\pm 0.022}$ | $0.077_{\pm 0.049}$ | $0.043_{\pm 0.010}$ |
| vicuna-7b-v1.5 | ACC | $0.740_{\pm 0.000}$ | $0.803_{\pm 0.013}$ | $0.834_{\pm 0.031}$ | $0.824_{\pm 0.054}$ | $\mathbf{0.835_{\pm 0.030}}$ | $0.832_{\pm 0.036}$ |
| | ECE | $0.063_{\pm 0.000}$ | $0.139_{\pm 0.012}$ | $0.108_{\pm 0.025}$ | $0.116_{\pm 0.034}$ | $0.114_{\pm 0.014}$ | $0.109_{\pm 0.034}$ |
| RTE | | | | | | | |
| Alpaca-7B | ACC | $0.672_{\pm 0.000}$ | $0.644_{\pm 0.015}$ | $0.687_{\pm 0.019}$ | $0.696_{\pm 0.020}$ | $\mathbf{0.703_{\pm 0.015}}$ | $0.690_{\pm 0.035}$ |
| | ECE | $0.175_{\pm 0.000}$ | $0.270_{\pm 0.018}$ | $0.212_{\pm 0.034}$ | $0.197_{\pm 0.028}$ | $0.184_{\pm 0.026}$ | $0.193_{\pm 0.025}$ |
| LLama2-Chat-7B | ACC | $0.729_{\pm 0.000}$ | $0.685_{\pm 0.042}$ | $0.687_{\pm 0.048}$ | $0.699_{\pm 0.040}$ | $0.709_{\pm 0.034}$ | $\mathbf{0.731_{\pm 0.033}}$ |
| | ECE | $0.165_{\pm 0.000}$ | $0.218_{\pm 0.031}$ | $0.205_{\pm 0.033}$ | $0.198_{\pm 0.033}$ | $0.184_{\pm 0.030}$ | $0.172_{\pm 0.020}$ |
| LLama2-7B | ACC | $0.682_{\pm 0.000}$ | $0.684_{\pm 0.034}$ | $\mathbf{0.698_{\pm 0.049}}$ | $0.676_{\pm 0.058}$ | $0.689_{\pm 0.068}$ | $0.685_{\pm 0.050}$ |
| | ECE | $0.044_{\pm 0.000}$ | $0.076_{\pm 0.021}$ | $0.084_{\pm 0.029}$ | $0.085_{\pm 0.034}$ | $0.105_{\pm 0.031}$ | $0.083_{\pm 0.032}$ |
| Mistral-7B-v0.1 | ACC | $0.686_{\pm 0.000}$ | $0.731_{\pm 0.025}$ | $0.756_{\pm 0.015}$ | $0.768_{\pm 0.019}$ | $\mathbf{0.776_{\pm 0.016}}$ | $0.773_{\pm 0.025}$ |
| | ECE | $0.054_{\pm 0.000}$ | $0.121_{\pm 0.047}$ | $0.080_{\pm 0.042}$ | $0.084_{\pm 0.033}$ | $0.087_{\pm 0.025}$ | $0.085_{\pm 0.035}$ |
| vicuna-7b-v1.5 | ACC | $0.610_{\pm 0.000}$ | $0.731_{\pm 0.015}$ | $0.756_{\pm 0.011}$ | $0.762_{\pm 0.013}$ | $0.765_{\pm 0.019}$ | $\mathbf{0.770_{\pm 0.026}}$ |
| | ECE | $0.234_{\pm 0.000}$ | $0.101_{\pm 0.021}$ | $0.073_{\pm 0.028}$ | $0.067_{\pm 0.016}$ | $0.057_{\pm 0.015}$ | $0.052_{\pm 0.015}$ |
| SST-2 | | | | | | | |
| Alpaca-7B | ACC | $0.730_{\pm 0.000}$ | $0.868_{\pm 0.088}$ | $0.939_{\pm 0.018}$ | $0.949_{\pm 0.015}$ | $0.955_{\pm 0.012}$ | $\mathbf{0.952_{\pm 0.014}}$ |
| | ECE | $0.139_{\pm 0.000}$ | $0.068_{\pm 0.048}$ | $0.025_{\pm 0.009}$ | $0.021_{\pm 0.006}$ | $0.020_{\pm 0.009}$ | $0.026_{\pm 0.010}$ |
| LLama2-Chat-7B | ACC | $0.867_{\pm 0.000}$ | $0.951_{\pm 0.008}$ | $0.942_{\pm 0.018}$ | $\mathbf{0.953_{\pm 0.012}}$ | $0.952_{\pm 0.016}$ | $0.952_{\pm 0.015}$ |
| | ECE | $0.039_{\pm 0.000}$ | $0.033_{\pm 0.006}$ | $0.044_{\pm 0.015}$ | $0.032_{\pm 0.012}$ | $0.035_{\pm 0.014}$ | $0.037_{\pm 0.014}$ |
| LLama2-7B | ACC | $0.530_{\pm 0.000}$ | $0.754_{\pm 0.140}$ | $0.829_{\pm 0.121}$ | $0.874_{\pm 0.105}$ | $0.904_{\pm 0.062}$ | $\mathbf{0.925_{\pm 0.045}}$ |
| | ECE | $0.018_{\pm 0.000}$ | $0.180_{\pm 0.058}$ | $0.119_{\pm 0.076}$ | $0.085_{\pm 0.072}$ | $0.062_{\pm 0.027}$ | $0.040_{\pm 0.012}$ |
| Mistral-7B-v0.1 | ACC | $0.563_{\pm 0.000}$ | $0.958_{\pm 0.007}$ | $0.941_{\pm 0.058}$ | $0.956_{\pm 0.030}$ | $0.961_{\pm 0.022}$ | $\mathbf{0.969_{\pm 0.006}}$ |
| | ECE | $0.058_{\pm 0.000}$ | $0.133_{\pm 0.029}$ | $0.086_{\pm 0.033}$ | $0.078_{\pm 0.032}$ | $0.072_{\pm 0.032}$ | $0.052_{\pm 0.020}$ |
| vicuna-7b-v1.5 | ACC | $0.893_{\pm 0.000}$ | $0.946_{\pm 0.011}$ | $0.956_{\pm 0.008}$ | $0.961_{\pm 0.012}$ | $0.964_{\pm 0.008}$ | $\mathbf{0.968_{\pm 0.009}}$ |
| | ECE | $0.041_{\pm 0.000}$ | $0.032_{\pm 0.009}$ | $0.025_{\pm 0.008}$ | $0.026_{\pm 0.006}$ | $0.023_{\pm 0.005}$ | $0.021_{\pm 0.005}$ |

Table 11: The full results (mean and standard deviation) for various experimental configurations extending Figure 3.

| Dataset | Case | Reasoning | $\hat{y}$ | $p$ |
|---|---|---|---|---|
| Strategy QA | Question: Is the voice of the Genie from Disney's Aladdin still alive? Choose the answer from True and False | | | |
| | Options: A) True, B) False | | | |
| | Ground Truth: A | | | |
| | 7B | The voice of the Genie from Disney's Aladdin is still alive. | B | 0.6249 |
| | 13B | The voice of the Genie from Disney's Aladdin is Robin Williams. Robin Williams died on August 11, 2014. | B | 0.7654 |
| | 30B | Robin Williams was the voice of the Genie in Disney's Aladdin. He died on August 11, 2014. | B | 0.8471 |
| World Tree | Question: A bird eats a brightly-colored insect that tastes bad. The bird avoids preying on this type of insect again. This example is best described as ? | | | |
| | Options: A) a physical characteristic, B) a learned behavior, C) an inherited behavior, D) an adaptation | | | |
| | Ground Truth: B | | | |
| | 7B | ing the juice from fruit is a kind of physical change. A physical change is a change in the physical state of a substance. A physical change is not a change in the chemical composition of a substance. A physical change is not a change in the chemical composition of a substance. | D | 0.5249 |
| | 13B | An adaptation is a change in an organism that makes it better suited to its environment. | D | 0.7651 |
| | 30B | Adaptation means a change in the body of an organism that helps it survive in its environment. Adaptation is a kind of behavior. | D | 0.8764 |

Table 12: Qualitative Results of LLaMA on Strategy QA and WorldTree