

Evaluating and Calibrating LLM Confidence on Questions with Multiple Correct Answers

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Abstract

Confidence calibration is essential for making large language models (LLMs) reliable, yet existing training-free methods have been primarily studied under single-answer question answering. In this paper, we show that these methods break down in the presence of multiple valid answers, where disagreement among equally correct responses leads to systematic underestimation of confidence. To enable a systematic study of this phenomenon, we introduce MACE, a benchmark of 12,000 factual questions spanning six domains with varying numbers of correct answers. Experiments across 15 representative calibration methods and four LLM families (7B–72B) reveal that while accuracy increases with answer cardinality, estimated confidence consistently decreases, causing severe miscalibration for questions with mixed answer counts. To address this issue, we propose Semantic Confidence Aggregation (SCA), which aggregates confidence over multiple high-probability sampled responses. SCA achieves state-of-the-art calibration performance under mixed-answer settings while preserving strong calibration on single-answer questions.

1 Introduction

Confidence calibration aims to align a model’s expressed confidence with its true predictive performance (Guo et al., 2017; Desai and Durrett, 2020), and has long been a central research topic for improving the reliability of machine learning systems. In recent years, confidence calibration for large language models (LLMs) has attracted increasing attention, as honesty has been recognized as a fundamental aspect of aligning LLMs with human values (Aspell et al., 2021). When properly calibrated,

LLMs’ confidence can serve as a meaningful indicator of their uncertainty, reflecting the likelihood of hallucination (Maynez et al., 2020; Min et al., 2023) and guiding when retrieval augmentation is required (Ni et al., 2024).

Confidence calibration methods can be divided into training-based and training-free approaches. Training-based methods learn to align confidence with ground-truth accuracy and can achieve strong in-domain calibration (Lin et al., 2022a; Ni et al., 2025b). However, they require substantial annotation and often generalize poorly to other questions or domains (Ni et al., 2025a). In this paper, we focus on training-free methods, which can be roughly categorized into three approaches: 1) leveraging token-level generation probabilities (Guo et al., 2017; Desai and Durrett, 2020; Jiang et al., 2021; Si et al., 2022), 2) prompting models to explicitly verbalize confidence (Lin et al., 2022a; Yin et al., 2023; Xiong et al., 2024; Ni et al., 2024), and 3) measuring semantic consistency across multiple sampled responses (Manakul et al., 2023; Kuhn et al., 2023; Zhang et al., 2023). Among these, response-consistency-based methods achieve the state-of-the-art (SOTA) performance.

Response-consistency-based approaches rely on the implicit assumption that higher agreement among generated responses indicates greater correctness. While this assumption often holds for single-answer questions, it breaks down for questions with multiple valid answers. In such cases, disagreement among equally correct responses can lead to low confidence estimates, even when the model possesses the relevant knowledge. For example, as shown in Figure 1, when asked “name one person who received the Nobel Prize in Physics in 1995”, the model may correctly generate either “Martin Lewis Perl” or “Frederick Reines” across samples. However, answer-level inconsistency results in low estimated confidence, similar to situations in which the model fluctuates

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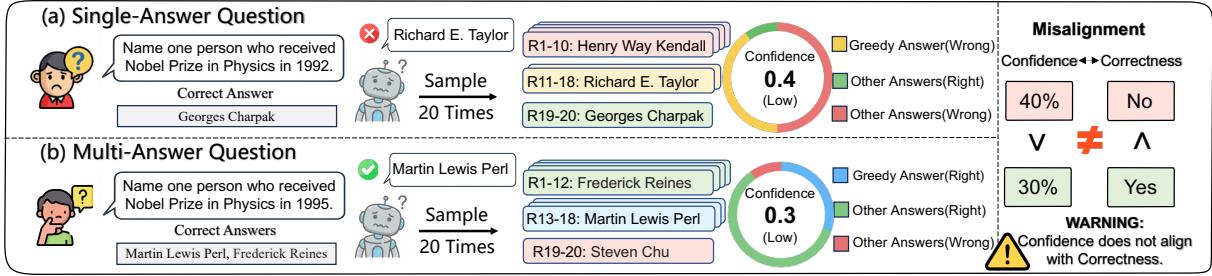


Figure 1: Failure of consistency-based calibration on multi-answer questions. Disagreement among sampled correct answers yields low estimated confidence, indistinguishable from uncertainty caused by alternation between correct and incorrect answers in single-answer settings.

among potentially wrong answers.

Because existing datasets predominantly contain single-answer questions, prior calibration studies have largely overlooked multi-answer settings, leaving it unclear how training-free confidence calibration methods—especially consistency-based approaches—behave in this scenario. Although multi-answer questions can be easier, as any correct answer suffices and accuracy may increase, consistency-based methods may assign low confidence due to disagreement among equally valid answers, potentially reducing overconfidence (Yin et al., 2023; Xiong et al., 2024) but in a miscalibrated manner. To systematically study confidence estimation under multi-answer question answering (QA), we introduce MACE (**M**ulti-**A**nswer **C**onfidence **E**stimation), a benchmark of 12,000 question–answer pairs spanning six factual domains, where each question has 1, 2, 4, or 6 correct answers.

Grounded on MACE, we evaluate 15 representative confidence calibration methods, including token-probability-based, verbalized, and consistency-based approaches, across four LLM families (LLaMA, Qwen, DeepSeek, and GPT), ranging from 7B to 72B parameters. Our experiments reveal that: (1) as the number of correct answers increases, LLMs achieve higher QA accuracy but exhibit lower confidence; (2) in realistic settings with mixed ground-truth answer cardinalities, methods that achieve SOTA calibration on single-answer questions collapse due to severe miscalibration on multi-answer questions; and (3) this confidence degradation is more pronounced for larger models (e.g., 70B), as they tend to alternate among a wider set of correct answers than smaller models.

To address this, we propose SCA (**S**emantic **C**onfidence **A**ggregation), which calibrates confidence by aggregating the probabilities of multi-

ple high-confidence answers rather than relying on the most confident one. Specifically, we use the token-level sequence generation probability of each sampled response as its confidence signal. Since low-confidence responses contribute minimally, a simple summation over sampled responses yields improved calibration under mixed-answer settings, while preserving calibration performance on single-answer questions, outperforming SOTA baselines.

In summary, this work advances confidence calibration from single-answer QA to a more general setting with mixed numbers of ground-truth answers. We introduce the MACE benchmark, conduct a comprehensive evaluation across four LLM families, and propose SCA, which achieves state-of-the-art calibration performance in this general QA scenario.

2 Related Work

Calibration in Large Language Models. Existing calibration methods for large language models (LLMs) can be training-based and training-free. Training-based methods require finetuning to enhance knowledge boundary perception (Lin et al., 2022a; Zhang et al., 2024; Yang et al., 2024). Training-free methods can be broadly categorized into three approaches: *Probability-based* methods leverage the model’s internal representations, such as token probabilities, logits, or hidden activations (Jiang et al., 2021; Kadavath et al., 2022; Ren et al., 2023; Wightman et al., 2023; Ling et al., 2024; Ni et al., 2025b). *Verbalized-based* methods prompt LLMs to directly express confidence in natural language (Lin et al., 2022a; Tian et al., 2023; Tanneru et al., 2024). *Consistency-based* methods estimate reliability by measuring agreement across multiple generations or reasoning chains (Manakul et al., 2023; Cole et al., 2023; Lyu et al., 2024; Ni et al., 2025a). While existing calibration studies

primarily focus on single-answer scenarios, our work broadens this scope to encompass realistic and complex multi-answer settings.

Datasets for Confidence Estimation. Existing datasets are not fully suitable for studying confidence estimation under varying ground-truth answer counts. Most datasets contain questions with a single answer. *Question-Answering benchmarks* include ParaRel (Elazar et al., 2021), HotpotQA (Yang et al., 2018), SelfAware (Yin et al., 2023), HaluEval (Li et al., 2023), FalseQA (Hu et al., 2023), and NEC (Liu et al., 2023a). *Multiple-Choice benchmarks* include MMLU (Hendrycks et al., 2021), FEVER (Thorne et al., 2018) and WiCE (Kamoi et al., 2023). However, existing benchmarks remain limited by the insufficient volume of questions for specific fixed answer counts and the lack of completed ground-truth annotations, restricting their utility for investigation into confidence estimation within multi-answer settings.

3 The MACE Benchmark

In this section, we provide the overview and construction process of the MACE benchmark.

3.1 Overview

To study how existing confidence calibration methods perform on multi-answer questions, we introduce MACE (**M**ulti-**A**nswer **C**onfidence **E**stimation), a benchmark comprising questions with one or multiple correct answers. MACE spans six factual domains: Honorable Award (Award), Political Office (Office), Regional Affiliation (Region), Mathematical Concept (Math), Natural River (River), and Linguistic Culture (Language). For each domain, MACE includes four question types with 1, 2, 4, or 6 correct answers, respectively (abbreviated as 1a, 2a, 4a, and 6a, in the paper), with 500 questions per type. The construction of MACE has three key phases, shown in Figure 2: **knowledge collection** that collects knowledge triplets {subject, relation, object} in the domains except Math, **knowledge filtering** that filters out low-quality triplets and ensure answer completeness, and **QA pair generation** that construct natural language QA pairs based on the triplets. Dataset statistics are summarized in Table 1.

3.2 Knowledge Collection

Domain Identification. We collaborate with LLMs to identify domains in which ground-truth

Table 1: Statistics of the six factual domains in MACE. #Sub.: Number of subjects collected from Wikidata. #Obj.: Number of objects associated with the subjects and used as answers. Obj-Type: Types of the target objects. #Q.: Total number of questions in MACE, including those with 1, 2, 4, and 6 correct answers. #UsedQ: Used questions sampled from constructed questions.

| Domain | Sub. | Obj. | Obj-Type | #Q | #UsedQ |
|----------|------|-------|----------|-------|--------|
| Award | 175 | 2,370 | Person | 9,384 | 2,000 |
| Office | 159 | 1,923 | Person | 6,177 | 2,000 |
| Region | 99 | 1,536 | Country | 5,120 | 2,000 |
| Math | 5 | – | Number | 2,000 | 2,000 |
| River | 810 | 810 | Country | 2,000 | 2,000 |
| Language | 933 | 933 | Country | 2,000 | 2,000 |

answers are clear and complete. Mathematical questions are straightforward to verify, while factual questions—such as award recipients or regional affiliations—are generally uncontroversial and supported by reliable evidence. Balancing coverage and annotation cost, we ultimately select six domains for inclusion in MACE.

Triplet Collection. For Math questions, the knowledge is derived via predefined rules. For other domains, we first use Wikidata¹, a widely recognized, reliable knowledge source, to identify all possible subjects and then retrieve their corresponding objects via the predefined relations. The subject type, relation, and object type of each domain can be found in Table 6. The subject counts are reported in the Raw column of Table 2.

3.3 Knowledge Filtering

To ensure answer correctness and completeness, we conduct heuristic filtering and manual verification. The count of the remaining subjects after each step is shown in Table 2.

Heuristic-Based Filtering. We use a two-stage pipeline to remove low-quality data: (i) *Popularity Filter*: retains only high-traffic subjects based on Wikipedia pageviews; (ii) *Validity Filter*: applies domain-specific rules to eliminate invalid or noisy subjects. This step removes 92.4% of the initial data, retaining a high-quality subset and substantially reducing the workload for human verification.

Manual Verification. We recruit ten domain experts to manually audit the remaining triplets, recognizing any remaining factual errors and enriching incomplete entries. Finally, they remove an

¹<https://query.wikidata.org/sparql>

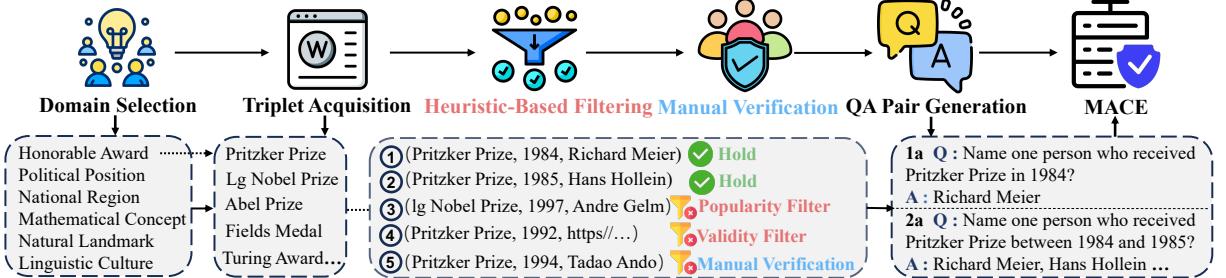


Figure 2: **The MACE benchmark construction pipeline**, illustrated using the *Honorable Award* domain. ①② **Valid triplet** (e.g., Pritzker Prize winners) are retained. ③ **Low-popularity triplet** (e.g., obscure awards like the Ig Nobel Prize) are removed via *Popularity Filter*. ④ **Noisy triplet** containing invalid formats (e.g., URLs) are removed via a *Validity Filter*. ⑤ **Factually incorrect triplet** are identified and removed during the *Manual Verification*. Finally, QA pairs are generated using triplet under four ground-truth counts settings (1a, 2a, 4a, 6a).

Table 2: **Counts of subjects remaining after each filtering step.** **Raw:** Total count of retrieved subjects. **Pop.:** Count after popularity filter. **Val.:** Count after validity filter. **Man.:** Count after manual verification.

| Domain | Raw | Pop. | Val. | Man. |
|----------|--------|-------|-------|------|
| Award | 8,422 | 4,168 | 206 | 175 |
| Office | 7,306 | 5,000 | 289 | 159 |
| Region | 183 | 183 | 129 | 99 |
| River | 10,357 | 3,726 | 910 | 810 |
| Language | 7,251 | 3,830 | 1,012 | 933 |

additional 14.5% of subjects, achieving high inter-annotator agreement (Cohen’s $\kappa = 0.94$).

3.4 QA Pair Generation

For each domain, we design a corresponding prompt template (See Table 5) and use the remaining triplets to generate QA pairs. We create questions by selecting a subject and its associated relation, with the object serving as the answer. By varying the subjects and relations, we can generate questions with different numbers of correct answers, e.g., “Name one person who received {award} between {lower_year} and {upper_year}”. For each domain, the number of constructed questions varies, shown in the #Q column of Table 1. To prevent any domain from dominating the evaluation, we sample 500 questions for each setting (1a, 2a, 4a, and 6a) in each domain for evaluation, resulting in 2,000 QA pairs per domain.

3.5 Construction Characteristics

Our construction pipeline ensures that: 1) all questions in MACE have clear, complete, and correct ground-truth answers; 2) questions with different numbers of valid answers are explicitly separated, enabling analysis of answer-count effects and re-

alistic mixed-question scenarios; and 3) questions across varying answer-count settings are grounded in the same knowledge types, differing only in factors such as year range, thereby maintaining comparable difficulty.

4 Experimental Setup

4.1 Confidence Estimation Methods

We categorize existing confidence estimation methods into more fine-grained approaches: **Single-turn** and **Double-turn** approaches. Detailed formulations are provided in Appendix § B.1.

Single-turn. Most of these methods estimate confidence based on whether the model concentrates on a single response for a given question. We further divide them into two types:

- **Question-level Confidence** (Malinin and Gales, 2021; Kadavath et al., 2022; Kuhn et al., 2023). These methods quantify the entropy of the model’s output distribution. *Prediction Entropy* (*Prob Entropy*) directly measures the entropy of the answer probability space; *Length-Normalize Prediction Entropy* (*N-Prob Entropy*) refines this by normalizing for sequence length; and *Semantic Entropy* (*Sem Entropy*) focuses on the semantic meaning regardless of the specific formatting.
- **Answer-level Confidence** (Jiang et al., 2021; Manakul et al., 2023; Xiong et al., 2024). These methods evaluate the confidence of specific answers. *Verb* prompts the model to directly express confidence in natural language, while *Verb-Topk* outputs confidence scores for top- k candidates. *Consistency* (*Consis*) measures confidence via agreement across multiple sampled outputs. *Consis-Verb* and *Consis-Verb-Topk* further weight this consistency using the verbalized

scores from *Verb* and *Verb-Topk*. *Perplexity* directly derives confidence from the sequence’s generation probability.

Double-turn. These methods adopt a post-hoc approach, measuring confidence through a secondary query after the initial answer is produced, rather than assessing the model’s generation probability for that answer.

- P_{True} (Kadavath et al., 2022). The model verifies its answer via a binary True/False judgment. Specifically, $P_{\text{True}}\text{-Censis}$ approximates the confidence of True via black-box sampling, whereas $P_{\text{True}}\text{-Prob}$ directly extracts the token’s probability. Their conditioned variants, $P_{\text{True}}\text{-Censis-Cand}$ and $P_{\text{True}}\text{-Prob-Cand}$, augment the verification prompt with multiple candidate answers to assist the judgment.
- **Self-Ask** (Tian et al., 2023). The model explicitly verbalizes a numerical confidence score in natural language. *Self-Ask* performs this assessment directly, while *Self-Ask-Cand* incorporates multiple candidate answers as assistance.

4.2 Models

We evaluate a diverse set of representative language models across different scales and series. For open-source models, we include Qwen2.5-Instruct series (7B, 14B, 32B, 72B) (Yang et al., 2025), LLaMA3.1-Instruct series (8B, 70B) (Grattafiori et al., 2024), and DeepSeek-V3 (DeepSeek-AI, 2024). Additionally, we include two state-of-the-art closed-source models GPT-4o-mini and GPT-4o (Hurst et al., 2024).

4.3 Evaluation

Metrics. We evaluate the model using three metrics: **Accuracy** measures the correctness of the model’s predictions. **Confidence** quantifies the model’s certainty regarding its predictions. **Area Under the Receiver Operating Characteristic Curve (AUROC)** (Hanley and McNeil, 1982) is used to evaluate calibration ability. It quantifies the model’s ability to discriminate between correct and incorrect predictions, where a higher AUROC indicates that the model consistently assigns higher confidence to its correct outputs. For each metric, we report the average across all domains.

Correctness and Consistency Evaluator. Given the diversity of output formats, we use GPT-4o as our primary evaluator, following (Liu et al., 2023b).

Table 3: Confidence scores of LLaMA-3.1-70B-Instruct under different counts of correct answers. “1a” denotes questions with a single correct answer, and the remaining settings follow the same convention.

| Method | 1a | 2a | 4a | 6a |
|--------------------------------------|------|------|------|------|
| Accuracy | 48.0 | 55.4 | 59.9 | 61.7 |
| Single-turn | | | | |
| <i>Question-level</i> | | | | |
| Prob Entropy | 71.6 | 70.0 | 66.6 | 65.6 |
| N-Prob Entropy | 91.5 | 90.9 | 89.9 | 89.7 |
| Sem Entropy | 60.8 | 57.9 | 49.7 | 45.2 |
| <i>Answer-level</i> | | | | |
| Verb | 94.8 | 94.7 | 93.1 | 92.3 |
| Verb-Topk | 81.9 | 73.9 | 62.1 | 56.9 |
| Censis | 51.3 | 48.9 | 40.2 | 35.9 |
| Censis-Verb | 50.3 | 47.9 | 40.5 | 36.4 |
| Censis-Verb-Topk | 47.6 | 45.9 | 38.4 | 34.2 |
| Perplexity | 77.6 | 76.4 | 73.0 | 71.0 |
| Double-turn | | | | |
| $P_{\text{True}}\text{-Censis}$ | 79.3 | 79.3 | 77.0 | 75.5 |
| $P_{\text{True}}\text{-Prob}$ | 79.2 | 79.0 | 76.8 | 75.4 |
| $P_{\text{True}}\text{-Censis-Cand}$ | 88.1 | 87.9 | 87.1 | 87.9 |
| $P_{\text{True}}\text{-Prob-Cand}$ | 88.1 | 87.8 | 87.1 | 87.8 |
| Self-Ask | 63.6 | 60.9 | 56.1 | 54.4 |
| Self-Ask-Cand | 64.5 | 63.5 | 59.6 | 56.8 |

An answer is deemed correct if GPT-4o determines that it matches any of the ground-truth answers. GPT-4o is also employed to assess semantic consistency between pairs of responses. To validate the reliability of these automatic judgments, we perform human evaluation on 300 randomly sampled instances, observing a Cohen’s κ of 0.92, which indicates high agreement among annotators.

5 Results and Analysis

In this section, we examine how existing confidence estimation methods behave in multi-answer settings. We first analyze how QA performance and estimated confidence vary on questions with more correct answers, and then evaluate calibration performance under mixed questions with different answer counts. Due to space constraints, we focus on LLaMA-3.1-70B-Instruct, which shows trends consistent with other models; full results are provided in Appendix § C.1.

5.1 Model Confidence Decreases as the Number of Correct Answers Increases

As demonstrated in Table 3, increasing the number of ground-truth answers leads to a steady improvement in accuracy, suggesting that the questions become empirically easier. However, Table 3 re-

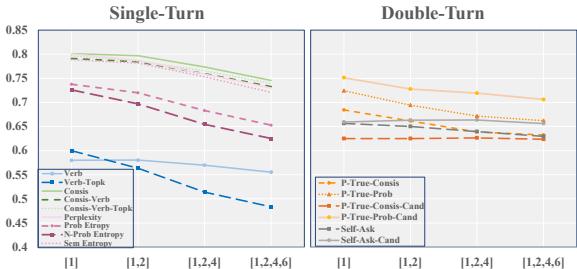


Figure 3: AUROC of LLaMA-3.1-70B-Instruct on mixed questions with varying counts of correct answers.

veals a consistent downward trend in confidence across most estimation methods. This indicates that miscalibration between confidence and QA performance arises in multi-answer settings not only for response-consistency-based methods, but for nearly all existing approaches. Across different domains, the overall trend is similar. In more challenging domains, such as Region, the model’s confidence decreases less sharply (see Figure 9).

Notably, consistency-based methods exhibit the best calibration performance among existing methods (See Figure 3 and Table 18). On single-answer questions, consistent with prior studies, the estimated confidence exceeds QA performance, indicating overconfidence. However, when the ground-truth answers become more, the estimated confidence changes from overconfident to over-prudent.

Larger Models Experience a Sharper Confidence Drop. This phenomenon is shown in Figure 4. For instance, within the LLaMA series, the 70B model exhibits a significant confidence decrement of **0.154** from single-answer to six-answer settings, while the 8B model drops only **0.056**; notably, its confidence even shows a slight increase when moving from the 1a to the 2a setting. We speculate that this is because larger models possess a much broader knowledge coverage. As the number of correct answers increases, larger models tend to generate a wider range of potential valid answers. In contrast, smaller models have limited knowledge coverage, so their generation space is often confined to a narrow subset of the possible answers. We provide a granular investigation into the impact of knowledge coverage, with detailed findings presented in Section 5.3.

5.2 Calibration Degrades on Mixed Questions with Varying Answer Counts

To evaluate existing methods in a more realistic scenario where questions can have different num-

bers of valid answers, we mix the questions and examine overall calibration performance for each domain. AUROC results are illustrated in Figure 3. We observe a *consistent downward trend in AUROC as questions become more heterogeneous in the number of correct answers for most of the methods*. This stems from the misalignment between rising accuracy and declining confidence estimates.

Compared to double-turn methods, single-turn methods typically exhibit stronger calibration performance except for verbalized approaches due to models’ inherent overconfidence (Kadavath et al., 2022; Lin et al., 2022b). As we expected in Section § 4 show greater sensitivity to fluctuations in the number of valid answers. This is because they directly use the generation distribution to measure confidence while double-turn methods rely on the model’s post-hoc judgement.

5.3 Why Does Confidence Decline More Sharply in Larger Models?

Definition of Knowledge Coverage. We consider the knowledge possessed by a model to be reflected in the answers for which it assigns high confidence. Accordingly, we define knowledge coverage as the number of high-confidence answer clusters, where sampled responses are grouped into clusters based on semantic consistency. Specifically, we apply a token-level probability-based filter and retain only clusters whose cumulative probability exceeds a threshold of $\tau = 0.1$. A detailed analysis of the cluster probability distribution and the choice of threshold is provided in Appendix § C.2.

Figure 5 illustrates how knowledge coverage scales with model size, and Figure 6 shows the distribution of cluster sizes. Larger models consistently exhibit a greater knowledge coverage than smaller ones, with the gap widening as the number of ground-truth answers increases. This suggests that larger models encode broader knowledge, whereas smaller models may fail to produce effective answers even when more correct answers exist.

Consequently, as the number of correct answers increases, larger models—due to their broader knowledge—tend to generate a wider range of potentially correct answers, reducing response consistency and thus lowering estimated confidence. In contrast, smaller models are constrained to a narrower candidate set, leading to a more gradual decline in confidence. As a result, larger models exhibit a sharper confidence decline due to more

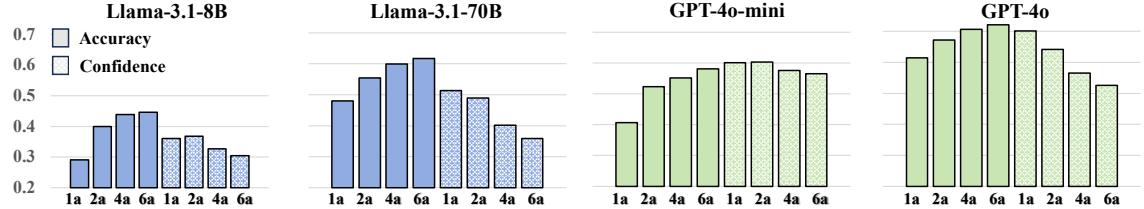


Figure 4: QA performance and confidence variation with the number of correct answers across model scales.

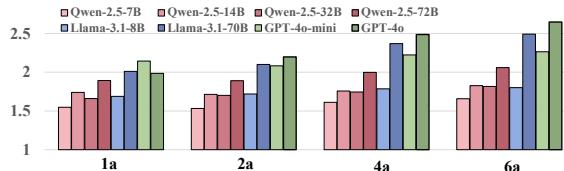


Figure 5: Knowledge coverage across ground-truth (GT) set sizes. Different color schemes denote different model families. Color intensity increases from light to dark to indicate increasing model size.

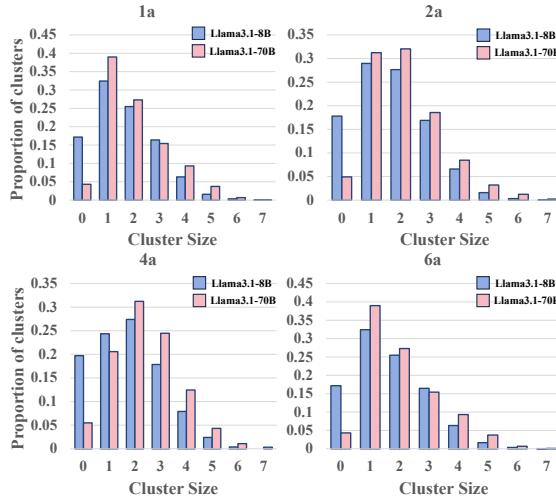


Figure 6: Distribution of the cluster sizes after filtering. rapidly increasing knowledge coverage. Further analysis is provided in Appendix § C.3.

6 Semantic Confidence Aggregation

In this section, we propose Semantic Confidence Aggregation (SCA), a method for confidence calibration in realistic multi-answer scenarios. The key idea is that overall confidence should reflect the aggregate confidence of all valid answers rather than rely on the single most confident response, and that response inconsistency (e.g., high entropy) does not necessarily imply low confidence.

6.1 Methodology

Similar to Sem Entropy, we begin by sampling multiple answers and clustering them based on se-

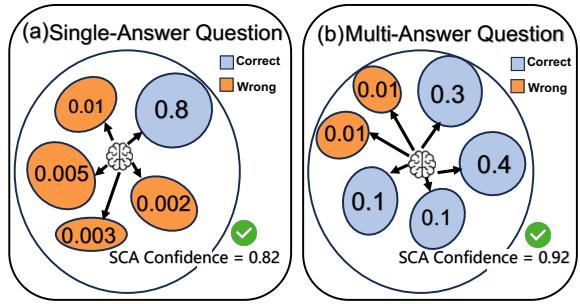


Figure 7: **Illustration of SCA method without tuning.** As shown, confidence estimation is dominated by high-confidence clusters. SCA sums probabilities across all clusters, achieving consistent strong calibration performance in both single-answer and multi-answer settings.

mantic similarity. Let $\mathcal{S} = \{s_1, \dots, s_N\}$ denote N sampled responses for a given question. We partition \mathcal{S} into M clusters $\mathcal{C} = \{C_1, \dots, C_M\}$. Since token-level generation probabilities reflect the model’s certainty, for a cluster C_m , we compute its confidence as the sum of the token-level probabilities of all responses within the cluster, rather than relying on the proportion of samples it contains. The formulation is:

$$P_{\text{SCA}}(C_m) = \sum_{s \in C_m} p(s), \quad (1)$$

where $p(s)$ represents the token-level generation probability of sequence s .

Since low-probability responses may be generated by chance rather than representing answers the model considers likely correct, we sum only the probabilities of clusters whose confidence exceeds a threshold τ . The set of valid clusters is defined as $\mathcal{C}_{\text{valid}} = \{C_m \in \mathcal{C} \mid P(C_m) > \tau\}$ and the final confidence score for the question is computed as:

$$\text{Confidence} = \sum_{C_m \in \mathcal{C}_{\text{valid}}} P(C_m). \quad (2)$$

Experimental results show that SCA achieves comparable performance at $\tau = 0$ to that obtained with the optimal τ (Table 4). This indicates that simply summing token-level probabilities over all sampled

Table 4: AUROC score on LLaMA-3.1-70B-Instruct of different calibration methods under increasing answer mixture. $\tau = 0$ denotes no-filtering, while $\tau \neq 0$ uses the threshold value that achieves the best AUROC on the development set. **Bold** marks the best, and underlined the second-best, in each column.

| Method | [1] | [1,2] | [1,2,4] | [1,2,4,6] |
|-----------------------------------------|-------------|-------------|-------------|-------------|
| Single-turn | | | | |
| <i>Question-level</i> | | | | |
| Prob Entropy | 74.5 | 72.6 | 69.0 | 66.1 |
| N-Prob Entropy | 73.8 | 70.4 | 66.2 | 63.3 |
| Sem Entropy | 78.9 | 78.6 | 75.8 | 72.5 |
| <i>Answer-level</i> | | | | |
| Verb | 58.4 | 58.4 | 57.2 | 55.8 |
| Verb-Topk | 60.7 | 56.2 | 51.2 | 48.4 |
| Consis | 80.2 | <u>80.3</u> | 78.1 | <u>75.3</u> |
| Consis-Verb | 79.7 | 79.1 | 76.6 | 73.8 |
| Consis-Verb-Topk | 80.0 | 79.0 | 77.0 | 74.3 |
| Perplexity | 80.9 | 79.4 | 76.5 | 73.8 |
| Double-turn | | | | |
| P _{True} -Consis | 68.1 | 66.4 | 64.1 | 63.5 |
| P _{True} -Prob | 72.9 | 70.1 | 67.6 | 66.7 |
| P _{True} -Consis-Cand | 62.6 | 62.7 | 62.9 | 62.5 |
| P _{True} -Prob-Cand | 76.0 | 73.5 | 72.5 | 71.1 |
| Self-Ask | 66.5 | 66.1 | 65.0 | 63.9 |
| Self-Ask-Cand | 66.5 | 66.8 | 66.9 | 66.1 |
| Confidence Aggregation Baselines | | | | |
| SNCA ($\tau = 0.5$) | 77.9 | 77.3 | 74.2 | 70.5 |
| SNCA ($\tau = 0$) | 50.0 | 50.0 | 50.0 | 50.0 |
| SFCA ($\tau = 0.25$) | 77.1 | 77.2 | 75.2 | 73.0 |
| SFCA ($\tau = 0$) | 50.0 | 50.0 | 50.0 | 50.0 |
| Ours | | | | |
| SCA ($\tau = 0.05$) | <u>80.6</u> | 81.2 | 79.2 | 76.7 |
| SCA ($\tau = 0$) | 80.5 | 81.2 | <u>79.1</u> | 76.7 |

responses is sufficient, without requiring clustering or filtering, thereby reducing computational cost.

6.2 Experimental Setup

Additional Aggregation Methods. To verify whether using token-level probabilities to compute cluster confidence is appropriate, we compare two additional methods. These methods differ only in how cluster confidence is calculated.

- **SNCA (Semantic Normalized Confidence Aggregation):** normalizes the aggregated token-level probabilities across all clusters to capture relative magnitudes: $P_{\text{SNCA}}(C_m) = \frac{P_{\text{SCA}}(C_m)}{\sum_{j=1}^M P_{\text{SCA}}(C_j)}$.
- **SFCA (Semantic Frequency Confidence Aggregation):** defines probability of a cluster based on the count of samples within it without considering token-level probability: $P_{\text{SFCA}}(C_m) = \frac{|C_m|}{N}$.

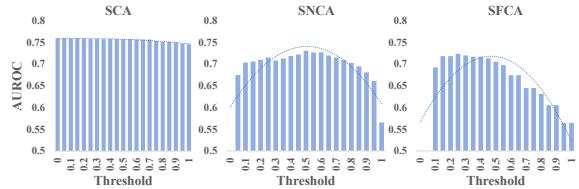


Figure 8: Sensitivity of average AUROC across answer settings to the threshold for our methods.

Models and Datasets. Due to space constraints, experiments focus on LLaMA-3.1-70B-Instruct; results for other models are reported in Appendix § D.1. We randomly sample 20% of MACE as a development set and use the remaining data for testing. For each aggregation method, two settings are evaluated: a fixed threshold $\tau = 0$ and an optimal threshold tuned on the development set.

6.3 Results and Analysis

Table 4 shows calibration performance on the test set, and Figure 8 shows how the three aggregation methods vary with the threshold on the development set. We observe that *SCA matches the best-performing existing methods in the single-answer setting and achieves the strongest results across all three mixed multi-answer scenarios with $\tau = 0$* . This means that SCA achieves strong calibration performance without clustering or any filtering, simply by summing the token-level probabilities of all responses. Compared with SNCA and SFCA, SCA is less sensitive to the threshold. This indicates that the absolute values of token-level probabilities inherently capture the model’s perception of answer correctness, assigning high probabilities to likely correct answers and low probabilities to spurious ones, as shown in Figure 7.

7 Conclusion

This work extends confidence calibration from single-answer QA to a more general setting with mixed numbers of ground-truth answers. We introduce the MACE benchmark, containing 12,000 QA pairs across six factual domains, with 1, 2, 4, or 6 correct answers per question. Using MACE, we evaluate 15 existing calibration methods and find that, as the number of correct answers increases, LLMs achieve higher QA accuracy but lower estimated confidence, leading to severe miscalibration. Consequently, all these methods collapse in realistic settings with mixed answer cardinalities. To address this, we propose SCA (Semantic Confi-

dence Aggregation), which aggregates probabilities of multiple high-confidence answers rather than relying on the top one, achieving state-of-the-art calibration in this general multi-answer setting.

Limitations

While this study offers novel insights into confidence estimation within multi-answer settings, several limitations warrant further consideration. First, our evaluation is currently restricted to English-language datasets; extending this analysis to multilingual or cross-lingual contexts remains essential for a more global understanding of calibration. Second, our scope primarily encompasses short factual responses. Since real-world applications often involve open-ended and compositional generation, investigating confidence behavior in long-form contexts is a crucial next step. Nonetheless, we believe our work provides a useful perspective for more robust calibration frameworks in realistic scenarios.

Ethics Statement

All data used in this study are derived from publicly available and legally accessible sources. We employ both open-weight and API-based large language models under their respective usage policies. All experiments are conducted strictly for academic research purposes, without involving human subjects or sensitive content.

References

- Amanda Askell and 1 others. 2021. A general language assistant as a laboratory for alignment. *arXiv preprint arXiv:2112.00861*.
- Jeremy Cole, Michael Zhang, Daniel Gillick, Julian Eisenschlos, Bhwan Dhingra, and Jacob Eisenstein. 2023. Selectively answering ambiguous questions. In *Proceedings of EMNLP 2023*, pages 530–543.
- DeepSeek-AI. 2024. Deepseek-v3: Scaling open-source language models with dense and mixture-of-experts architecture. *arXiv preprint arXiv:2412.19437*.
- Shrey Desai and Greg Durrett. 2020. Calibration of pre-trained transformers. *arXiv preprint arXiv:2003.07892*.
- Yanai Elazar, Nora Kassner, Shauli Ravfogel, Eduard Ravichander, Abhilasha andHovy, Hinrich Schütze, and Yoav Goldberg. 2021. Measuring and improving consistency in pre-trained language models. In *Transactions of the Association for Computational Linguistics (TACL)*.
- Aaron Grattafiori, Abhimanyu Dubey, Abhinav Jauhri, Abhinav Pandey, Abhishek Kadian, and ... 2024. The llama 3 herd of models. *arXiv preprint arXiv:2407.21783*. [cs.AI].
- Chuan Guo, Geoff Pleiss, Yu Sun, and Kilian Q Weinberger. 2017. On calibration of modern neural networks. In *International conference on machine learning*, pages 1321–1330. PMLR.
- James A Hanley and Barbara J McNeil. 1982. The meaning and use of the area under a receiver operating characteristic (roc) curve. *Radiology*, 143(1):29–36.
- Dan Hendrycks, Collin Burns, Steven Basart, Andy Zou, Mantas Mazeika, Dawn Song, and Jacob Steinhardt. 2021. Measuring massive multitask language understanding. In *Proceedings of the International Conference on Learning Representations (ICLR)*.
- Joue-An Hu and 1 others. 2023. Uncertainty in natural language generation: From theory to practice. *ArXiv preprint*. (Note: Verify specific title for Hu et al 2023 depending on context, assuming FalseQA refers to recent hallucination work).
- Aaron Hurst, Adam Lerer, Adam P. Goucher, Adam Perelman, Aditya Ramesh, Aidan Clark, AJ Ostrow, Akila Welihinda, Alan Hayes, Alec Radford, Aleksander Mądry, ..., Rowan Zellers, and ... 2024. Gpt-4o system card. *arXiv preprint arXiv:2410.21276*. [cs.CL].
- Zhengbao Jiang, Jun Araki, Haibo Ding, and Graham Neubig. 2021. How can we know when language models know? on the calibration of language models for question answering. *Transactions of the Association for Computational Linguistics*, 9:962–977.
- Saurav Kadavath, Tom Conerly, Amanda Askell, Tom Henighan, Dawn Drain, Ethan Perez, Nicholas Schiefer, Zac Hatfield-Dodds, Nova DasSarma, Eli Tran-Johnson, and 1 others. 2022. Language models (mostly) know what they know. *arXiv preprint arXiv:2207.05221*.
- Ryo Kamoi and 1 others. 2023. Wice: Real-world entailment for claims in wikipedia. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing (EMNLP)*.
- Lorenz Kuhn, Yarin Gal, and Sebastian Farquhar. 2023. Semantic uncertainty: Linguistic invariances for uncertainty estimation in natural language generation. In *International Conference on Learning Representations (ICLR)*.
- Junyi Li, Xiaoxue Cheng, Wayne Xin Zhao, Jian-Yun Nie, and Ji-Rong Wen. 2023. Halueval: A large-scale hallucination evaluation benchmark for large language models. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing (EMNLP)*.
- Stephanie Lin, Jacob Hilton, and Owain Evans. 2022a. Teaching models to express their uncertainty in words. *Transactions on Machine Learning Research*.
- Stephanie Lin, Jacob Hilton, and Owain Evans. 2022b. Truthfulqa: Measuring how models mimic human falsehoods. *arXiv preprint arXiv:2109.07958*.

- Chen Ling, Xujiang Zhao, Xuchao Zhang, Wei Cheng, Yanchi Liu, Yiyou Sun, Mika Oishi, Takao Osaki, Katsushi Matsuda, Jie Ji, Guangji Bai, Liang Zhao, and Haifeng Chen. 2024. **Uncertainty quantification for in-context learning of large language models**. In *Proceedings of NAACL 2024*, pages 3357–3370.
- Xiao Liu and 1 others. 2023a. Evaluating the necessary and sufficient conditions for knowledge understanding in large language models. *ArXiv preprint*.
- Yang Liu, Dan Iter, Yichong Xu, Shuohang Wang, Ruochen Xu, and Chenguang Zhu. 2023b. **G-eval: NLg evaluation using gpt-4 with better human alignment**. *arXiv preprint arXiv:2303.16634*.
- Qing Lyu, Kumar Shridhar, Chaitanya Malaviya, Li Zhang, Yanai Elazar, Niket Tandon, Marianna Apidianaki, Mrinmaya Sachan, and Chris Callison-Burch. 2024. **Calibrating large language models with sample consistency**. *arXiv preprint arXiv:2402.13904*.
- Andrey Malinin and Mark Gales. 2021. **Uncertainty estimation in autoregressive structured prediction**. In *International Conference on Learning Representations (ICLR)*.
- Potsawee Manakul, Adian Liusie, and Mark Gales. 2023. **Selfcheckgpt: Zero-resource black-box hallucination detection for generative large language models**. In *Proceedings of EMNLP 2023*, pages 9004–9017.
- Joshua Maynez, Shashi Narayan, Bernd Bohnet, and Ryan McDonald. 2020. On faithfulness and factuality in abstractive summarization. In *Proceedings of ACL 2020*, pages 1906–1919.
- Sewon Min, Kalpesh Krishna, Xinyan Velocity, Sameer Singh, and Hannaneh Hajishirzi. 2023. Factscore: Fine-grained atomic evaluation of factual precision in long form text generation. In *Proceedings of ACL 2023*.
- Shiyu Ni, Keping Bi, Jiafeng Guo, and Xueqi Cheng. 2024. When do llms need retrieval augmentation? mitigating llms’ overconfidence helps retrieval augmentation. *arXiv preprint arXiv:2402.11457*.
- Shiyu Ni, Keping Bi, Jiafeng Guo, Minghao Tang, Jing-tong Wu, Zengxin Han, and Xueqi Cheng. 2025a. Annotation-efficient universal honesty alignment. *arXiv preprint arXiv:2510.17509*.
- Shiyu Ni, Keping Bi, Jiafeng Guo, Lulu Yu, Baolong Bi, and Xueqi Cheng. 2025b. Towards fully exploiting Ilm internal states to enhance knowledge boundary perception. *arXiv preprint arXiv:2502.11677*.
- Jie Ren, Jiaming Luo, Yao Zhao, Kundan Krishna, Mohammad Saleh, Balaji Lakshminarayanan, and Peter J. Liu. 2023. **Out-of-distribution detection and selective generation for conditional language models**. In *International Conference on Learning Representations (ICLR)*.
- Chenglei Si, Zhe Gan, Zhengyuan Yang, Shuohang Wang, Jianfeng Wang, Jordan Boyd-Graber, and Li-juan Wang. 2022. Prompting gpt-3 to be reliable. *arXiv preprint arXiv:2210.09150*.
- Sree Harsha Tanneru, Chirag Agarwal, and Himabindu Lakkaraju. 2024. **Quantifying uncertainty in natural language explanations of large language models**. In *Proceedings of the 27th International Conference on Artificial Intelligence and Statistics (AISTATS)*, volume 238 of *Proceedings of Machine Learning Research*, pages 1072–1080. PMLR.
- James Thorne, Andreas Vlachos, Christos Christodoulopoulos, and Arpit Mittal. 2018. Fever: a large-scale dataset for fact extraction and verification. In *Proceedings of the 2018 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies (NAACL-HLT)*.
- Katherine Tian, Eric Mitchell, Allan Zhou, Archit Sharma, Rafael Rafailov, Huaxiu Yao, Chelsea Finn, and Christopher Manning. 2023. Just ask for calibration: Strategies for eliciting calibrated confidence scores from language models fine-tuned with human feedback. In *Proceedings of EMNLP 2023*, pages 5433–5442, Singapore. Association for Computational Linguistics.
- Gwenyth Portillo Wightman, Alexandra Delucia, and Mark Dredze. 2023. **Strength in numbers: Estimating confidence of large language models by prompt agreement**. In *Proceedings of the 3rd Workshop on Trustworthy Natural Language Processing (TrustNLP 2023)*, pages 326–362.
- Miao Xiong, Zhiyuan Hu, Xinyang Lu, Yifei Li, Jie Fu, Junxian He, and Bryan Hooi. 2024. Can llms express their uncertainty? an empirical evaluation of confidence elicitation in llms. In *International Conference on Learning Representations (ICLR 2024)*.
- An Yang, Baosong Yang, Beichen Zhang, Binyuan Hui, Bo Zheng, Bowen Yu, Chengyuan Li, Dayiheng Liu, Fei Huang, Haoran Wei, Huan Lin, Jian Yang, Jian-hong Tu, Jianwei Zhang, Jianxin Yang, Jiaxi Yang, Jingren Zhou, Junyang Lin, Kai Dang, and 23 others. 2025. **Qwen2.5 technical report**. *arXiv preprint arXiv:2412.15115*. [cs.CL].
- Yuqing Yang, Ethan Chern, Xipeng Qiu, Graham Neubig, and Pengfei Liu. 2024. **Alignment for honesty**. In *Proceedings of the 38th Annual Conference on Neural Information Processing Systems (NeurIPS)*.
- Zhilin Yang, Peng Qi, Saizheng Zhang, Yoshua Bengio, William W Cohen, Ruslan Salakhutdinov, and Christopher D Manning. 2018. Hotpotqa: A dataset for diverse, explainable multi-hop question answering. In *Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing (EMNLP)*.
- Zhangyue Yin, Qiushi Sun, Qipeng Guo, Jiazhao Wu, Xipeng Qiu, and Xuanjing Huang. 2023. Do large

language models know what they don’t know? In *Findings of the Association for Computational Linguistics: ACL 2023*.

Hanning Zhang, Shizhe Diao, Yong Lin, Yi R. Fung, Qing Lian, Xingyao Wang, Yangyi Chen, Heng Ji, and Tong Zhang. 2024. R-tuning: Instructing large language models to say ‘I don’t know’. In *Proceedings of the 2024 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies (Volume 1: Long Papers)*, pages 7106–7132.

Jiaxin Zhang, Zhuohang Li, Kamalika Das, Bradley Malin, and Sricharan Kumar. 2023. Sac3: reliable hallucination detection in black-box language models via semantic-aware cross-check consistency. In *Findings of the Association for Computational Linguistics: EMNLP 2023*, pages 15445–15458.

A The MACE Benchmark

A.1 Domain Identification

To ensure the quality and utility of the benchmark, we establish three core selection principles: objective verifiability, knowledge diversity, and cross-difficulty coverage. Guided by these criteria, we conduct iterative LLM prompting (e.g., GPT-4o, DeepSeek-V3) followed by expert deliberation to refine candidate topics. Ultimately, we finalize six representative factual domains: Honorable Award (Award), Political Office (Office), Regional Affiliation (Region), Mathematical Concept (Math), Natural River (River), and Linguistic Culture (Language).

A.2 Triplet Collection

In our setting, knowledge is represented as a triplet (s, r, \mathcal{O}) , where each component is defined as follows: (1) The **subject** s represents the primary entity or anchor of the query (e.g., *Nobel Prize in Physics*); (2) The **relation** r denotes the semantic predicate or attribute connecting the subject to the answers (e.g., *laureate of*); (3) The **object set** $\mathcal{O} = \{o_1, o_2, \dots, o_k\}$ contains the set of all valid ground-truth entities that satisfy the relation r for subject s . By varying the cardinality of the object set $|\mathcal{O}| \in \{1, 2, 4, 6\}$.

Except for the *Math* domain, which is generated through rule synthesis, all other domains are collected via the Wikidata SPARQL endpoint². Specifically, for each domain, we query Wikidata to retrieve relevant subjects and their associated factual objects based on defined relations (see Table 6).

For instance, in the *Award* domain, we retrieve the entity *Nobel Prize in Physics* as the subject and obtain its *laureates* in a specific year as the objects based on relations “is officially awarded to”. To ensure alignment with common model knowledge, we restrict the temporal coverage to the years 1800–2023.

A.3 Heuristic-Based Filtering

To ensure data quality, we apply a two-stage filtering process: *Popularity Filter* followed by a *Validity Filter*. *Popularity Filter* is applied to the subjects of the knowledge triplets while *Validity filter* is applied to subjects and objects. *Popularity Filter* ranks all entity labels within each domain by their 12-month Wikipedia pageviews, retaining the top 5K entries and any items with more than 1K views. Afterward, *Validity Filter* removes entries with empty or invalid fields (e.g., missing labels, broken links, unresolved QIDs) and applies domain-specific refinement criteria. Because raw Wikidata outputs are often incomplete or noisy, we further impose structured constraints to ensure factual consistency and completeness:

- **Award:** retain only subjects granted to a single laureate per year, with continuous yearly records and at least three objects per subject.
- **Office:** preserve subjects held by exactly one person per year, requiring a minimum of ten recorded years per subject.
- **Region:** include only countries with at least three administrative subdivisions.
- **River & Language:** keep entities associated with no more than six countries to avoid overly generic mappings. To control annotation cost, we sample 600 instances from objects associated with a single subject.

A.4 Manual Verification

To ensure the factual accuracy and internal consistency of all harvested labels, we conduct a multi-stage human verification process. Two domain experts independently review each domain’s entries for factual correctness, completeness, and consistency with Wikidata metadata. Each label is cross-checked against its supporting evidence (e.g., year, person, or country linkage) to confirm semantic validity and eliminate potential entity mismatches. Disagreements are resolved through consensus discussions. Annotation reliability, measured using

²<https://query.wikidata.org/sparql>

| Domain | Core Prompt Template |
|----------|-----------------------------------------------------------------------------------------------------------------------------------|
| Award | Name one person who received {award} between {lower_year} and {upper_year}. |
| Office | Name one person from who officially assumed the office of {office name} between {lower_year} and {upper_year}. |
| Country | Name one first-level administrative division of {country} whose area lies between {lower_area} and {upper_area} km ² . |
| Math | Name one {number type} number between {lower_num} and {upper_num}. |
| Language | Name one country where {language_1}, {language_2} or {language_3} was predominantly spoken by native speakers. |
| River | Name one country through which the {river_1}, {river_2}, or {river_3} flows. |

Table 5: Core prompt templates for each factual domain.

Table 6: **Detailed schema of relations and entity types across six factual domains.** This table outlines the semantic categories for subjects and objects, along with the specific predicates used to query the knowledge graph.

| Domain | Subject Type | Relation Description | Object Type |
|----------------------|--------------------|------------------------------|-------------------------------------|
| Honorable Award | Award Name | Is officially awarded to | Person |
| Political Office | Political Position | Is officially held by | Person |
| Regional Affiliation | Sovereign Country | Contains | First-level Administrative Division |
| Mathematical Concept | Number Types | Includes as an instance | Number |
| Natural River | River Name | Flows through geographically | Country |
| Linguistic Culture | Human Language | Is spoken widely in | Country |

Cohen’s $\kappa = 0.94$ across all domains, indicating strong agreement. We further perform iterative spot-checking for quality assurance: for each domain, a random sample of 50 instances is revalidated to confirm factual soundness and formatting consistency. This verification–revision loop is repeated until no residual errors remain (two full rounds in total).

A.5 QA Pair Generation

Our prompt templates are summarized in Table 5.

Retrieval-based Domains. Each domain consists of a unique set of factual subjects, where each subject is linked to one or more objects, forming the foundational knowledge triplets (s, r, \mathcal{O}) . To construct questions with a specific number of correct answers ($k \in \{1, 2, 4, 6\}$), we dynamically adjust the constraints within each domain.

Specifically, we employ a *constraint relaxation* strategy to obtain triplets with the desired number of ground-truth objects based on the initial subject-to-object mapping. We implement this through two distinct approaches:

(1) **One-to-Many Expansion (Intra-subject):** Include domains *Award*, *Office*, and *Region*. For subjects that naturally possess multiple objects under a broad relation, we relax the relational constraints while keeping the subject fixed. For instance, instead of querying for the "winner of the 1995 Nobel Prize in Physics" (single-answer), we expand the relation to "winners of the Nobel Prize

in Physics between 1990 and 1995" to harvest a larger, pre-defined set of objects.

(2) **One-to-Few Aggregation (Cross-subject):** Include domains *Language* and *River*. For scenarios where a single subject-relation pair cannot naturally yield enough objects, we construct multi-answer instances by systematically combining multiple subjects that share the same relation. For example, we may aggregate two subjects that each possess only one or two correct answers into a single question (e.g., "Name one country speaking language A or language B") to satisfy the required answer count.

This dual-path approach ensures that the factual density of our benchmark is systematically controlled while maintaining logical coherence and high relevance across different answer counts.

Rule-based Domain. The *Math* domain is defined through five numeric subjects. (Table 7), each acting as a pseudo-label. As these categories span broad numerical ranges, we do not construct natural questions explicitly. Instead, we generate queries by uniformly sampling numbers from the interval $[0, 1,000,000]$, providing wide coverage of numerical reasoning behaviors.

Quality control All generated QA instances first undergo rigorous deduplication, and we ensure that no label appears in multiple domains to prevent cross-domain leakage. To construct a representative and balanced dataset, we employ a clustering-

| Number Type | Definition |
|-------------|-------------------------------------------------------------|
| prime | $p > 1, p \in \mathbb{N}, \nexists d \in (1, p) : d \mid p$ |
| square | $n = k^2, k \in \mathbb{N}$ |
| cube | $n = k^3, k \in \mathbb{N}$ |
| fibonacci | $F_n = F_{n-1} + F_{n-2}, F_1 = F_2 = 1$ |
| triangular | $T_n = \frac{n(n+1)}{2}, n \in \mathbb{N}$ |

Table 7: Five mathematical number types used to construct questions in the *Math* domain. Each defines a distinct numeric sequence within $[0, 10^6]$.

based sampling strategy. Specifically, for each answer setting within a domain, we perform K-Means clustering to partition the instances into $k = 500$ clusters and select the sample closest to the centroid of each cluster. This process yields 2,000 distinct samples per domain, resulting in a final dataset totaling 12,000 instances.

B Experiment Setup

B.1 Calibration Methods

- **Prediction Entropy.** (Kadavath et al., 2022)

To capture uncertainty across M generated responses, we compute the mean token-level entropy over all samples:

$$U_{\text{Prob Entropy}} = -\frac{1}{M} \sum_{j=1}^M \sum_{i=1}^{|r_j|} p_{z_i} \log p_{z_i}, \quad (3)$$

where p_{z_i} represents the normalized probability distribution over tokens within the j -th generation.

- **Length-Normalized Prediction Entropy.**

(Malinin and Gales, 2021) To avoid bias toward longer sequences, we normalize the entropy of each sampled response by its length:

$$U_{\text{N-Prob Entropy}} = -\frac{1}{M} \sum_{j=1}^M \frac{1}{|r_j|} \sum_{i=1}^{|r_j|} p_{z_i} \log p_{z_i}. \quad (4)$$

This normalization ensures comparable uncertainty estimates across outputs of varying lengths.

- **Semantic Entropy.** (Kuhn et al., 2023) Given a set of semantic clusters $\{C_1, \dots, C_K\}$ obtained from multiple sampled responses, we compute a probability distribution over clusters by aggregating the sentence-level probabilities. Specifically, the probability assigned to cluster C_k is

$$P(C_k) = \sum_{r_j \in C_k} P(r_j), \quad (5)$$

where $P(r_j)$ denotes the generation probability of response r_j .

In standard semantic-entropy settings, these cluster probabilities are typically normalized to form a valid distribution:

$$\tilde{P}(C_k) = \frac{P(C_k)}{\sum_{i=1}^K P(C_i)}, \quad (6)$$

yielding $\tilde{P}(C_k) \in [0, 1]$ and $\sum_k \tilde{P}(C_k) = 1$.

The semantic entropy is then computed as the Shannon entropy of the normalized cluster distribution:

$$U_{\text{SE}} = -\sum_{k=1}^K \tilde{P}(C_k) \log \tilde{P}(C_k), \quad (7)$$

which quantifies the degree of semantic dispersion in the model’s outputs—high values indicate diverse or inconsistent answer patterns, while low values correspond to concentrated semantic predictions.

- **Verb.** (Jiang et al., 2021) This method elicits confidence by prompting the model to verbalize a numeric confidence score alongside its answer. Given a question x , the model generates a textual response containing both the answer \hat{y} and a confidence expression. The confidence value C is then extracted from the generated text:

$$C_{\text{Verb}} = \text{LLM}(x). \quad (8)$$

Example prompt:

[Instruction] You are a knowledgeable assistant. Please answer the following question and provide your confidence as a numeric value between 0 and 1 (e.g., 0.85 means you are 85% confident).

[Input] Question: {question}

[Output format] Answer: {answer} Confidence: {confidence between 0 and 1, with two-decimal precision}

- **Verb_{Topk}.** (Xiong et al., 2024) This variant extends the verbalization setting by asking the model to provide k distinct candidate answers $\{\hat{y}_1, \hat{y}_2, \dots, \hat{y}_k\}$ along with their respective confidences $\{C_1, C_2, \dots, C_k\}$. The final confidence is defined as the maximum confidence among semantically valid candidates:

$$C_{\text{Verb}_{\text{Topk}}} = \max_{1 \leq i \leq k} (C_i \cdot \mathbb{I}\{\hat{y}_i \in \mathcal{Y}^*\}), \quad (9)$$

where \mathcal{Y}^* denotes the set of semantically valid answers.

Example prompt:

[Instruction] You are a knowledgeable assistant. Please list your top-\$k\$ most likely answers to the following question. For each answer, report your numeric confidence between 0 and 1 (e.g., 0.85 means 85% confident). Use two-decimal precision for all confidence values.

[Input] Question: {question}

[Output format] 1. Answer: {answer_1}, Confidence: {confidence_1} 2. Answer: {answer_2}, Confidence: {confidence_2} 3. Answer: {answer_3}, Confidence: {confidence_3} ... up to \$k\$ answers.

- **Consistency.** (Manakul et al., 2023) Consistency score measures the proportion of model samples that agree with the aggregated prediction \tilde{Y} among M sampled outputs:

$$C_{\text{consistency}} = \frac{1}{M} \sum_{i=1}^M \mathbb{I}\{\hat{Y}_i = \tilde{Y}\}, \quad (10)$$

- **Weighted Consistency**(Xiong et al., 2024) To incorporate the self-reported confidence C_i of each sampled answer, we further introduce a weighted variant:

$$C_{\text{conf}} = \frac{\sum_{i=1}^M \mathbb{I}\{\hat{Y}_i = \tilde{Y}\} \times C_i}{\sum_{i=1}^M C_i}, \quad (11)$$

where higher-confidence answers contribute proportionally more to the final score. When C_i is obtained from the *Verb* or *Verb_{Topk}* methods, this variant corresponds to *Consistency-Verb* and *Consistency-Verb-Topk*, respectively.

- **Perplexity.**(Manakul et al., 2023) Perplexity is computed as the average negative log-likelihood of token probabilities:

$$U_{\text{Perplexity}} = -\frac{1}{|r|} \sum_{i=1}^N \log p_{z_i}, \quad (12)$$

where r denotes the generated sequence and p_{z_i} is the model-assigned probability for the i -th token.

- **P_{True}-Consis/P_{True}-Prob** (Kadavath et al., 2022). These methods estimate model confidence by prompting the LLM to explicitly verify whether its previously generated answer is correct. The verification prompt x' asks the model to respond with “True” or “False”, and the resulting confidence is defined as the probability of the token “True”:

$$C_{\text{P}_{\text{True}}} = p(z_{\text{true}} | x'). \quad (13)$$

We implement two variants: (1) In the **P_{True}-Consis** variant, confidence is obtained by performing multiple sampling runs and taking the empirical frequency of the “True” response across samples; (2) In the **P_{True}-Prob** variant, we directly use the model’s internal probability (logit-derived softmax value) assigned to the “True” token, without repeated sampling.

Example prompt:

[Instruction] You will be given a question and the model’s previous answer. Please respond with True if the answer is factually correct, or False if it is incorrect. Answer strictly with either “True” or “False” only.

[Input] Question: What is the capital of France?

Model answer: Paris.

[Output] True

- **P_{True}-Consis-Cand/P_{True}-Prob-Cand** (Kadavath et al., 2022). To better handle multi-answer scenarios, we extend the verification prompt x' by including a set of candidate answers $\{a_1, a_2, \dots, a_K\}$, allowing the model to evaluate its response in the context of multiple plausible answers:

$$C_{\text{P}_{\text{True}}-\text{Consis-Cand}} = p(z_{\text{true}} | x', \{a_1, a_2, \dots, a_K\}). \quad (14)$$

Similarly, two variants are considered: (1) In the **P_{True}-Consis-Cand** variant, confidence is computed as the empirical frequency of “True” responses across multiple sampling runs; (2) In the **P_{True}-Prob-Cand** variant, the probability assigned to the “True” token from the model’s logits is used directly as the confidence score.

Example prompt:

[Instruction] You will be given a question, the model’s answer, and several candidate answers. Please respond with True if the model’s answer is factually correct, or False if it is incorrect. Answer strictly with either “True” or “False” only.

[Input] Question: Which player won the UEFA Euro 2016 Best Young Player Award?

Model answer: Renato Sanches.

Candidate answers: Renato Sanches, Anthony Martial, Raheem Sterling.

[Output] True

- **SelfAsk**(Tian et al., 2023). This method prompts the model to *self-assess* and directly verbalize its own confidence score after producing an answer. Given a question–answer pair (x, \hat{y}) , the model is re-prompted with a

meta-instruction asking it to output a numerical confidence value (e.g., “0.85”) that reflects how certain it is about \hat{y} . The resulting confidence is defined as:

$$C_{\text{SelfAsk}} = \text{LLM}(x', \hat{y}), \quad (15)$$

where x' denotes the self-assessment prompt and $\text{LLM}(\cdot)$ returns a scalar confidence value verbalized by the model.

Example prompt:

Question: What is the capital of France?

Answer: Paris.

How confident are you that your answer is correct? Please output only a number between 0 and 1 (e.g., 0.85).

- **SelfAsk-Cand(Tian et al., 2023).** To better account for uncertainty among multiple plausible answers, this variant augments the verification prompt with a set of candidate answers $\{a_1, a_2, \dots, a_K\}$. The model is instructed to assess its confidence in \hat{y} given this broader context. The confidence is computed as:

$$C_{\text{SelfAsk-Cand}} = \text{LLM}(x', \hat{y}, \{a_1, a_2, \dots, a_K\}), \quad (16)$$

where x' includes both the original answer and the candidate list as context for self-evaluation.

Example prompt:

Question: What is the capital of France?

Candidate answers: Paris, Lyon, Marseille.

Considering these candidates, how confident are you that your original answer (Paris) is correct?

Please output only a number between 0 and 1 (e.g., 0.85).

B.2 Domain Effects: Relation Between Question Type and Difficulty

We analyze the domain-level calibration behavior of **LLaMA-3.1-70B-Instruct** across varying ground-truth set sizes. As illustrated in Figure 9, all configurations (1a/2a/4a/6a) exhibit a highly consistent trend: domains characterized by higher accuracy (lower intrinsic difficulty) also demonstrate

higher confidence levels. Crucially, due to the significant disparity in intrinsic difficulty across these specialized domains, we employ the macro-average as the primary metric. This approach prevents the aggregate performance from being disproportionately skewed by high-accuracy, low-difficulty domains, thereby ensuring a more representative evaluation of global calibration.

The observed variation in accuracy and confidence is primarily driven by the structural differences in question construction across domains (see Appendix § A.5). Each domain imposes unique constraints on how questions are formulated and how answers are distributed, which directly modulates the cognitive load and retrieval complexity of the task.

One-to-Few Domains (Language, River): Low Difficulty. Domains such as *Language* and *River* follow a one-to-few mapping, where each subject is associated with only a handful of factual objects. Multi-answer questions are constructed by relaxing constraints of subjects scope. Since the options consist of short, distinct noun phrases within a tightly bounded semantic space, the model encounters minimal ambiguity. Consequently, these domains yield the highest accuracy and confidence.

One-to-Many Domains (Award, Office, Region): Moderate to High Difficulty. In *Award*, *Office*, and *Region*, each subject corresponds to a vast pool of factual objects. To ensure answer uniqueness, questions must be grounded in specific contextual attributes (e.g., years, tenure, or administrative roles). This necessitates additional reasoning steps, such as linking a specific temporal constraint to a unique recipient, thereby increasing the complexity of the *answer space*. Among these, *Region* represents the most challenging domain; many entities share similar geopolitical or geographic features, leading to high semantic overlap and an increased likelihood of model confusion.

Rule-Based Numerical Questions (Math): Moderate Difficulty. The *Math* domain utilizes five numeric categories as subjects, with queries constructed by sampling values from broad numerical intervals. Unlike the factual retrieval required in other domains, these tasks demand the recognition of abstract numeric properties. The resulting performance is intermediate—outperforming the complex attribute-linking in *Award* and *Country*, but proving more difficult than the simple noun-phrase



Figure 9: Domain-specific accuracy and confidence under different ground-truth sizes.

enumeration found in *Language* and *River*.

C Results and Analysis

C.1 Estimated Confidence Drops on Questions with More Correct Answers.

We report the **confidence** of all evaluated models under different numbers of valid answers (1a/2a/4a/6a), as shown in Tables 8–15. Note that for API-based models (e.g., GPT-4o, GPT-4o-mini, and DeepSeek-V3), we do not report methods that rely on logit probabilities or internal token distributions, such as Prob-Entropy, N-Prob-Entropy and Sem Entropy. Across model families and parameter scales, a clear and consistent pattern emerges: model accuracy follows a steady upward trend as the number of valid answers increases. However, the model confidence exhibits a diametrically opposite decline over the same range. This diverging behavior reveals a significant misalignment between the models’ actual performance and their certainty: as the task environment becomes more “favorable” (i.e., more valid answers are available), the models paradoxically become increasingly “underconfident.” Such a monotonic decline in confidence despite rising accuracy demonstrates that existing calibration methods are unable to remain stable when confronted with multi-answer

Table 8: **Confidence scores of Qwen2.5-7B-Instruct** under different ground truth(GT) set sizes.

| Method | 1a | 2a | 4a | 6a |
|--------------------------------|------|------|------|------|
| Single-turn | | | | |
| <i>Question-level</i> | | | | |
| Prob Entropy | 67.8 | 68.2 | 66.9 | 66.6 |
| N-Prob Entropy | 92.1 | 92.3 | 92.0 | 91.9 |
| Sem Entropy | 64.7 | 65.5 | 63.6 | 62.9 |
| <i>Answer-level</i> | | | | |
| Verb | 94.7 | 95.4 | 94.8 | 94.7 |
| Verb _{Topk} | 82.5 | 81.3 | 73.7 | 71.8 |
| Consistency | 53.1 | 54.7 | 52.6 | 51.9 |
| Consis-Verb | 44.9 | 44.3 | 41.2 | 40.5 |
| Consis-Verb-Topk | 35.1 | 35.3 | 31.1 | 30.7 |
| Perplexity | 79.2 | 79.6 | 79.4 | 79.1 |
| Double-turn | | | | |
| P _{True} -Consis | 46.9 | 47.0 | 45.0 | 46.9 |
| P _{True} -Prob | 46.8 | 46.9 | 44.9 | 46.8 |
| P _{True} -Consis-Cand | 59.3 | 61.0 | 62.9 | 65.0 |
| P _{True} -Prob-Cand | 59.4 | 61.1 | 63.0 | 65.2 |
| Self _{Ask} | 73.7 | 73.8 | 73.0 | 73.7 |
| Self _{Ask} -Cand | 70.5 | 71.5 | 71.1 | 72.2 |

variation, highlighting a fundamental limitation of current approaches.

C.2 Analysis of Cluster Probability Distribution

To obtain a reliable measure of the *effective* answer space, it is important to examine how probability mass is distributed across semantic clusters

Table 9: **Confidence scores of Qwen2.5-14B-Instruct** under different ground truth(GT) set sizes.

| Method | 1a | 2a | 4a | 6a |
|--------------------------------|-----------|-----------|-----------|-----------|
| Single-turn | | | | |
| <i>Question-level</i> | | | | |
| Prob Entropy | 73.4 | 73.3 | 72.4 | 71.7 |
| N-Prob Entropy | 93.7 | 93.6 | 93.5 | 93.2 |
| Sem Entropy | 70.6 | 71.3 | 69.9 | 68.4 |
| <i>Answer-level</i> | | | | |
| Verb | 87.4 | 87.1 | 85.6 | 85.4 |
| Verb _{Topk} | 87.6 | 84.0 | 74.1 | 70.5 |
| Consistency | 62.7 | 63.3 | 62.5 | 61.0 |
| Congis-Verb | 42.2 | 45.6 | 43.4 | 41.7 |
| Congis-Verb-Topk | 45.5 | 44.8 | 42.7 | 40.7 |
| Perplexity | 85.6 | 85.8 | 85.8 | 85.4 |
| Double-turn | | | | |
| P _{True} -Cognis | 50.1 | 52.2 | 49.4 | 49.5 |
| P _{True} -Prob | 50.1 | 52.2 | 49.4 | 49.5 |
| P _{True} -Cognis-Cand | 67.1 | 69.8 | 71.8 | 71.9 |
| P _{True} -Prob-Cand | 67.1 | 69.8 | 71.8 | 71.9 |
| Self _{Ask} | 77.5 | 78.7 | 76.0 | 75.2 |
| Self _{Ask} -Cand | 76.2 | 78.2 | 78.0 | 77.4 |

formed from multiple sampled responses. Our statistical analysis of cluster probabilities shows that over **70%** of clusters lie within the 0–0.1 range, indicating that most clusters carry only negligible probability mass and predominantly represent spurious or semantically irrelevant outputs. In contrast, a small number of clusters receive substantially higher mass and represent the dominant semantic modes of the model’s response distribution.

Because each cluster’s probability is defined as the *sum of absolute probabilities* of its member responses, applying a threshold effectively filters out clusters whose cumulative probability is intrinsically small. In other words, clusters with $P(C_m) < \tau$ contribute only negligible absolute probability mass and primarily reflect sampling noise rather than meaningful alternative answers.

Motivated by the empirical distribution, we retain only clusters whose cumulative probability satisfies

$$P(C_m) \geq 0.1.$$

This value serves as a natural dividing point between the large concentration of near-zero clusters and the smaller set of semantically coherent ones. Across domains and models, clusters above this threshold consistently exhibit stable semantics, while those below it are dominated by fragmented or degenerate responses.

Applying this threshold yields a more faithful estimate of the *effective* answer space and provides a clearer view of how semantic dispersion influences

Table 10: **Confidence scores of Qwen2.5-32B-Instruct** under different ground truth(GT) set sizes.

| Method | 1a | 2a | 4a | 6a |
|--------------------------------|-----------|-----------|-----------|-----------|
| Single-turn | | | | |
| <i>Question-level</i> | | | | |
| Prob Entropy | 74.9 | 74.2 | 73.4 | 72.7 |
| N-Prob Entropy | 94.1 | 94.1 | 93.8 | 93.6 |
| Sem Entropy | 72.8 | 72.4 | 71.2 | 69.1 |
| <i>Answer-level</i> | | | | |
| Verb | 88.6 | 88.1 | 87.3 | 87.7 |
| Verb _{Topk} | 87.6 | 82.4 | 75.1 | 72.4 |
| Consistency | 64.9 | 63.9 | 62.9 | 61.2 |
| Congis-Verb | 54.1 | 52.7 | 51.8 | 50.5 |
| Congis-Verb-Topk | 48.1 | 45.9 | 44.7 | 42.2 |
| Perplexity | 85.9 | 85.7 | 85.5 | 85.0 |
| Double-turn | | | | |
| P _{True} -Cognis | 69.4 | 76.2 | 78.2 | 78.4 |
| P _{True} -Prob | 69.5 | 76.2 | 78.3 | 78.5 |
| P _{True} -Cognis-Cand | 74.9 | 78.7 | 81.0 | 81.9 |
| P _{True} -Prob-Cand | 74.9 | 78.7 | 81.1 | 81.9 |
| Self _{Ask} | 72.8 | 72.5 | 70.7 | 72.4 |
| Self _{Ask} -Cand | 73.2 | 75.2 | 75.6 | 76.1 |

confidence.

C.3 Spearman Validity Across Knowledge Coverage

To assess the reliability of the Spearman correlation between model confidence and answer space size, we first analyze how the distribution of semantic clusters changes across different ground-truth cardinalities (1a, 2a, 4a, 6a). As shown in Figure 6, all GT settings exhibit a smooth distribution, with no domination by a small number of cluster sizes. For 1a, the majority of clusters are of size 1–3, with a light tail. As GT increases to 2, 4, and 6, the distribution shifts toward larger cluster sizes, remaining well-dispersed without skewing toward any particular cluster size.

This consistent shift suggests that the answer space expands in a stable and balanced manner: higher GT increases the space without collapsing it into a narrow mode or generating extreme outliers that might bias rank-based correlation measures. Because cluster frequencies remain diverse and avoid dominance effects, the Spearman correlation is not artificially skewed by outlier cluster sizes.

Results in Table 17 show the Spearman correlation between confidence and knowledge coverage. We find a notable negative correlation between these two metrics across multiple models, suggesting that higher confidence does not necessarily align with broader knowledge coverage.

Table 11: **Confidence scores of Qwen2.5-72B-Instruct** under different ground truth(GT) set sizes.

| Method | 1a | 2a | 4a | 6a |
|---------------------------------|-----------|-----------|-----------|-----------|
| Single-turn | | | | |
| <i>Question-level</i> | | | | |
| Prob Entropy | 76.4 | 75.4 | 74.3 | 73.4 |
| N-Prob Entropy | 94.1 | 93.9 | 93.5 | 93.3 |
| Sem Entropy | 71.8 | 70.3 | 68.3 | 66.6 |
| <i>Answer-level</i> | | | | |
| Verb | 87.9 | 87.3 | 86.2 | 86.8 |
| Verb _{Topk} | 85.9 | 79.5 | 70.8 | 69.9 |
| Consistency | 65.4 | 64.2 | 61.5 | 59.8 |
| Consis-Verb | 59.0 | 58.2 | 55.5 | 53.7 |
| Consis-Verb-Topk | 53.2 | 52.8 | 48.1 | 45.0 |
| Perplexity | 87.7 | 87.2 | 86.2 | 85.5 |
| Double-turn | | | | |
| P _{True} -Cconsis | 75.1 | 73.3 | 68.6 | 73.7 |
| P _{True} -Prob | 75.2 | 73.3 | 68.8 | 73.9 |
| P _{True} -Cconsis-Cand | 75.8 | 76.0 | 73.4 | 77.6 |
| P _{True} -Prob-Cand | 75.8 | 76.1 | 73.5 | 77.7 |
| Self _{Ask} | 84.9 | 79.7 | 72.9 | 75.3 |
| Self _{Ask} -Cand | 83.5 | 81.8 | 76.6 | 79.5 |

D Semantic Confidence Aggregation

D.1 Generalization Across Models

To evaluate the generalization capability of our methods, we extend our experiments to the **Qwen-2.5-72B-Instruct** model. As reported in Table 16, our methods consistently achieve superior performance on this alternative architecture. This consistent improvement demonstrates that SCA is robust and model-agnostic, maintaining its effectiveness across different large language models.

Table 12: **Confidence scores of LLaMA-3.1-8B-Instruct** under different ground truth(GT) set sizes.

| Method | 1a | 2a | 4a | 6a |
|---------------------------------|-----------|-----------|-----------|-----------|
| Single-turn | | | | |
| <i>Question-level</i> | | | | |
| Prob Entropy | 63.4 | 62.5 | 60.6 | 59.5 |
| N-Prob Entropy | 89.7 | 89.3 | 88.8 | 88.6 |
| Sem Entropy | 49.9 | 51.4 | 47.5 | 45.1 |
| <i>Answer-level</i> | | | | |
| Verb | 96.2 | 96.1 | 96.2 | 96.2 |
| Verb _{Topk} | 95.8 | 96.3 | 96.2 | 96.3 |
| Consistency | 36.0 | 36.8 | 32.7 | 30.4 |
| Consis-Verb | 37.1 | 37.0 | 33.5 | 30.7 |
| Consis-Verb-Topk | 30.4 | 29.8 | 26.9 | 24.6 |
| Perplexity | 67.0 | 67.6 | 65.9 | 64.4 |
| Double-turn | | | | |
| P _{True} -Cconsis | 53.3 | 50.8 | 46.2 | 45.9 |
| P _{True} -Prob | 53.1 | 50.9 | 46.4 | 45.7 |
| P _{True} -Cconsis-Cand | 64.8 | 65.7 | 66.1 | 65.7 |
| P _{True} -Prob-Cand | 64.7 | 65.7 | 65.9 | 65.9 |
| Self _{Ask} | 37.7 | 31.7 | 26.8 | 27.2 |
| Self _{Ask} -Cand | 45.4 | 47.8 | 46.3 | 46.1 |

Table 13: **Confidence scores of GPT-4o-mini** under different ground truth(GT) set sizes.

| Method | 1a | 2a | 4a | 6a |
|---------------------------------|-----------|-----------|-----------|-----------|
| Single-turn | | | | |
| <i>Question-level</i> | | | | |
| Sem Entropy | 49.6 | 50.1 | 46.2 | 44.9 |
| <i>Answer-level</i> | | | | |
| Verb | 93.2 | 92.1 | 91.1 | 90.8 |
| Verb _{Topk} | 83.7 | 73.0 | 61.5 | 56.5 |
| Consistency | 60.1 | 60.3 | 57.6 | 56.5 |
| Consis-Verb | 54.1 | 54.3 | 51.2 | 50.2 |
| Consis-Verb-Topk | 48.7 | 46.3 | 42.4 | 41.1 |
| Double-turn | | | | |
| P _{True} -Cconsis | 62.5 | 67.7 | 68.3 | 70.5 |
| P _{True} -Cconsis-Cand | 72.3 | 77.0 | 77.6 | 79.1 |
| Self _{Ask} | 76.3 | 76.1 | 73.7 | 74.9 |
| Self _{Ask} -Cand | 73.7 | 76.4 | 76.9 | 76.6 |

Table 14: **Confidence scores of GPT-4o** under different ground truth(GT) set sizes.

| Method | 1a | 2a | 4a | 6a |
|---------------------------------|-----------|-----------|-----------|-----------|
| Single-turn | | | | |
| <i>Question-level</i> | | | | |
| Sem Entropy | 63.0 | 54.1 | 45.4 | 40.4 |
| <i>Answer-level</i> | | | | |
| Verb | 92.1 | 90.7 | 88.8 | 88.5 |
| Verb _{Topk} | 89.6 | 85.6 | 71.8 | 67.4 |
| Consistency | 70.1 | 64.3 | 56.5 | 52.6 |
| Consis-Verb | 68.8 | 62.8 | 54.8 | 50.6 |
| Consis-Verb-Topk | 65.1 | 58.5 | 48.8 | 45.8 |
| Double-turn | | | | |
| P _{True} -Cconsis | 64.3 | 66.8 | 68.4 | 70.4 |
| P _{True} -Cconsis-Cand | 80.0 | 81.0 | 80.5 | 80.0 |
| Self _{Ask} | 77.8 | 75.8 | 74.9 | 75.3 |
| Self _{Ask} -Cand | 80.5 | 80.4 | 79.0 | 77.9 |

Table 15: **Confidence scores of DeepSeek-V3** under different ground truth(GT) set sizes.

| Method | 1a | 2a | 4a | 6a |
|---------------------------------|------|------|------|------|
| Single-turn | | | | |
| <i>Question-level</i> | | | | |
| Sem Entropy | 80.9 | 78.6 | 76.2 | 72.9 |
| <i>Answer-level</i> | | | | |
| Verb | 85.3 | 85.5 | 85.8 | 86.0 |
| Verb _{Topk} | 63.5 | 57.5 | 52.7 | 50.5 |
| Consistency | 81.1 | 79.1 | 76.7 | 73.2 |
| Consis-Verb | 69.0 | 65.9 | 60.6 | 55.6 |
| Consis-Verb-Topk | 63.4 | 58.5 | 53.6 | 49.0 |
| Double-turn | | | | |
| P _{True} -Cconsis | 64.3 | 64.6 | 64.7 | 66.2 |
| P _{True} -Cconsis-Cand | 82.4 | 81.5 | 82.5 | 80.5 |
| Self _{Ask} | 76.5 | 72.8 | 69.8 | 71.2 |
| Self _{Ask} -Cand | 83.8 | 81.3 | 80.8 | 78.7 |

Table 17: **Spearman correlation of confidence with knowledge coverage** across ground-truth(GT) set sizes.

| Model | 1a | 2a | 4a | 6a |
|---------------|--------|--------|--------|--------|
| Qwen2.5-7B | 0.009 | -0.000 | -0.000 | -0.012 |
| Qwen2.5-14B | -0.443 | -0.438 | -0.427 | -0.421 |
| Qwen2.5-32B | -0.421 | -0.421 | -0.407 | -0.399 |
| Qwen2.5-72B | -0.616 | -0.551 | -0.533 | -0.516 |
| Llama-3.1-8B | 0.242 | 0.227 | 0.325 | 0.366 |
| Llama-3.1-70B | -0.393 | -0.314 | -0.167 | -0.055 |
| GPT-4o-mini | -0.590 | -0.563 | -0.567 | -0.544 |
| GPT-4o | -0.821 | -0.779 | -0.729 | -0.684 |
| DeepSeek-V3 | -0.854 | -0.827 | -0.820 | -0.807 |

Table 16: **AUROC score on Qwen-2.5-72B-Instruct** of different calibration methods under increasing answer mixture. $\tau = 0$ denotes no-filtering, while $\tau \neq 0$ uses the threshold value that achieves the best AUROC on the development set. **Bold** marks the best, and underlined the second-best, in each column.

| Method | [1] | [1,2] | [1,2,4] | [1,2,4,6] |
|-----------------------------------------|-------------|-------------|-------------|-------------|
| Single-turn | | | | |
| <i>Question-level</i> | | | | |
| Prob Entropy | 82.4 | 79.1 | 78.4 | <u>77.5</u> |
| N-Prob Entropy | 81.8 | 78.4 | 77.0 | <u>76.2</u> |
| Sem Entropy | 77.3 | 75.6 | 75.1 | 73.9 |
| <i>Answer-level</i> | | | | |
| Verb | 64.3 | 60.6 | 58.5 | 57.4 |
| Verb-Topk | 67.7 | 64.1 | 59.9 | 57.7 |
| Consis | 78.2 | 77.1 | 76.7 | 75.8 |
| Consis-Verb | 77.5 | 75.8 | 75.4 | 74.1 |
| Consis-Verb-Topk | 75.1 | 73.3 | 72.3 | 71.0 |
| Perplexity | <u>82.0</u> | 79.9 | <u>78.5</u> | 77.4 |
| Double-turn | | | | |
| P _{True} -Consis | 73.7 | 70.0 | 69.4 | 69.6 |
| P _{True} -Prob | 81.3 | 77.2 | 76.2 | 76.3 |
| P _{True} -Consis-Cand | 71.1 | 69.2 | 68.3 | 68.2 |
| P _{True} -Prob-Cand | 81.5 | 77.5 | 75.8 | 75.6 |
| Self-Ask | 67.1 | 64.1 | 62.1 | 61.6 |
| Self-Ask-Cand | 74.4 | 70.6 | 67.2 | 66.0 |
| Confidence Aggregation Baselines | | | | |
| SNCA ($\tau = 0.2$) | 76.5 | 74.9 | 73.6 | 72.0 |
| SNCA ($\tau = 0$) | 50.0 | 50.0 | 50.0 | 50.0 |
| SFCA ($\tau = 0.2$) | 76.4 | 75.2 | 74.2 | 73.4 |
| SFCA ($\tau = 0$) | 50.0 | 50.0 | 50.0 | 50.0 |
| Ours | | | | |
| SCA ($\tau = 0.3$) | 82.0 | 80.3 | 79.5 | 78.4 |
| SCA ($\tau = 0$) | <u>82.0</u> | 80.4 | 79.5 | 78.4 |

Table 18: **ECE score on LLaMA-3.1-70B-Instruct** of different calibration methods under increasing answer mixture. **Bold** marks the best (lowest), and underlined the second-best, in each column.

| Method | [1] | [1,2] | [1,2,4] | [1,2,4,6] |
|--------------------------------|------------|------------|-------------|-------------|
| Single-turn | | | | |
| <i>Question-level</i> | | | | |
| Prob Entropy | 26.2 | 21.7 | 20.8 | 19.4 |
| N-Prob Entropy | 43.5 | 35.5 | 31.7 | 30.3 |
| Sem Entropy | 12.5 | 9.6 | 16.6 | 21.3 |
| <i>Answer-level</i> | | | | |
| Verb | 46.8 | 39.5 | 34.6 | 33.1 |
| Verb _{Topk} | 35.8 | 22.5 | <u>19.3</u> | 21.9 |
| Consistency | 8.6 | 10.4 | 21.6 | 27.0 |
| Consis-Verb | 11.7 | 12.3 | 21.5 | 27.1 |
| Consis-Verb-Topk | 12.4 | 14.3 | 23.6 | 29.1 |
| Perplexity | 30.6 | 23.4 | 20.9 | <u>19.6</u> |
| Double-turn | | | | |
| P _{True} -Consis | 35.3 | 34.1 | 33.0 | 31.5 |
| P _{True} -Prob | 35.1 | 33.7 | 32.7 | 31.4 |
| P _{True} -Consis-Cand | 41.7 | 35.6 | 30.4 | 30.6 |
| P _{True} -Prob-Cand | 41.6 | 35.4 | 30.2 | 30.0 |
| Self _{Ask} | 36.6 | 40.9 | 45.8 | 46.7 |
| Self _{Ask} -Cand | 26.3 | 22.8 | 23.5 | 25.6 |