Contextualized Sequence Likelihood: Enhanced Confidence Scores for Natural Language Generation

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Abstract

The advent of large language models (LLMs) has dramatically advanced the state-of-the-art in numerous natural language generation tasks. For LLMs to be applied reliably, it is essential to have an accurate measure of their confidence. Currently, the most commonly used confidence score function is the likelihood of the generated sequence, which, however, conflates semantic and syntactic components. For instance, in question-answering (QA) tasks, an awkward phrasing of the correct answer might result in a lower probability prediction. Additionally, different tokens should be weighted differently depending on the context. In this work, we propose enhancing the predicted sequence probability by assigning different weights to various tokens using attention values elicited from the base LLM. By employing a validation set, we can identify the relevant attention heads, thereby significantly improving the reliability of the vanilla sequence probability confidence measure. We refer to this new score as the Contextualized Sequence Likelihood (CSL). CSL is easy to implement, fast to compute, and offers considerable potential for further improvement with task-specific prompts. Across several QA datasets and a diverse array of LLMs, CSL has demonstrated significantly higher reliability than state-of-the-art baselines in predicting generation quality, as measured by the AUROC or AUARC. The code to replicate our experiments is available at https://github.com/zlin7/ContextSL.

1 Introduction

The development of large language models (LLMs) has afforded tremendous advancements in natural language generation (NLG). Recently, LLMs have been widely applied across various natural language domains (Zhang et al., 2023; Wang et al., 2023a; Alves et al., 2023; Zhang et al., 2024), even extending to tasks and domains traditionally dominated by other machine learning algorithms,

such as graph data (Fatemi et al., 2024), tabular data (Borisov et al., 2023; Hegselmann et al., 2023), time series (Gruver et al., 2023; Rasul et al., 2024), predictive chemistry (Jablonka et al., 2024; Shi et al., 2023), computer vision (Wang et al., 2023b), amongst others. As LLMs continue to demonstrate outstanding performance, their reliability is increasingly scrutinized. Uncertainty quantification, an area of research that can provide some guidance on reliability, has recently gained much attention. Despite its long history in other machine learning tasks (Gawlikowski et al., 2023), our understanding of uncertainty quantification in NLG remains relatively limited.

During pre-training, (autoregressive) LLMs are optimized to predict high logits for the target token to minimize (variants of) the negative log likelihood. Consequently, one of the most natural and widely used confidence scores in selective NLG, conformal NLG, or uncertainty quantification is the (sometimes normalized) likelihood of the sequence, equivalent to the sum/mean of token logits. At first glance, sequence likelihood appears to be the most faithful reflection of a model's confidence, as it represents the (log of) the predicted probability of the output sequence, or $\log \hat{p}(\mathbf{s}|x)$. However, this measure often lacks proper contextualization and disregards the specific nature of the task at hand. $\hat{p}(\mathbf{s}|x)$ conflates syntactic and semantic likelihoods, though we typically prioritize the semantic aspect, to a varying degree depending on the task. For example, depending on whether the question is "Which country won the World Cup in 2022" or "When did Messi win the World Cup," the answer "Messi emerged victorious in the 2022 World Cup" could be considered correct or incorrect. Further, the somewhat unusual expression here could adversely impact $\hat{p}(\mathbf{s}|x)$.

Despite its limitations, relatively limited attention has been paid to improving the vanilla sequence likelihood. A recent study by Duan et al. (2023) proposed assessing token relevance using an external natural language inference (NLI) model. The relevance score of a token is negatively proportional to the similarity between the original sequence and the sequence with this token removed, which is then applied to weight the token logits. However, since modern LMs rely on sub-word tokenizers, removing one sub-word token at a time results in non-words, is computationally expensive for longer texts, and remains context-unaware.

In this paper, we investigate the potential of utilizing the LLM's own attention mechanism to develop a weighted sequence likelihood as an enhanced confidence score. Specifically, the LLM is prompted to concentrate on the relevant tokens in its own generation. The most appropriate attention heads are then employed to re-weight the original token logits. The main contributions of this paper are summarized as thus:

- We introduce a straightforward yet effective method to reweight token logits, resulting in <u>Contextualized Sequence Likelihood (CSL)</u>, a more reliable confidence measure.
- We improve current automatic evaluation methods for confidence measures on Question-Answering (QA) datasets and manually verify their effectiveness.
- In popular free-form QA datasets, and on a variety of LLMs, we verify that CSL significantly outperforms baselines. Case studies suggest the attention weights are meaningful.

2 Related Works

With the rapid proliferation of LLMs and their swift adoption across various domains, uncertainty quantification (UQ) for natural language generation (NLG) is a fast-growing area of research (see Baan et al. (2023) and references therein). Adopting the language used by Lin et al. (2023), uncertainty measures the predictive distribution, while confidence (our focus) further depends on the specific generation. A common approach involves reducing NLG to a de facto classification problem and utilizing or enhancing classical UQ methods for classification (Desai and Durrett, 2020; Jiang et al., 2021; Kamath et al., 2020; Wang et al., 2022; Xiong et al., 2023). Recognizing the unique challenges posed by the inherently high (potentially infinite) dimensionality of NLG, recent research increasingly considers UQ for NLG from a sequence perspective (Hou et al., 2023; Kuhn et al., 2023; Malinin and Gales,

2021; Lin et al., 2023).

Relatively less attention has been devoted to confidence measures. Sequence likelihood, or the logprobability of the generated sequence, remains one of the most popular proxies for assessing the quality of individual answers (Quach et al., 2023; Kuhn et al., 2023; Cole et al., 2023). Another natural approach, given the versatility and strong performance of LLMs, involves using prompts to elicit the LLM's own confidence level (Kadavath et al., 2022; Lin et al., 2022a; Mielke et al., 2020; Chen and Mueller, 2023; He et al., 2023; Li et al., 2024; Wightman et al., 2023). For free-form generation datasets, this is typically done by arranging answers as options and extracting the model's logits for each option. While our method also employs prompts, they primarily guide the model to focus on tokens relevant to the context of the question. Another approach involves sampling additional generations and comparing their similarities (Lin et al., 2023; Cole et al., 2023), which demonstrates good discriminative capability but can be rather expensive. Although this approach has the advantage that it can work for black-box LLMs. Ensemble methods have also been proposed (Chen and Mueller, 2023).

Recently, Duan et al. (2023) proposed an improvement to sequence likelihood by weighting the tokens using their importance, which is computed by removing one token at a time from the original sequence and computing the NLI dissimilarity between the new and original sequences. The removal of sub-word tokens, however, introduces drastically grammatically incorrect sentences, which could confuse the NLI model. In addition, such a method could incur high computation overhead by making n NLI comparisons, where n is the length of the generation. In contrast, our method incurs no artificial grammatical errors and miniscule overhead.

An important downstream application of confidence measures is **abstention in LLMs**. Classification with rejection (Corbière et al., 2019; Fumera et al., 2000; Geifman and El-Yaniv, 2017; Jiang et al., 2018; Lin et al., 2022b) could be considered the direct antecedent of selective NLG—both aiming to determine when to trust a model. Naturally, approaches similar to those in the classification with rejection literature have been applied to NLP applications (Varshney et al., 2022a,b). More recently, Cole et al. (2023); Yadkori et al. (2024); Lin et al. (2023); Quach et al. (2023) started investigating NLG with abstention from UQ or risk control perspectives. Calibration is another crucial and relevant topic that has been extensively studied (Mielke et al., 2022; Si et al., 2022; Xiong et al., 2023; Zhu et al., 2023). Although calibration is not directly related to our primary focus—our main interest lies in ranking the confidence of different measures—we include results on the calibrated performance in the Appendix. Conformal prediction (Vovk et al., 2005) could also be considered a form of calibration at the distribution level, and has been extended to NLG to bound variants of error rates (Quach et al., 2023; Yadkori et al., 2024).

3 Contextualized Sequence Likelihood

3.1 Background: Sequence Likelihood

In this section we describe our approach: contextualized sequence likelihood (CSL). We first fix notation and introduce relevant definitions. We will focus on auto-regressive LMs, the current dominant paradigm. Denoting the model as \mathcal{M} , for any given input prompt denoted as x, the response s is a sequence of tokens $[s_1, \ldots, s_n]$ sampled from the predictive distribution $P(S; x, \mathcal{M})$. We will denote $s_{<i}$ as the truncated sequence $[s_1, \ldots, s_{i-1}]$. Given the auto-regressive assumption, the (log-softmax'd) logit for the *i*-th token represent \mathcal{M} 's prediction of the log probability of token s_i at this location. Consequently, the sum of all the logits for the sequence represents the log of the model's predicted probability of the output sequence:

$$C_{SL} = \sum_{i=1}^{n} l_i = \log \prod_{i=1}^{n} \hat{p}(s_i | \mathbf{s}_{< i}, x).$$
(1)

Eq. (1) is commonly used as a confidence score (Quach et al., 2023; Cole et al., 2023), and often normalized by the length n, as otherwise longer sequences tend to receive lower confidence (Kuhn et al., 2023; Malinin and Gales, 2021):

$$\mathbf{C}_{\mathsf{SL}(norm)} = \frac{1}{n} \sum_{i=1}^{n} l_i. \tag{2}$$

As pointed out by Cole et al. (2023), in practice C_{LL} is far from the actual log-probability of the sequence s, $\log \hat{p}(s|x)$. Techniques like nucleus sampling or top-k sampling will reduce the sum of the predicted probability of all tokens below 1. However, if we view this new distribution that s is effectively sampled from as $P'(S|x, \mathcal{M})$, then we at least have:

$$\forall \mathbf{s}, P'(\mathbf{s}|x) \propto \prod_{i=1}^{n} \hat{p}(s_i|\mathbf{s}_{< i}, x).$$
(3)

Thus, C_{SL} still faithfully preserves the ranking of LM's predicted probability of all possible generated sequences, which is all we care about for a good (pre-calibrated) confidence measure. However, as we shall see next, this does not imply sequence likelihood is a good confidence measure.

3.2 Contextualized Likelihood via Attention

While intuitively natural as confidence measures, Eqs. (1) and (2) sweep a crucial consideration under the proverbial rug: While sequence-likelihood reflects the model's predicted probability of the sequence s, what does this probability actually mean? Unfortunately, there is an inherent ambiguity here. For instance, let's say we are classifying an image x from ImageNet (Deng et al., 2009), and take the first-choice confidence score $\hat{p}(y|x)$ as predicted by a ResNet (He et al., 2016). However, $\hat{p}(y = \operatorname{cat}|x)$ could mean the (model's predicted) probability of "the input image is that of a cat", "there is a cat in the input image", or probably more precisely speaking, "this image should be labeled as a cat by ImageNet standards"¹. Similarly, strictly speaking, $\hat{p}(\mathbf{s}|x)$ only reflects the LM's prediction of the probability of "s follows x, according to the training data".

To illustrate further, consider the questionanswer pair where x is "Q: What did Neil Armstrong do on July 20, 1969?". A response s which goes "A: On July 20, 1969, Armstrong and Buzz Aldrin landed on the Moon for the first time in human history." appears appropriate and highly probable. However, the confidence of "whether s correctly answers x" is minimally influenced by the redundant mention of the date or Armstrong's fellow astronaut, Buzz Aldrin. Generally speaking, the confidence that we are concerned with in a response s depends on the context, with some tokens being significantly more relevant than others.

How can we systematically identify the most relevant tokens? To address this, we propose using a prompt (Fig. 1) to elicit the LM's attention on its own response s. Essentially, we prompt the LM to assess whether its generated response correctly answers the question. Unlike previous approaches that rely on similar prompts, we disregard the actual judgment and instead extract the attention values of the LM on s during this process to reweight the token logits. Assuming the s_i becomes the *i*'-th token in the attention-eliciting prompt, the new

¹See a similar discussion in Beyer et al. (2020).

confidence score could be written as:

$$C_{CSL} = \sum_{i=1}^{n} w_i l_i$$
 where $w_i = \frac{a_i}{\sum_{i'=1}^{n} a_{i'}}$ (4)

where $a_{i'}$ is the attention of the last token of the attention-eliciting prompt on the s_i .

```
Read the following question with
      optional context and decide if the
      answer correctly answer the question
      . Focus on the answer, and reply Y
      or N.
  . . .
  Context: Harry is a good witcher.
3
4 Question: How old is Harry?
 Answer: Harry practices witchcraft.
5
   Decision: N. (The answer does not
6
      mention Harry's age.)
8 [$optional_context]
9
 Question: [$question]
10 Answer: [$response]
  Decision:
```

Figure 1: The attention-eliciting prompt used in this paper (full version deferred to the Appendix due to space constraints). **\$optional_context**, **\$question** and **\$response** are replaced with the corresponding values of a sample. In our experiments, **\$optional_context** refers to the story and conversation history that accompanies each question in CoQA (Reddy et al., 2019).

Fig. 2 illustrates how the attention-eliciting prompt (Fig. 1) induces varying emphases on the same response for different questions. For instance, when the question focuses on "when", the section of the response detailing the event date receives greater attention weight across all heads. This indicates that the weighting scheme introduced in Eq. (4) effectively overweights relevant tokens and underweights irrelevant ones, resulting in a more contextualized version of sequence likelihood.

Besides using a prompt, a more straightforward source of attention weights is the original generating process. Specifically, when the LM completes generating s, we retrieve the attention for the next token. We refer to this variant as CSL-Next, in contrast to CSL with the prompt. Our hypothesis is that the LM induces some internal attention on the critical words of the generation even without an explicit prompt asking for it, and we will explain how to identify such attention in Section 3.3.

3.3 The Choice of Heads

While the prompt can enhance overall attention on relevant tokens, averaging attention across heads—even with the prompt—is unwise. Many attention

heads likely focus, for example, on ensuring grammatical correctness, with only a fraction dedicated to the response. Selecting only the useful heads from the multitude of heads (e.g., out of 1,600 in LLaMA2-13B) remains a challenging task.

We present a systematic approach to identify the appropriate heads. Let w^h denote the attention weights from head h, and C_{CSL}^{h} the associated confidence score computed via Eq. (4). For each head h and a subset of the samples, we use the associated confidence C_{CSL}^h to predict the accuracy of responses, and compute an AUROC (similar to Kuhn et al., 2023), denoted as $AUROC_h$. Notably, we found that the "functionality" of the heads appears relatively stable: That is, if we compare the $AUROC_h$ on two subsets of the population, the ranking of these heads is highly consistent across the two subsets, as shown in Fig. 3. As a result, we propose to pick the top k = 10 heads on the validation dataset and average the attention weights of only these heads. The reason why we pick more than one head is because picking only the best head is likely affected by noise due to the size of the validation set. In Section 4, we show that leveraging the attention from about k = 10 top heads performs better than either the average attention of all heads, or the top head.

4 Experiments

4.1 Datasets

We use the following standard benchmark datasets, largely following the practices in Kuhn et al. (2023); Lin et al. (2023):

- CoQA (coqa) (Reddy et al., 2019), an open-book conversational question answering dataset. We use the development split of coqa with 7,983 questions.
- TriviaQA (trivia) (Joshi et al., 2017), a closedbook QA dataset. We use the validation split of the rc.nocontext subset of trivia with 9,960 (de-duplicated) questions.
- Natural Questions (nq) (Kwiatkowski et al., 2019), a closed-book QA dataset. We use the validation split of nq with 3,610 questions.

Following (Lin et al., 2023), for each experiment we use a random subset of 1,000 questions as the validation set, and the remaining as the test set. We report the mean and standard deviation of all evaluation metrics (see Section 4.4) on the test set, calculated from 10 random data splittings.



Figure 2: Depending on the question, the attention-eliciting prompt introduced in Fig. 1 induces attention focusing on different parts of the same response ("when", "who" and "what"). In the plot on the right, we show the CDF of Δ_{attn} , the change of attention weight on the corresponding concept when asked the relevant question, on all 1,024 heads of Mistral-7B. For example, for "when", we compute Δ_{attn} as the attention weight on "On July 20, 1969" when asked the "when" question minus the average of the cases where the other two questions were asked. In all cases, the attention significantly increases on the relevant tokens (p-value from one-sided t-test is at most 9e-90).



Figure 3: Scatter plot of test vs validation AUROC for confidence measures computed via Eq. (4) with different heads' attention weights, on Natural Questions (nq) with Mistral-7B model. The ranking is highly consistent—the best heads on the validation set continue to perform well on the test set. In this case, the Spearman correlation (Spearman, 1961) is > 97%. We can thus pick only a small subset of the 1024 heads (or more for other LMs) to construct the final confidence measure C_{CSL} .

4.2 Baselines

We compare CSL (and CSL-Next) with several recent confidence measures:

- Deg, a confidence score based on the degree of similarity graph from Lin et al. (2023). Note that this method requires sampling multiple responses, and we set the number of additional generations to 5. We use the "Entailment" version as suggested by Lin et al. (2023).
- P(true) (Kadavath et al., 2022), which elicits the confidence by asking the LM itself whether its response is correct. We use the prompt from Kadavath et al. (2022); Lin et al. (2023).
- Sequence Likelihood (SL): This is the sequence likelihood measure discussed in Eq. (1), and widely in literature as a confidence score (Lin et al., 2023; Quach et al., 2023; Huang et al., 2024) or as a building block for predictive en-

tropy (Kuhn et al., 2023; Kadavath et al., 2022; Malinin and Gales, 2021). We include the lengthnormalized version in Eq. (2), SL(norm), as well.

TokenSAR (Duan et al., 2023): It proposes to estimate the relevance of each token as w_i in Eq. (4), with w_i ∝ 1 − sim(s, s_{-i}) where sim is similarity measured by an NLI model and s_{-i} is the response of interest s without token i.

In addition, we also replace the sequence likelihood used in Semantic Entropy (SE,Kuhn et al., 2023), which is an *uncertainty*² measure, with CSL, and report results in Section 4.6

4.3 Language Model and Generation

For the base LLMs, we include the most popular open LLMs: LLaMA2 (Touvron et al., 2023b), Mistral (Jiang et al., 2023) and Gemma (Team et al., 2024). We use the 13B version for LLaMA, and the 7B version for Mistral and Gemma due to their improved performance. Response generation largely follows Kuhn et al. (2023) with some improvements: The original pipeline often removes content after periods in abbreviations (such as "Dr."), so we modified the prompt to ensure each response s ends with a newline character but keeps contents after punctuations. Like Kuhn et al. (2023), we focus on the greedily-decoded generation s for each question and use a temperature of 0.5 for baselines that require additional response sampling.

4.4 Evaluation

For an effective confidence measure, low confidence should correlate with a higher probability of incorrect generation. To assess the quality of confi-

²See Lin et al. (2023) for a discussion distinguishing between confidence and uncertainty.

Table 1: Agreement with human annotation, on 720 sampled question-response pairs in total.

Agreement with Human (%)	coqa	nq	trivia
acc _{agree}	98.2	91.8	98.2
acc _{llama2}	97.0	86.7	95.0
acc _{gpt}	94.1	85.8	96.6

dence measures, we adhere to established methodologies (Kuhn et al., 2023; Band et al., 2022). This involves utilizing them to predict the correctness of a generation and calculating the Area Under the Receiver Operating Characteristic curve (AUROC) for this prediction task. Formally, let acc_i represent the indicator function $1{s_i correctly answers x_i}$. We compute the AUROC using the confidence measure C(x, s.) to predict acc. This approach allows us to systematically evaluate how well the confidence measures distinguish between correct and incorrect responses across multiple samples.

In addition to AUROC, following Lin et al. (2023), we also report Area Under Accuracy-Rejection Curve (AUARC) (Nadeem et al., 2009). The Accuracy-Rejection Curve (ARC) computes the average the accuracy when a subset of samples is rejected based on C. As we exclude more low-confidence samples, the accuracy of the remaining samples should increase. The *upper bound* is achieved by predicting only the correct s (i.e. set C to accuracy), and the AUARC of a *random* predictor is equal to the base accuracy without rejection.

Correctness of Generations: A critical requirement for computing AUROC or AUARC is a reliable acc_i , the accuracy of each response. This is a unique challenge in UQ for NLG, and deserves separate research. Prior work typically relies on lexical similarity measures such as ROUGE (Kuhn et al., 2023; Quach et al., 2023) or BLEU (Huang et al., 2024). Lin et al. (2023) uses gpt-3.5 to evaluate the correctness of each response given a reference answer³, and considers anything with a rating above 70% as correct. Inspired by (Lin et al., 2023), we use the agreement of both LLaMA2-70B and gpt-3.5-turbo-0125's evaluations as acc (More details are in Appendix B). As shown in Table 1, this notably improves the correctness evaluation and thus the reliability of AUROC/AUARC. We include the results using accllama2 in the Appendix D since acc_{agree} and acc_{qpt} may not remain reproducible in the future.

4.5 Results

Table 2 presents the AUROC of different confidence measures. Clearly, all the confidence baselines consistently detect good s over bad ones, but CSL outperforms baselines. Similar results are observed for AUARC in Table 3 as well: As the LMs have good base accuracy (from the "Random" column) for coqa and trivia, the gap between different confidence measures is relatively small, but generally significant. In particular, among likelihood-based methods, it is sometimes confusing whether normalized or unnormalized likelihood should be used (Kuhn et al., 2023; Malinin and Gales, 2021), and TokenSAR does not always outperform the better of the two. However, CSL consistently outperforms all three. Thanks to the additional sampling, Deg performs quite well, especially if we further increase the temperature of the base LM (see Appendix), but in practice it could significantly increase the computation cost as it requires m additional generations and $O(m^2)$ similarity comparisons. Finally, after the head selection process, the difference between CSL and CSL-Next is small, but still extremely significant if we perform a pooled test. The observed similar performance is because chosen attention heads exhibit highly correlated patterns (see Section 4.7). We recommend CSL over CSL-Next as they share similar overhead (close to none) but the attention-eliciting prompt is more structured compared with the more arbitrary prompt used to generate s, and therefore the "good" heads are likely to be more stable.

4.6 Improving Uncertainty Measures

As noted earlier, sequence likelihood is widely used in entropy computation, which is used as an uncertainty measure for NLG. Semantic Entropy (Kuhn et al., 2023) is a state-of-the-art uncertainty measure that groups sampled generations into semantic sets and computes the entropy over these sets. In doing so, it uses sequence likelihood (sometimes normalized). We simply replace it with CSL to create a new uncertainty measure, SE+CSL. The comparison is shown in Table 4. SE+CSL consistently outperforms either the normalized or the unnormalized version of SE, showing potential in replacing sequence likelihood in other domains such as conformal NLG (Quach et al., 2023).

4.7 Is the Improvement a Fluke?

Despite not using an explicit attention-eliciting prompt, CSL-Next performs close to CSL, outper-

³The original paper uses gpt-3.5-turbo-0301 which is no longer accessible.

Table 2: AUROC of using confidence measures C to predict the accuracy of responses. Methods not significantly different from the best are in **bold**.

	Deg (E)	P(true)	SL	SL(norm)	TokenSAR	CSL	CSL-Next
trivia (llama2)	81.74±0.25	$64.82{\pm}0.18$	88.19±0.12	87.86±0.12	87.91±0.13	89.70±0.19	89.61±0.18
trivia (gemma)	$84.00 {\pm} 0.19$	$81.82{\pm}0.18$	$88.72{\pm}0.11$	$88.11{\pm}0.08$	$88.09{\pm}0.08$	89.71±0.14	$89.42 {\pm} 0.11$
trivia (mistral)	$81.85 {\pm} 0.30$	$68.78{\pm}0.28$	$88.81{\pm}0.15$	$88.64{\pm}0.14$	$88.74{\pm}0.13$	90.76±0.18	90.73±0.15
coqa (llama2)	$69.93 {\pm} 0.57$	$53.64{\pm}0.41$	$69.50{\pm}0.40$	$72.59{\pm}0.44$	$72.78{\pm}0.47$	$73.34{\pm}0.74$	73.36±0.57
coqa (gemma)	$70.03 {\pm} 0.68$	$55.99{\pm}0.42$	$70.83{\pm}0.46$	$71.96{\pm}0.57$	$72.38{\pm}0.55$	$73.30{\pm}0.57$	73.64±0.63
coqa (mistral)	$69.84{\pm}0.52$	$52.33{\pm}0.42$	$68.97{\pm}0.38$	$70.60{\pm}0.38$	$70.87{\pm}0.41$	$71.79{\pm}0.75$	71.91±0.63
nq (llama2)	$71.61 {\pm} 0.51$	$52.51{\pm}0.47$	$66.57{\pm}0.33$	$69.48{\pm}0.50$	$70.43{\pm}0.46$	73.73±0.49	$73.54{\pm}0.46$
nq (gemma)	$73.32{\pm}0.68$	$63.66{\pm}0.46$	$72.09{\pm}0.65$	$75.81{\pm}0.65$	$75.88{\pm}0.68$	$\textbf{77.95}{\pm}\textbf{0.58}$	$77.17 {\pm} 0.65$
nq (mistral)	73.03 ± 0.52	$54.77{\pm}0.51$	$69.22{\pm}0.53$	$71.06{\pm}0.54$	$72.61{\pm}0.48$	$76.65{\pm}0.43$	75.73±0.68

Table 3: AUARC of using confidence measures C to predict the accuracy of responses. Methods not significantly different from the best are in **bold**.

	Random	Upper Bound	$\text{Deg}\left(E ight)$	P(true)	SL	SL(norm)	TokenSAR	CSL	CSL-Next
trivia (llama2)	82.60±0.14	$98.39{\pm}0.03$	$92.84{\pm}0.28$	87.50±0.12	95.99±0.06	$95.95{\pm}0.05$	$95.96{\pm}0.05$	96.32±0.08	96.29±0.06
trivia (gemma)	$78.14{\pm}0.13$	$97.41 {\pm} 0.03$	$91.48{\pm}0.19$	$91.83{\pm}0.11$	$94.61{\pm}0.05$	$94.38{\pm}0.04$	$94.38{\pm}0.04$	$\textbf{94.79}{\pm}\textbf{0.04}$	$94.65{\pm}0.04$
trivia (mistral)	$79.94{\pm}0.12$	$97.84{\pm}0.03$	$91.91 {\pm} 0.31$	$87.55{\pm}0.13$	$95.27{\pm}0.06$	$95.21{\pm}0.05$	$95.22{\pm}0.05$	95.68±0.09	95.68±0.07
coqa (llama2)	$91.36{\pm}0.17$	$99.62{\pm}0.01$	$94.71{\pm}0.22$	$92.24{\pm}0.18$	$95.69{\pm}0.13$	$96.09{\pm}0.14$	$96.17{\pm}0.14$	$96.26{\pm}0.18$	$96.26{\pm}0.16$
coqa (gemma)	$92.64{\pm}0.14$	$99.72 {\pm} 0.01$	$95.46{\pm}0.20$	$94.13{\pm}0.15$	$96.54{\pm}0.10$	$96.63{\pm}0.11$	$96.68{\pm}0.11$	$96.85{\pm}0.11$	96.90±0.13
coqa (mistral)	$92.04{\pm}0.14$	$99.67 {\pm} 0.01$	$95.09{\pm}0.33$	$92.62{\pm}0.16$	$95.92{\pm}0.10$	$96.13 {\pm} 0.11$	$96.22{\pm}0.10$	96.37±0.13	96.38±0.12
nq (llama2)	$56.49{\pm}0.68$	$88.74 {\pm} 0.39$	$70.59{\pm}1.27$	$57.68{\pm}0.68$	$70.51{\pm}0.76$	$71.01{\pm}0.81$	$71.97{\pm}0.80$	$73.46{\pm}0.66$	$73.31{\pm}0.87$
nq (gemma)	$47.16{\pm}0.65$	$82.59 {\pm} 0.49$	$62.96{\pm}0.94$	$57.30{\pm}0.67$	$65.78{\pm}0.95$	$66.41{\pm}0.92$	$67.02{\pm}0.93$	$67.78{\pm}1.07$	$66.89{\pm}1.03$
nq (mistral)	$52.90{\pm}0.74$	86.57±0.47	67.48±1.00	$56.47{\pm}0.93$	69.15±0.82	69.27±0.72	$70.62{\pm}0.65$	72.25±0.74	71.85±0.69

Table 4: AUROC of using variants of Semantic Entropy to predict the accuracy of responses. SE+CSL significantly improves the original version based on vanilla sequence likelihoods.

	SE(norm)	SE	SE+CSL
trivia (llama2)	89.88±0.11	89.33±0.12	90.50±0.12
trivia (gemma)	90.33±0.10	$90.02{\pm}0.12$	90.75±0.13
trivia (mistral)	90.35±0.12	$89.78{\pm}0.15$	91.13±0.13
coqa (llama2)	75.26±0.33	$72.50{\pm}0.34$	75.58±0.51
coqa (gemma)	74.81±0.48	$72.95{\pm}0.48$	75.08±0.50
coqa (mistral)	74.06 ± 0.41	$71.54{\pm}0.32$	74.56±0.51
nq (llama2)	74.13±0.51	$69.62{\pm}0.38$	76.33±0.50
nq (gemma)	77.93±0.58	$73.67{\pm}0.77$	79.50±0.52
nq (mistral)	75.71±0.40	$71.85{\pm}0.49$	78.66±0.35

forming baselines significantly. It is reasonable to then worry that the improvement is just the result of black-box data-mining by the head-selection step in Section 3.3. This section presents evidence that CSL most likely identifies meaningful concepts.

Fig. 4 shows the correlation between the w_i vectors used for CSL and CSL-Next—which is almost always positive and usually close to 1. As the prompts used to induce these attention weights are quite different, such agreement could be taken as preliminary evidence that these weights are "meaningful" and less likely to be purely the results of two independent black-box "fitting" processes.

Fig. 5 shows a few examples of the induced at-



Figure 4: Histogram of the correlation between attentions from CSL and CSL-Next (top 10 heads' average). We keep only generations with more than 2 tokens. For most responses, the chosen heads' attentions are highly correlated, suggesting that both methods focus on the same tokens, as exemplified in Fig. 5.

tention weights, illustrating how CSL makes the confidence measure more focused on important tokens. Given the nature of soft attention, despite the fact that w_i chosen by Section 3 generally identifies the important tokens and improves upon vanilla sequence likelihood, it is still sometimes difficult to interpret why each token is under/over-weighted. For interpretability reasons, a future research direction might be to directly use natural language to identify such tokens. For example, one might directly ask the LM to list the important entities with respect to a question. The challenge, then, transfers to identifying the actual tokens implied by the natural language output listing important entities in the original s.

Question 1: how early did he want to get there?
Response 1: an hour before the time
Question 2: What does Barwell think of him?
Response 2: he is not fit to be his guardian
Question 3: who is Susan Boyle?
Response 3: Susan Boyle is a Scottish singer who be-
came famous after appearing on the TV show "Britain's
Got Talent" in 2009.

Figure 5: Tokens whose attention is increased are marked (others decreased). As expected, such re-weighting are not always interpretable, but help locating the more relevant tokens in general.

Table 5: AUROC using heads picked from coqa. Despite the big distribution shift from coqa to nq/trivia, the heads chosen on coqa still provides attention weights that significantly improves the AUROC.

	SL(norm)	CSL	CSL-Next
trivia (llama2)	87.86±0.12	$88.59{\pm}0.85$	$88.37{\pm}0.87$
trivia (gemma)	88.11±0.08	$\textbf{89.03}{\pm}\textbf{0.61}$	$87.43{\pm}0.94$
trivia (mistral)	88.64±0.14	$\textbf{89.70}{\pm}\textbf{1.43}$	$88.46{\pm}1.93$
nq (llama2)	$69.48 {\pm} 0.50$	$\textbf{70.94}{\pm}\textbf{1.66}$	$70.10{\pm}2.09$
nq (gemma)	75.81±0.65	$\textbf{77.21}{\pm}\textbf{1.06}$	$74.99{\pm}1.30$
nq (mistral)	71.06±0.54	72.71±3.32	72.27±2.72

Finally, if the attention weights are actually focusing on the important concepts as intended, one might expect that they should transfer *between datasets* and be more robust to distribution shifts. In Table 5, we select heads based on validation sets from coqa and apply them on the other two datasets, which are quite different from coqa (e.g. in the format of questions). CSL still provides consistent performance boost, while CSL-Next sometimes lags behind SL(norm). This suggests both the prompt and the head selection step increase the weights on the more relevant tokens.

4.8 Ablation: Choice of Attention Heads



Figure 6: AUROC gain compared with SL(norm) for different k (number of attention heads to keep), from 1 to all heads. The performance peaks around k = 10 and is stable. CSL is also consistently better than CSL-Next-notably, when we average the attention from all heads, CSL still outperforms SL(norm), but CSL-Next is significantly worse.

In Fig. 6, we compute the *gain* in AUROC compared with SL(norm) (i.e. equal weighting), keeping different number of attention heads. The solid lines represent CSL, and the dotted lines denote CSL-Next. Note that using only one head is also significantly better than the baseline, but performance increases and peaks around 10 heads (sometimes more). We believe using a small number of "good" heads can reduce the noise introduced by using a small validation set, making CSL more contextualized to the question.

5 Discussion and Conclusion

In this paper, we explore enhancements to the widely used confidence measure, sequence likelihood, which serves as a quality metric for model generations in selective generation and risk control for natural language generation. We introduce Contextualized Sequence Likelihood, or CSL, a novel approach that utilizes attention weights on generated tokens to re-weight the logits in sequence likelihood computation. This new confidence measure surpasses existing methods across several popular datasets and large language models by more accurately predicting the accuracy of each response.

Despite these improvements, there are limitations to the current approach. First, the interpretability of attention weights is often obscured by the nature of the self-attention mechanism. While attention re-weighting generally enhances the confidence measure, there are individual cases where selected heads do not align with tokens that humans would typically consider important in the context of the question. As discussed in Section 4, a possible solution involves identifying key tokens through a language model via natural language, though this introduces the additional challenge of matching these words to the original response.

Another limitation is the applicability of the current prompt, which is tailored for questionanswering and may require modifications for other tasks. Additionally, like many baseline methods, the current approach cannot leverage external information for "fact-checking." Integrating confidence from multiple models could potentially bridge the gap between a language model's perceived confidence and the actual correctness of a response. We hope that future research will address these issues and expand the toolkit available to practitioners for assessing the reliability of large language models.

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A Prompts

In this section, we present the full prompts used in various aspects of our experiments.

A.1 Question-Answering Generation Prompts

We use the following prompts when generating responses for the question-answering datasets.

```
CoQA:

Read the context and answer the

questions below.

*Context*: [$context]

[additional question-answer pairs]

*Question*: [$question]

*Answer*:
```

where additional question-answer pairs are preceding turns of the conversation about the paragraph consisting of questions and reference answers.

TriviaQA:

Natural Questions is a much harder dataset than TriviaQA, so we use the same 5-shot prompt ver-²⁴ sion of the prompt in (Touvron et al., 2023a) (with ²⁵₂₆ 5 questions randomly picked from the training set). ²⁷

```
Answer these questions:
 *Question*: who makes up the state
     council in russia
4 *Answer*: governors and presidents
  *Question*: when does real time with
5
     bill maher come back
6 *Answer*: November 9, 2018
 *Question*: where did the phrase
      american dream come from
  *Answer*: the mystique regarding
      frontier life
9 *Question*: what do you call a group of
      eels
10 *Answer*: bed
11 *Question*: who wrote the score for
     mission impossible fallout
12 *Answer*: Lorne Balfe
13 *Question*: [$question]
14 *Answer*:
```

A.2 Attention-eliciting Prompt

In the following, we provide the full prompt previewed in Fig. 1.

```
Read the following question with
optional context and decide if the
answer correctly answer the question
. Focus on the answer, and reply Y
or N.
Context: Luxor International Airport is
a airport near Luxor in Egypt (EG).
It is 353km away from the nearest
```

```
seaport (Duba). The offical IATA for
       this airport is LXR
  Question: Luxor international airport is
       in which country?
6 Answer: It is in the United States, and
      its IATA is LXR.
   Decision: N. (The airport is in Egypt,
      not the United States.)
9
10 Context: Harry is a good witcher.
11 Question: How old is Harry?
  Answer: Harry practices witchcraft.
12
   Decision: N. (The answer does not
      mention Harry's age.)
16 Question: What is the capital of Kenya?
17 Answer: Nairobi is the capital of Kenya.
18
   Decision: Y.
19
20
21 Question: Who has won the most Premier
      League titles since 2015?
22 Answer: Manchester City have win the
      most Premier League title after
      2015.
   Decision: Y. (Grammar errors are
      ignored.)
26 [$optional context]
  Question: [$question]
27
28 Answer: [$response]
29 Decision:
```

A.3 Automatic Accuracy Evaluation

For the prompts used to elicit judgment from gpt-3.5-turbo-0125 and LLaMA2-70B, we use the same ones from the Appendix of Lin et al. (2023).

B Automatic Accuracy Evaluation

To verify the efficacy of automatic accuracy evaluation by gpt-3.5-turbo-0125 and LLaMA2-70B, we compare their judgements' alignment with human annotations. Specifically, we first sample 80 (question, response) pairs for each (model, dataset), resulting in 720 samples in total. We then manually compare each sample's response with the reference answer, and decide if the generated response is correct (given the context if any). Then, we retrieve the ratings on these 720 samples from gpt-3.5-turbo-0125 and LLaMA2-70B, and find the thresholds that result in the highest agreement. The resulting accuracy-threshold relation is illustrated in Fig. 7. From the results, we chose 0.2 as the threshold for LLaMA2-70B and 0.6 for gpt-3.5-turbo-0125. In other words, denote the rating from LLaMA2-70B on a generated response s as $r_{llama2}(s)$, then $\operatorname{acc}_{llama2}(s) = \mathbb{1}\{r_{llama2}(s) \ge 0.2\}$. Note that we found 20 out of the 720 samples hard to decide during our manual annotation process, usually due to incorrect reference answers or intrinsic ambiguity in the questions. We ignore them during the computation of Fig. 7.



Figure 7: Agreement with human annotation with different thresholds over all 720 samples.

C Temperature of Base Language Model

We include results using a high temperature of 1.0 in Tables 6 and 7. Higher temperature increases the sampling diversity of Deg and P(true), which increases the performance of Deg significantly, but brings mixed results to P(true). We also note that with 5 additional generations (6 in total) Deg is sometimes better than CSL or CSL-Next. We repeat the uncertainty experiments with higher temperature as well, in Table 8, and found that SE+CSL is the most predictive of the generations' quality at this temperature.

The experiments here suggest that sampling from an appropriate temperature really helps quantifying the reliability of the generations, but it should be noted that either sampling based confidence measures (Deg,P(true)) or sampling-based uncertainty measures (SE(norm), SE, SE+CSL) bear a significantly higher computational overhead - $(m+1) \times$ the generation cost and up to $(m^2 - m)$ pairwise NLI inference, with m being the additional generations. On the other hand, CSL requires one inference (not generation) call to the base LM which is only a fraction of the overhead. In practice, one might choose the best practice basing on cost and latency tolerance as well as difference in performance for the particular data distribution, and as shown in SE+CSL, CSL could be combined with sampling to yield better results as well.

D Results Using acc_{llama2}

We include results using acc_{llama2} (accuracy as judged by LLaMA2-70B) for reproducibility purposes in Tables 9 and 10. Conclusions stay the same as in the main text.

E Calibration Quality

We perform post-hoc calibration using the default sklearn.calibration.CalibratedClassifierCV. Fig. 8 shows the reliability diagrams (similar to those in Kull et al. (2019)) after calibration for CSL. The resulting probabilities are overall quite calibrated.

	Deg (E)	P(true)	SL	SL(norm)	TokenSAR	CSL	CSL-Next
3 generations							
trivia (llama2)	86.49±0.14	$61.63{\pm}0.27$	$88.16{\pm}0.13$	$87.84{\pm}0.13$	$87.89{\pm}0.13$	89.65±0.20	89.58±0.17
trivia (gemma)	87.00±0.12	$77.87{\pm}0.17$	$88.83{\pm}0.11$	$88.10{\pm}0.09$	$88.07{\pm}0.09$	89.73±0.16	$89.43 {\pm} 0.10$
trivia (mistral)	87.01±0.21	$73.75{\pm}0.16$	$88.85{\pm}0.15$	$88.66{\pm}0.14$	$88.75{\pm}0.13$	90.77±0.17	90.75±0.13
coqa (llama2)	72.51±0.29	$53.83{\pm}0.40$	$69.48{\pm}0.39$	$72.67{\pm}0.43$	$\textbf{72.88}{\pm}\textbf{0.46}$	73.46±0.69	$73.45{\pm}0.56$
coqa (gemma)	73.27±0.44	$56.82{\pm}0.57$	$70.78{\pm}0.47$	$72.07{\pm}0.52$	$72.46{\pm}0.49$	73.07±0.52	$73.60{\pm}0.52$
coqa (mistral)	71.86±0.57	$55.04{\pm}0.47$	$68.98{\pm}0.38$	$70.61{\pm}0.38$	$70.89{\pm}0.41$	71.79±0.74	71.91±0.63
nq (llama2)	72.47±0.50	$50.33{\pm}0.55$	$66.64{\pm}0.35$	$69.48{\pm}0.50$	$70.41{\pm}0.46$	73.83±0.52	$73.59{\pm}0.48$
nq (gemma)	75.78±0.68	$62.57{\pm}0.41$	$72.09{\pm}0.65$	$75.81{\pm}0.65$	$75.88{\pm}0.68$	77.96±0.57	$77.19{\pm}0.63$
nq (mistral)	73.76±0.70	$58.65{\pm}0.51$	$69.22{\pm}0.53$	$71.06 {\pm} 0.54$	$72.61{\pm}0.48$	76.65±0.43	$75.73{\pm}0.68$
5 generations							
trivia (llama2)	88.79±0.12	61.63±0.27	88.16±0.13	87.84±0.13	87.89±0.13	89.65±0.20	89.58±0.17
trivia (gemma)	89.19±0.11	$77.87{\pm}0.17$	$88.83{\pm}0.11$	$88.10{\pm}0.09$	$88.07{\pm}0.09$	89.73±0.16	$89.43 {\pm} 0.10$
trivia (mistral)	89.39±0.21	$73.75{\pm}0.16$	$88.85{\pm}0.15$	$88.66{\pm}0.14$	$88.75{\pm}0.13$	90.77±0.17	90.75±0.13
coqa (llama2)	75.73±0.30	$53.83{\pm}0.40$	$69.48{\pm}0.39$	$72.67{\pm}0.43$	$72.88{\pm}0.46$	73.46±0.69	$73.45{\pm}0.56$
coqa (gemma)	76.40±0.50	$56.82{\pm}0.57$	$70.78{\pm}0.47$	$72.07{\pm}0.52$	$72.46{\pm}0.49$	73.07±0.52	$73.60{\pm}0.52$
coqa (mistral)	74.41±0.51	$55.04{\pm}0.47$	$68.98{\pm}0.38$	$70.61{\pm}0.38$	$70.89{\pm}0.41$	71.79±0.74	$71.91{\pm}0.63$
nq (llama2)	74.09±0.53	$50.33{\pm}0.55$	$66.64{\pm}0.35$	$69.48{\pm}0.50$	$70.41{\pm}0.46$	73.83±0.52	$73.59{\pm}0.48$
nq (gemma)	77.40±0.74	$62.57{\pm}0.41$	$72.09{\pm}0.65$	$75.81{\pm}0.65$	$75.88{\pm}0.68$	77.96±0.57	$77.19{\pm}0.63$
nq (mistral)	76.31±0.65	$58.65{\pm}0.51$	$69.22{\pm}0.53$	$71.06 {\pm} 0.54$	$72.61{\pm}0.48$	76.65±0.43	75.73±0.68

Table 6: Similar to Table 2, but with different number of generations at temperature of 1.0.

Table 7: Similar to Table 3, but with different number of generations at temperature of 1.0.

	Random	Upper Bound	$\text{Deg}\left(E\right)$	P(true)	SL	SL(norm)	TokenSAR	CSL	CSL-Next
3 generations									
trivia (llama2)	82.61±0.14	$98.39{\pm}0.03$	$95.04{\pm}0.18$	87.06±0.16	95.99±0.06	$95.95{\pm}0.05$	$95.96{\pm}0.05$	96.33±0.08	96.30±0.07
trivia (gemma)	$78.11{\pm}0.12$	$97.41 {\pm} 0.03$	$93.52{\pm}0.12$	$91.01{\pm}0.11$	$94.62{\pm}0.05$	$94.37{\pm}0.04$	$94.37{\pm}0.04$	$\textbf{94.79}{\pm}\textbf{0.04}$	$94.66{\pm}0.04$
trivia (mistral)	$79.90{\pm}0.12$	$97.83{\pm}0.03$	$94.12{\pm}0.16$	$90.17{\pm}0.10$	$95.27{\pm}0.06$	$95.20{\pm}0.05$	$95.21{\pm}0.05$	$95.67{\pm}0.09$	95.67±0.07
coqa (llama2)	$91.36{\pm}0.17$	$99.62{\pm}0.02$	$95.52{\pm}0.20$	$92.20{\pm}0.21$	$95.69{\pm}0.13$	$96.11 {\pm} 0.14$	$\textbf{96.19}{\pm}\textbf{0.14}$	$96.28{\pm}0.17$	$96.27{\pm}0.15$
coqa (gemma)	$92.63{\pm}0.14$	$99.72 {\pm} 0.01$	$96.14{\pm}0.19$	$94.33{\pm}0.17$	$96.53{\pm}0.11$	$96.66{\pm}0.10$	$96.70{\pm}0.10$	$96.82{\pm}0.09$	96.90±0.11
coqa (mistral)	$92.04{\pm}0.14$	$99.67 {\pm} 0.01$	$95.80{\pm}0.26$	$93.06{\pm}0.19$	$95.92{\pm}0.10$	$96.13{\pm}0.11$	$96.22{\pm}0.10$	$96.37{\pm}0.14$	96.39±0.11
nq (llama2)	$56.48{\pm}0.68$	$88.74 {\pm} 0.39$	$72.37{\pm}0.89$	$56.84{\pm}0.70$	$70.50 {\pm} 0.77$	$71.00{\pm}0.81$	$71.95{\pm}0.80$	$\textbf{73.49}{\pm}\textbf{0.67}$	$73.28{\pm}0.86$
nq (gemma)	$47.16{\pm}0.65$	$82.59{\pm}0.49$	$66.59{\pm}0.87$	$56.54{\pm}0.78$	$65.78{\pm}0.95$	$66.41{\pm}0.92$	$67.02{\pm}0.93$	$\textbf{67.78}{\pm}\textbf{1.07}$	$66.89{\pm}1.03$
nq (mistral)	$52.90{\pm}0.74$	$86.57{\pm}0.47$	$70.09{\pm}0.84$	$59.77{\pm}0.52$	$69.15{\pm}0.82$	$69.27{\pm}0.72$	$70.62{\pm}0.65$	$72.24{\pm}0.74$	$71.83{\pm}0.67$
5 generations									
trivia (llama2)	82.61±0.14	$98.39{\pm}0.03$	95.80±0.09	87.06±0.16	95.99±0.06	95.95±0.05	$95.96{\pm}0.05$	96.33±0.08	96.30±0.07
trivia (gemma)	$78.11{\pm}0.12$	$97.41 {\pm} 0.03$	$94.51{\pm}0.08$	$91.01{\pm}0.11$	$94.62{\pm}0.05$	$94.37{\pm}0.04$	$94.37{\pm}0.04$	$\textbf{94.79}{\pm}\textbf{0.04}$	$94.66{\pm}0.04$
trivia (mistral)	$79.90{\pm}0.12$	$97.83{\pm}0.03$	$95.15{\pm}0.11$	$90.17{\pm}0.10$	$95.27{\pm}0.06$	$95.20{\pm}0.05$	$95.21{\pm}0.05$	95.67±0.09	95.67±0.07
coqa (llama2)	$91.36{\pm}0.17$	$99.62{\pm}0.02$	$96.13{\pm}0.15$	$92.20{\pm}0.21$	$95.69{\pm}0.13$	$96.11 {\pm} 0.14$	$\textbf{96.19}{\pm}\textbf{0.14}$	$96.28{\pm}0.17$	$96.27{\pm}0.15$
coqa (gemma)	$92.63{\pm}0.14$	$99.72{\pm}0.01$	$96.74{\pm}0.20$	$94.33{\pm}0.17$	$96.53{\pm}0.11$	$96.66{\pm}0.10$	$96.70{\pm}0.10$	$96.82{\pm}0.09$	96.90±0.11
coqa (mistral)	$92.04{\pm}0.14$	$99.67 {\pm} 0.01$	$96.22{\pm}0.16$	$93.06{\pm}0.19$	$95.92{\pm}0.10$	$96.13{\pm}0.11$	$96.22{\pm}0.10$	$96.37{\pm}0.14$	96.39±0.11
nq (llama2)	$56.48{\pm}0.68$	$88.74{\pm}0.39$	$73.77{\pm}0.89$	$56.84{\pm}0.70$	$70.50{\pm}0.77$	$71.00{\pm}0.81$	$71.95{\pm}0.80$	$73.49{\pm}0.67$	$73.28{\pm}0.86$
nq (gemma)	$47.16{\pm}0.65$	$82.59 {\pm} 0.49$	67.47±0.98	$56.54{\pm}0.78$	$65.78{\pm}0.95$	$66.41 {\pm} 0.92$	$67.02{\pm}0.93$	67.78±1.07	$66.89{\pm}1.03$
nq (mistral)	$52.90{\pm}0.74$	$86.57{\pm}0.47$	$72.07{\pm}0.84$	$59.77{\pm}0.52$	$69.15{\pm}0.82$	$69.27{\pm}0.72$	$70.62{\pm}0.65$	$72.24{\pm}0.74$	$71.83{\pm}0.67$



Figure 8: Reliability diagrams of CSL. Bins with fewer than 10 samples are ignored due to noise.

	SE(norm)	SE	SE+CSL
3 generations			
trivia (llama2)	88.18±0.11	$87.90{\pm}0.08$	88.99±0.13
trivia (gemma)	88.05±0.13	$88.08{\pm}0.15$	88.73±0.15
trivia (mistral)	88.90±0.16	$88.50{\pm}0.18$	89.84±0.16
coqa (llama2)	75.26±0.46	$72.11{\pm}0.32$	75.27±0.57
coqa (gemma)	75.42±0.38	$72.81{\pm}0.36$	75.25±0.42
coqa (mistral)	73.53±0.35	$70.49{\pm}0.37$	73.89±0.50
nq (llama2)	72.91±0.42	$68.44{\pm}0.34$	74.05±0.47
nq (gemma)	77.36±0.73	$72.73{\pm}0.80$	78.33±0.69
nq (mistral)	75.65±0.66	71.15 ± 0.72	77.37±0.59
5 generations			
trivia (llama2)	89.40±0.11	89.17±0.10	89.95±0.11
trivia (gemma)	89.32±0.09	$89.31{\pm}0.12$	89.82±0.12
trivia (mistral)	90.38±0.13	$89.86{\pm}0.16$	90.91±0.14
coqa (llama2)	77.08±0.40	$73.87{\pm}0.33$	77.25±0.47
coqa (gemma)	77.24±0.51	$74.39{\pm}0.46$	77.11±0.46
coqa (mistral)	75.65±0.31	$72.58{\pm}0.29$	76.04±0.50
nq (llama2)	74.45±0.37	$70.33{\pm}0.35$	75.90±0.41
nq (gemma)	78.31±0.54	$74.17{\pm}0.69$	79.33±0.57
nq (mistral)	77.02 ± 0.68	$73.17{\pm}0.65$	$78.82{\pm}0.55$

Table 8: Similar to Table 4, but with different number of generations at temperature of 1.0.

	Deg (E)	P(true)	SL	SL(norm)	TokenSAR	CSL	CSL-Next
trivia (llama2)	80.30±0.30	63.90±0.17	86.33±0.11	85.83±0.12	85.86±0.13	87.72±0.24	87.61±0.22
trivia (gemma)	81.92±0.16	$79.94{\pm}0.18$	$86.21{\pm}0.10$	$85.56{\pm}0.09$	$85.51{\pm}0.08$	87.14±0.14	$86.89{\pm}0.11$
trivia (mistral)	79.95±0.25	$67.67{\pm}0.27$	$86.33{\pm}0.13$	$86.14{\pm}0.13$	$86.23{\pm}0.11$	88.31±0.18	$\textbf{88.22}{\pm}\textbf{0.13}$
coqa (llama2)	68.32 ± 0.62	$53.41{\pm}0.41$	$68.17{\pm}0.33$	$71.04{\pm}0.53$	$71.29{\pm}0.54$	71.93±0.68	$71.70{\pm}0.63$
coqa (gemma)	69.19±0.62	$54.90{\pm}0.36$	$69.67{\pm}0.42$	$70.39{\pm}0.63$	$70.73{\pm}0.59$	71.65±0.63	$\textbf{71.96}{\pm 0.64}$
coqa (mistral)	68.52 ± 0.52	$52.66{\pm}0.37$	$67.72{\pm}0.30$	$69.07{\pm}0.39$	$69.30{\pm}0.40$	70.31±0.79	$\textbf{70.18}{\pm}\textbf{0.66}$
nq (llama2)	68.69±0.42	$51.70{\pm}0.38$	$64.47{\pm}0.44$	$66.07{\pm}0.42$	$66.64{\pm}0.36$	69.86±0.52	$69.53{\pm}0.45$
nq (gemma)	69.73±0.57	$60.51{\pm}0.55$	$69.34{\pm}0.47$	$70.84{\pm}0.58$	$70.60{\pm}0.62$	73.51±0.52	$72.27{\pm}0.59$
nq (mistral)	69.45±0.55	$52.60{\pm}0.39$	$66.70{\pm}0.49$	$67.14{\pm}0.42$	$68.07{\pm}0.44$	72.34±0.45	$71.19{\pm}0.58$

Table 9: Like Table 2, but using accuracy from LLaMA2-70B.

Table 10: Like Table 3, but using accuracy from LLaMA2-70B.

	Random	Upper Bound	Deg (E)	P(true)	SL	SL(norm)	TokenSAR	CSL	CSL-Next
trivia (llama2)	82.71±0.13	98.41±0.03	92.48±0.20	87.25±0.13	$95.60{\pm}0.06$	95.51±0.05	$95.49{\pm}0.05$	95.91±0.06	95.86±0.07
trivia (gemma)	$78.58{\pm}0.12$	$97.52{\pm}0.03$	$91.02{\pm}0.23$	$91.35{\pm}0.14$	$94.12{\pm}0.05$	$93.85{\pm}0.04$	$93.85{\pm}0.05$	$94.29{\pm}0.04$	$94.14{\pm}0.05$
trivia (mistral)	$80.23{\pm}0.11$	$97.90{\pm}0.02$	$91.48{\pm}0.33$	$87.38{\pm}0.13$	$94.75{\pm}0.06$	$94.67{\pm}0.05$	$94.66{\pm}0.05$	$95.16{\pm}0.06$	$95.15{\pm}0.04$
coqa (llama2)	$91.00{\pm}0.17$	$99.58{\pm}0.02$	$94.19{\pm}0.16$	$91.86{\pm}0.17$	$95.30{\pm}0.14$	$95.65{\pm}0.16$	$95.73{\pm}0.16$	$95.88{\pm}0.17$	$95.81{\pm}0.17$
coqa (gemma)	$92.14{\pm}0.15$	$99.68 {\pm} 0.01$	$95.10{\pm}0.26$	$93.39{\pm}0.15$	$96.09{\pm}0.11$	$96.12{\pm}0.14$	$96.18{\pm}0.13$	$96.35{\pm}0.12$	$\textbf{96.39}{\pm}\textbf{0.14}$
coqa (mistral)	$91.61{\pm}0.16$	$99.64{\pm}0.01$	$94.81 {\pm} 0.34$	$92.28{\pm}0.18$	$95.47{\pm}0.11$	$95.63{\pm}0.13$	$95.71{\pm}0.12$	$95.86{\pm}0.18$	$95.86{\pm}0.15$
nq (llama2)	$56.74{\pm}0.60$	$88.89{\pm}0.34$	$68.96{\pm}1.00$	$57.57{\pm}0.60$	$68.96{\pm}0.70$	$69.01{\pm}0.73$	$69.72{\pm}0.71$	$71.10{\pm}0.64$	$70.80{\pm}0.78$
nq (gemma)	$48.50{\pm}0.60$	$83.59{\pm}0.44$	$61.92{\pm}1.07$	$56.26{\pm}0.62$	$64.78{\pm}0.73$	$64.47{\pm}0.85$	$64.75{\pm}0.85$	$65.96{\pm}0.85$	$64.95{\pm}0.99$
nq (mistral)	$53.65{\pm}0.59$	$87.05{\pm}0.37$	$65.99{\pm}0.99$	$56.07{\pm}0.86$	$67.63{\pm}0.69$	$67.29{\pm}0.57$	$68.31{\pm}0.54$	$69.88{\pm}0.64$	$69.46{\pm}0.54$