# Decomposing Uncertainty for Large Language Models through Input Clarification Ensembling

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#### Abstract

Uncertainty decomposition refers to the task of decomposing the total uncertainty of a model into data (aleatoric) uncertainty, resulting from the inherent complexity or ambiguity of the data, and model (epistemic) uncertainty, resulting from the lack of knowledge in the model. Performing uncertainty decomposition for large language models (LLMs) is an important step toward improving the reliability, trustworthiness, and interpretability of LLMs, but this research task is very challenging and remains unresolved. The existing canonical method, Bayesian Neural Network (BNN), cannot be applied to LLMs, because BNN requires training and ensembling multiple variants of models, which is infeasible or prohibitively expensive for LLMs. In this paper, we introduce an uncertainty decomposition framework for LLMs, called input clarifications ensemble, which bypasses the need to train new models. Rather than ensembling models with different parameters, our approach generates a set of clarifications for the input, feeds them into the fixed LLMs, and ensembles the corresponding predictions. We show that our framework shares a symmetric decomposition structure with BNN. Empirical evaluations demonstrate that the proposed framework provides accurate and reliable uncertainty quantification on various tasks. Code will be made publicly available at https://github.com/ UCSB-NLP-Chang/llm\_uncertainty.

#### **1** Introduction

With the wide application of Large language models (LLMs), it becomes crucial that the predictions of LLMs are trustworthy. One critical dimension of the trustworthiness of LLMs is the ability to indicate when their generations are reliable and correct, which falls into the topic of *uncertainty quantification* (UQ). As an effective risk assessment method, uncertainty quantification aims to measure the confidence level of neural networks on their predictions (Gal et al., 2016; Bhatt et al., 2021; Hüllermeier and Waegeman, 2021). A higher uncertainty implies the output of LLMs should be rejected or need further evaluation. The quality of uncertainty quantification is also influenced by how close the prediction confidence measure corresponds to the actual accuracy (*i.e.*, whether the model is *well-calibrated*).

Quantifying the total uncertainty for LLMs has received increasing research attention. Existing work observes that LLMs are relatively well-calibrated by ensembling multiple reasoning chains (Wang et al., 2022; Huang et al., 2022; Si et al., 2023), ensembling different prompts (Jiang et al., 2023), or prompting the LLMs to output their confidence levels (Kadavath et al., 2022; Lin et al., 2022; Tian et al., 2023). Besides these observations, several methods have been proposed to quantify the uncertainty of LLMs (Lin et al., 2022; Xiao et al., 2022; Kuhn et al., 2022; Lin et al., 2023; Duan et al., 2023; Huang et al., 2023; Park and Kim, 2023; Ren et al., 2023). An accurate quantification of the uncertainty can be used for various applications, such as out-of-distribution detection and misclassified data detection.

However, measuring the total uncertainty is just the first step towards understanding the uncertainty of LLM prediction. In order to draw a more holistic view of LLM's uncertainty structure, one would also need to understand different types of uncertainty and decompose the source into these types, a problem we refer to as *uncertainty decomposition*. Specifically, the total uncertainty can be decomposed into two categories of uncertainty, *data* (*aleatoric*) uncertainty and model (epistemic) uncertainty. Model uncertainty arises when the model lacks the knowledge to produce the correct output. For example, the question 'What is 2+3?' requires the knowledge of algebraic operations. Without such knowledge, the uncertainty will be high.

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On the other hand, the data uncertainty arises from the inherent complexities and ambiguities of data examples, such as ambiguous questions (Min et al., 2020; Guo et al., 2021; Kuhn et al., 2023) and unclear task instructions (Tamkin et al., 2022), and is irreducible no matter how well the model learns. For example, to answer the question 'Who is the president of this country?', without any context, the uncertainty would be high regardless of how well the LLM learns, because the question itself is ambiguous. Uncertainty decomposition provides important insights for users to improve the performance of LLM. If model uncertainty is high, users could supply the model with adequate knowledge through model adaptation, in-context learning, etc; if the data uncertainty is high, then users should modify the query to make it more concrete.

However, despite the existing work that studies the total uncertainty for LLMs, decomposing the uncertainty for LLMs remains understudied. Furthermore, existing methods for uncertainty decomposition cannot be directly applied, due to the black-box nature of LLMs and their prohibitive sizes. Bayesian Neural Network (BNN) (Gal and Ghahramani, 2016; Lakshminarayanan et al., 2017; Maddox et al., 2019), decomposes the uncertainty by training different variants of models, e.g., by having different random seeds, drop-out rates etc., to minimize the model uncertainty in the target task and then ensembling them. However, training multiple variants of LLMs such as GPT-4 and PaLM-2 will be either infeasible or extremely expensive. Given these challenges, we aim to address the following question: How to develop an effective uncertainty quantification framework that can decompose the uncertainty for LLMs?

In this paper, we propose an alternative framework for uncertainty decomposition, called input clarification ensemble, which is almost symmetrical to BNNs but can bypass the need to modify LLM parameters. In particular, we notice that, although it is very challenging to modify LLM's parameters, it is relatively easy to manipulate the input to LLMs. Inspired by this, rather than ensembling different model variants that minimize the model uncertainty, we introduce a set of *input* clarifications, which, when appended to the input, can minimize the data uncertainty. We then ensemble the LLM's predictions under different clarifications. Figure 1 shows the general pipeline. Unlike the BNN method that ensembles the predictions of several different models, the proposed method



Figure 1: Overview of the proposed uncertainty quantification method.

leverage input clarification ensemble to quantify the uncertainty. For example, for the question 'Who is the president of this country?', a possible clarification is 'This country refers to the US.' By ruling out the data uncertainty by clarification, we can ascribe the remaining uncertainty of each individual prediction to model uncertainty. Furthermore, by measuring the disagreement of the model predictions under different clarifications, we can gauge the data uncertainty. Our experiments verify that the proposed method provide accurate uncertainty quantification results on both total uncertainty and its decomposition.

#### 2 Related Work

In this section, we will discuss the existing work for uncertainty quantification.

#### 2.1 Related Work

Uncertainty quantification. Uncertainty quantification for machine learning models has been widely studied to quantify the reliability of model predictions (Gal et al., 2016; Gal and Ghahramani, 2016; Malinin and Gales, 2018; Ovadia et al., 2019; Malinin et al., 2020; Lin et al., 2022; Kuhn et al., 2022; Lin et al., 2023). Various reasons can cause uncertainty in model predictions, such as lack of knowledge and noisy data. Given the total uncertainty in model uncertainty (due to lack of knowledge in the model) and data uncertainty (due to the inherent randomness and noise in data).

Depending on how the uncertainty is obtained, existing uncertainty quantification methods can

be categorized into *intrinsic* and *extrinsic* methods. Intrinsic methods adopt machine learning models to provide an inherent uncertainty estimate, such as Bayesian approaches and deterministic approaches (Malinin and Gales, 2018). The Bayesian approaches (Blundell et al., 2015; Gal and Ghahramani, 2016; Teye et al., 2018; Mobiny et al., 2021; Lakshminarayanan et al., 2017; Malinin et al., 2020; He et al., 2020) can quantify both data and model uncertainty. In comparison, extrinsic methods quantify the uncertainty in a posthoc manner using auxiliary models (Kristiadi et al., 2021; Lahlou et al., 2022). Our method belongs to the intrinsic methods and is directly motivated by the Bayesian neural networks.

**Uncertainty Quantification and Model Calibra**tion for LLMs With the wide application of LLMs, how to accurately quantify the prediction uncertainty has also drawn attention (Xiao et al., 2022; Lin et al., 2022; Mielke et al., 2022; Zhou et al., 2023; Huang et al., 2023; Duan et al., 2023; Chen and Mueller, 2023). Additional challenges have been introduced since LLMs are more applied in generative tasks, which makes the output distribution measurement more difficult (Ott et al., 2018; Malinin and Gales, 2020). Semantic Uncertainty (Kuhn et al., 2022) has been proposed to alleviate the unstructured output space of LLMs for better uncertainty quantification. Lin et al. (2023) also aims to address the unstructured output space. Although there have been some explorations in this direction, existing methods can only estimate the total uncertainty. In comparison, we propose a more principled framework that can both quantify the total uncertainty and decompose it into data uncertainty and model uncertainty, leading to a more fine-grained understanding of LLMs.

Another line of research is the model calibration for LLMs. Model calibration is the process of ensuring that the predicted probabilities or confidence scores from a machine learning model align with the true probabilities or likelihoods of events occurring (*i.e.*, the prediction is correct). Wellcalibrated model predictions help improve the reliability of uncertainty quantification. Based on existing model calibration methods (Hendrycks and Gimpel, 2016; Guo et al., 2017; Ovadia et al., 2019; Riquelme et al., 2018; Desai and Durrett, 2020), prior work (Huang et al., 2022; Jiang et al., 2023, 2021; Ye and Durrett, 2022) has shown that LLMs are relatively well-calibrated on factual QA and complex reasoning tasks by properly prompting them. Specifically, Kadavath et al. (2022); Tian et al. (2023) estimate the prediction confidence of LLMs by prompting LLMs to output their confidence of their answers. For complex reasoning tasks, LLMs may output both the reasoning chains and the final answer. To estimate the confidence score, previous approaches (Huang et al., 2022) sample multiple outputs for the input question and use the answer frequency to indicate the confidence. Researchers further ensemble multiple prompts for better calibration performance (Jiang et al., 2023). Our uncertainty quantification is based on the wellcalibrated predictions of LLMs, which lead to a more precise and accurate quantification result.

### 3 Methodology

### 3.1 Notations and Problem Formulation

Denote X and Y as the input and output target of a given task, respectively, and  $\theta$  as the parameters of an LLM. Denote p(Y|X) and  $q(Y|X,\theta)$  as the ground-truth and predicted distribution of Y given X.

We then introduce three uncertainty concepts. First, the *total uncertainty* is defined as the entropy of the predicted distribution, *i.e.*,  $U_{total} = H(q(\boldsymbol{Y}|\boldsymbol{X}; \boldsymbol{\theta}))$ . If the overall uncertainty is high, then it means the LLM has low confidence in its output. The total uncertainty can be further decomposed into two different types of uncertainties.

The first type of uncertainty is referred to as the *model uncertainty*, which characterizes how well the LLM approaches the ground truth distribution, and thus learns the knowledge therein. For example, to answer '*What is* 2+3?', if the LLM were able to learn the true knowledge of the algebraic operation, it would be able to answer with certainty; otherwise, the uncertainty would be high.

The second type of uncertainty is referred to as the *data uncertainty*, which characterizes the fundamental uncertainty residing in the groundtruth distribution, and is irreducible no matter how well the LLM learns. For example, to answer *'Who is the president of this country?'*, even if the LLM were well acquainted with politics, it still could not answer it confidently, because this question is inherently ambiguous. The data uncertainty is often quantified by the entropy in the ground-truth distribution, *i.e.*,  $\mathcal{H}(p(\mathbf{Y}|\mathbf{X}))$ .

The goal of this paper is to estimate both the model and data uncertainties in LLMs.

#### 3.2 Background: Bayesian Neural Networks

One possible solution to our task is to apply the canonical Bayesian Neural Network (BNN) approach, which is a standard approach to uncertainty decomposition. Instead of having one set of parameters, BNN ensembles k models, each parameterized as  $\theta^{(k)}$ . Each of the k models seeks to minimize the training loss, usually the cross entropy loss for classification tasks, which is equivalent to solving the following optimization problem

$$\min_{\boldsymbol{\theta}} \operatorname{KL}(p(\boldsymbol{Y}|\boldsymbol{X}) \| q(\boldsymbol{Y}|\boldsymbol{X}, \boldsymbol{\theta}))).$$
(1)

However, different models have slightly different hyperparameter settings, such as initialization values, dropout weights, architectures, *etc.*, and thus the optimized values,  $\{\theta^{(k)}\}$ , are different across different *k*'s. Denote the resulting distribution of  $\{\theta^{(k)}\}$  as  $p(\theta|D)$  where D is the training dataset. Then the ensembled distribution of BNN can be represented as  $q(Y|X) = \mathbb{E}_{q(\theta|D)}[q(Y|X, \theta)]$ .

BNN decomposes the uncertainty as

$$\mathcal{H}(q(\boldsymbol{Y}|\boldsymbol{X})) = \underbrace{\mathcal{I}_q(\boldsymbol{Y},\boldsymbol{\theta}|\boldsymbol{X})}_{(1)} + \underbrace{\mathbb{E}_{q(\boldsymbol{\theta}|\mathcal{D})}\mathcal{H}(q(\boldsymbol{Y}|\boldsymbol{X},\boldsymbol{\theta}))}_{(2)},$$

where  $\mathcal{I}_q$  denotes the mutual information under the *q* distribution. ① measures the disagreement among the different models; ② measures the average uncertainty of each individual model. Under certain assumptions, ① and ② can approximate the model and data uncertainties, respectively (Gal et al., 2016). An illustration of the BNN framework is shown in the upper panel of Figure 1.

Here is an intuitive explanation of why this is the case. According to Eq. 1, the goal of each model is to approach the ground-truth distribution, and thus can be viewed as the process of reducing the model uncertainty. Therefore, if the optimization is successful, all the models will learn the true distribution, *i.e.*,  $q(Y|X, \theta^{(k)}) = p(Y|X), \forall k$ , which, by definition, results in zero model uncertainty. Meanwhile, ① will also be zero because all the models produce the same prediction. Thus ① equals model uncertainty in this case. ② would also equal the data uncertainty because the predicted distribution is equal to the true distribution.

On the other hand, if the models fail to learn the true distribution, in which case the model uncertainty will be large, ① will also be large because different models have different hyperparameter settings and will be stuck in very different local optima.

#### **3.3 Does BNN work for LLMs?**

Our goal of decomposing uncertainty for LLMs would be easily achieved if the BNN framework were readily applicable to LLMs. Unfortunately, this is not the case, because the key to the success of BNNs is the learning process in Eq. 1, which is very challenging for LLMs. Specifically, there are two types of methods for adapting LLMs to a particular task, supervised fine-tuning and prompting/incontext learning. Directly fine-tuning the model according to Eq. 1 is usually infeasible due to the limited access to model parameters and its huge requirement for computation. Even if it is feasible, it would be very time-consuming because it requires fine-tuning multiple LLMs.

On the other hand, the in-context learning method, though feasible, does not fit into the BNN framework because it does not directly aim to optimize Eq. 1, so the decomposition will be very inaccurate. To demonstrate this, we perform a simple experiment on the AmbigQA (Min et al., 2020) dataset, which contains both ambiguous questions with multiple answers and unambiguous questions. We use the BNN method to decompose the uncertainty of ChatGPT, where the different individual model is derived by providing different in-context examples. If the decomposition method is accurate, we would expect to see that the data uncertainty for the ambiguous questions is significantly larger than that of the unambiguous ones. However, as shown in Figure 2, the gap between the uncertainties of the two groups of questions is very small. More experiment details can be found in Section 4.



Figure 2: Data uncertainty distribution on the AmbigQA (Min et al., 2020) dataset using the BNN method. We use kernel density estimation to smooth the frequency distribution histogram. BNN is achieved by ensembling different in-context examples.

Although the BNN framework does not work for LLMs, it inspires us to design an alternative framework that is almost completely symmetrical to BNN, which we will introduce in the next subsection.

#### 3.4 Input Clarification Ensembling

Although modifying or adapting LLM models is challenging, it is relatively straightforward to modify the input to LLMs. Now that BNN works by ensembling different *models* that minimize *model uncertainty* (Eq. 1), can we design a framework that ensembles different *inputs* that minimize *data uncertainty*?

This is the motivation behind our proposed framework, which consists of the following two steps.

**Step 1: Input Clarification.** Given an input X, we first generate a set of texts,  $C^{(k)}$ , called *clarifications*. Each clarification  $C^{(k)}$  seeks to minimize the ambiguity in X (and thus the data uncertainty) when appended to X. Formally,

$$\min_{\boldsymbol{C}} \mathcal{H}(p(\boldsymbol{Y}|\boldsymbol{X} \oplus \boldsymbol{C})), \tag{3}$$

where  $\oplus$  denotes concatenation. In the aforementioned example, 'Who is the president of this country?', possible clarifications include 'This country refers to the US.' and many other countries. Since there can be many clarifications, { $C^{(k)}$ } is a set.

**Step 2: Ensemble.** Define q(C|X) as the distribution of the clarification given a particular input. The predicted distribution is derived by ensembling the predictions conditional on each clarified input, *i.e.*,  $q(Y|X) = \mathbb{E}_{q(C|X)}[q(Y|X \oplus C, \theta)]$ . Note that the model parameters,  $\theta$ , are kept constant, and thus will be omitted from the condition for brevity.

We then propose to decompose the uncertainty of the ensembled model as

$$\mathcal{H}(q(\boldsymbol{Y}|\boldsymbol{X})) = \underbrace{\mathcal{I}_q(\boldsymbol{Y}, \boldsymbol{C}|\boldsymbol{X})}_{\mathbb{Q}'} + \underbrace{\mathbb{E}_{q(\boldsymbol{C}|\boldsymbol{X})}\mathcal{H}(q(\boldsymbol{Y}|\boldsymbol{X} \oplus \boldsymbol{C}))}_{\mathbb{Q}'}.$$
(4)

We claim that 1' and 2' can approximate the data and model uncertainties, respectively. An illustration of the proposed framework is shown in the lower panel of Figure 1.

By comparing Eqs. 3 and 4 against Eqs. 1 and 2, we can notice the symmetry between our framework and BNN's — BNN seeks to pin down model uncertainty whereas ours data uncertainty; Eq. 4 takes almost an identical form to Eq. 2 but the corresponding uncertainties are swapped. Figure 1 also shows such symmetry.

Accordingly, the same explanation of why it works applies here. When the input is already

very clear, and hence data uncertainty is low, the clarifications will be identically empty, so  $\mathbb{T}'$  will approach zero. When the input is very ambiguous, the clarifications will be very different (think about the aforementioned president example), and so would the answers produced with different clarifications. In this case,  $\mathbb{T}'$  will be very high. On the other hand,  $\mathbb{T}'$  measures the average uncertainty on *clarified* input, which rules out most of the data uncertainty, so the remaining uncertainty can mostly be ascribed to model uncertainty.

#### 3.5 Input Clarification

Unlike in conventional neural networks, the input to LLMs usually contains multiple components, including instructions, in-context examples, questions *etc.* Therefore, we can separately measure the data uncertainties of different input components by clarifying only the corresponding components. For example, to measure the data uncertainty resulting from ambiguous instructions, we can clarify only the instruction. In this work, we will focus on measuring instruction uncertainty and question uncertainty, but the framework is readily generalizable to other input components.

To derive clarifications that approximately solve Eq. 3, we introduce a clarification LLM, where we provide an instruction and in-context example to guide the LLM to perform adequate clarification. Note that the clarification LLM can be different from the LLM for prediction. In this work, we will use gpt-3.5-turbo and gpt-4 as the clarification LLM to ensure the quality of clarification. Further implementation details are provided in Section 4.

### 3.6 Improving Performance via Soliciting Clarifications

Our framework not only provides a way of decomposing the uncertainties, but can also enable an interpretable and more effective human-LLM interaction experience. Currently, one of the major ways for humans to interact with LLMs is by designing appropriate input. However, the input designed by humans may not be clear enough to LLMs, often resulting in undesirable answers given by LLMs. With the proposed input clarification framework, we can design an interaction paradigm that alleviates this problem.

Given an input query, we can first gauge the uncertainties of different input components. If one of the components, say the instruction, contributes to high uncertainty (exceeding a threshold), we can provide feedback to the user that the LLM is not sure about the answer because the instruction is ambiguous, along with several clarification options produced by the clarification LLM for the user to choose from. This would help the user to perform directed improvement of the input query and obtain the desirable answer.

## 4 Experiments

In this section, we conduct empirical evaluations to demonstrate the validity and effectiveness of the proposed method. Specifically, we aims to answer the following two questions:

- 1. Can the proposed UQ framework quantify *to-tal uncertainty* effectively and correctly?
- 2. Can the proposed UQ framework *decompose the uncertainty* effectively and correctly?

To answer the first question, we conduct the mistake detection experiment, which will be introduced in Section 4.2. To answer the second question, we conduct three experiments: ambiguity detection, monotonicity check, and recall of correct answers, which will be presented in Sections 4.3-4.5, respectively.

### 4.1 Experiment Configurations

We use gpt-3.5-turbo-0613 as the default LLM for all experiments. We sample 10 model predictions with temperature 0.5 and use the answer frequency to estimate the output distribution. Since all the datasets we use are open-ended generation tasks, different generated answers could have the exactly same meaning. For example, to answer the question 'When did the world's population reach 7 billion?', the LLM may generate several different answers such as 'December 2017' and 'The world's population reached 7 billion in December 2017', which are essentially the same meaning. Regarding these two answers as distinct answers can lead to an overestimation of the entropy of output distribution. Previous work (Kuhn et al., 2022; Lin et al., 2023) uses a natural language inference model to cluster different generated sequences with the same semantic meanings into one group for better output distribution estimation. We empirically find that LLMs can achieve better clustering performance. Therefore, we prompt the LLM to cluster output answers into different groups for output distribution estimation on question-answering datasets.

For all the experiments, we introduce the following baselines: Semantic Uncertainty (Kuhn et al., 2022) (denoted as SE) directly computes the entropy of the output distribution as the estimated (total) uncertainty (named semantic entropy in their paper). Tian et al. (2023) first queries the LLM for the answer and then queries the LLM again for the confidence of the correctness of the answer. We denote this method as ASK4CONF. We also slightly modify the prompt for the ambiguity detection task to query LLM for the confidence of the ambiguity of the input (denoted as ASK4CONF-D). The BNN\* method is implemented by ensembling the output distributions of multiple different in-context example sets (we use 5 different sets). We add \* here since this method is different from standard BNN and does not directly optimize Eq. 1. We provide more details of the prompts used in the experiments in Appendix A.2.

#### 4.2 Mistake Detection

Correctly quantifying the total uncertainty is the premise of correctly decomposing the uncertainty. If the estimated total uncertainty is inaccurate, so will the estimated data and model uncertainty. A reliable total uncertainty measure should have a close correspondence to the model's prediction accuracy. For model predictions whose total uncertainty is high, the chances that the predictions are incorrect should also be high. Therefore, we will evaluate the total uncertainty quantification using the mistake detection task, following the previous work (Kuhn et al., 2022; Lin et al., 2023).

**Evaluation Settings** We evaluate the total uncertainty on the Natural Question (NQ) dataset (Kwiatkowski et al., 2019) and GSM8K (Cobbe et al., 2021). We compute the total uncertainty of each model and use it to predict whether the model's answer is correct. We report the area under the receiver operator characteristic curve (AUROC) as well as the best F1 score when using the total uncertainty to predict the correctness of the model answer. We use 5-shot in-context examples on the NQ dataset and 2-shot on the GSM8K dataset with chain-of-thoughts. For our method, we prompt the LLM to rephrase the input question to generate the clarification set. The detailed prompts are listed in Appendix A.2.

**Results** The experiment results are shown in Table 1, which confirms that the total uncertainty measured by the proposed approach is reliable. Specif-

Method	AUROC	F1 Score	Entropy (🖌)	Entropy (X)	
Natural Question					
SE	63.8	77.9	0.29	0.56	
ASK4CONF	70.4	83.9	-	-	
$BNN^*$	69.7	79.7	0.46	0.88	
OURS	72.3	80.2	0.58	1.18	
GSM8K					
SE	88.2	92.4	0.32	1.46	
ASK4CONF	58.1	92.3	-	-	
BNN*	88.3	94.6	0.57	1.94	
OURS	89.7	94.7	0.42	1.82	

Table 1: Uncertainty quantification for mistake detection. Entropy ( $\checkmark$ ) refers to the average total uncertainty of questions with correct answers, while Entropy ( $\bigstar$ ) refers to the average total uncertainty of question with wrong answers.

ically, we highlight the following observations. First, our method achieves comparable uncertainty quantification performance compared to the baselines, achieving a similar AUROC and F1 score. Second, as the proposed method shares a symmetry form with the BNN method, one would expect the total uncertainty quantification of the two should be similar. The above experimental results verify that the quantification results of these two methods are very close. Third, although ASK4CONF performs well on factual QA tasks, it provides a poor uncertainty estimation for the complex reasoning task (GSM8K), while our method can still provide good mistake detection performance.

#### 4.3 Ambiguity Detection

Now we can proceed to evaluate whether the decomposed uncertainty is reliable. As discussed, one of the main causes of data uncertainty is the ambiguity of the input. Therefore, we will test how well the measured data uncertainty is predictive of whether an input is ambiguous. In particular, we focus on two input components, the instruction and the question, and separately predict the ambiguity within each component using the respective data uncertainty (see Section 3.5).

**Datasets** For ambiguity detection of the question, we select the AmbigQA dataset (Min et al., 2020), which has annotations on the ambiguity of questions. The questions in AmbigQA are extracted from the NQ dataset (Kwiatkowski et al., 2019).

For ambiguity detection of the instruction, since there is no existing dataset, we created a dataset, called AmbigInst, where we generated ambiguous instructions, their disambiguated versions, and the input-output pairs using ChatGPT via in-context learning. We further manually verify each generated instruction. Each instruction is paired with around 15 questions. Since the focus of AmbigInst is to detect ambiguous instructions, we did not introduce ambiguity to the paired questions. More details about AmbigInst can be found in Appendix B.

Evaluation Settings We use 5-shot in-context examples on the AmbigQA dataset similar to the experiment on the NQ dataset. Since the questions in AmbigInst are relatively easy and straightforward, we directly prompt LLMs in a zero-shot setting. For ambiguous question detection, we perform clarifications on the input question only. Since the ambiguities in the AmbigQA dataset sometimes could be subtle and hard to detect, we retrieve the most similar 16 questions as in-context examples when prompting the LLMs to generate clarifications for a particular input question. Also, we use gpt-4 as the clarification LLM for the AmbigQA dataset. The similarity between two questions is measured by the cosine similarity of their sentence embeddings from SENTENCE-BERT (Reimers and Gurevych, 2019). For the AmbigInst dataset, we directly prompt gpt-3.5-turbo-0613 to generate instruction clarifications (details in Appendix A.2). We additionally include the performance of our method when using ground-truth disambiguation from the two datasets for reference (denoted as  $OURS^*$ )

The baselines are similar to the methods in the mistake detection task. The main difference is we use the quantified uncertainty to predict whether the input contains ambiguity. Note that we leverage the data uncertainty for BNN\* and OURS and the total uncertainty for SE in this task. Also, BNN\* is not included on the AmbigInst dataset since we do not include in-context examples in the experiments on that dataset.

**Results** The experiment results are shown in Table 2. We emphasize two observations. First, our method achieves the best ambiguity detection performance and significantly outperforms the baselines. Note that all the baselines, except for BNN\*, use the total uncertainty for ambiguity detection, and thus could not disentangle model uncertainty from the data uncertainty. Therefore, these results verify the importance of uncertainty decomposition. Second, the BNN\* method is not effective in the black-box LLM setting. As we have discussed in Section 3.3, simply varying the in-context ex-

Method	AUROC	F1 Score	Avg. DU (🖌)	Avg. DU (X)	
AmbigQA					
SE	54.9	46.8	0.24	0.47	
ASK4CONF-D	55.0	64.3	-	-	
BNN*	53.6	53.0	0.13	0.13	
OURS	71.7	70.1	0.28	0.67	
OURS*	89.8	85.6	0.53	1.52	
AmbigInst					
SE	66.0	53.7	0.07	0.50	
ASK4CONF-D	57.9	75.4	-	-	
OURS	81.3	77.9	0.10	0.75	
OURS*	96.7	92.6	0.10	1.04	

Table 2: Uncertainty quantification for ambiguity detection. Avg. DU (✓) refers to the average data uncertainty of unambiguous questions, while Avg. DU (✗) refers to the average data uncertainty of ambiguous questions.

amples cannot accurately estimate the parameter posterior distribution, while the proposed framework is specially designed for the black-box LLMs.

Another observation is that ambiguity detection performance varies across different datasets. On the AmbigQA dataset (Min et al., 2020), the ambiguities are more implicit and hard to find by the clarification models, which makes the detection performance relatively low (although still higher than baselines significantly). Min et al. (2020) also note that the ambiguity in the dataset is "sometimes subtle" and "many (ambiguities) are only apparent after examining one or more Wikipedia pages". In comparison, on the AmbigInst dataset where we design ambiguities to be very explicit, the clarification model can generate effective clarifications for most cases, leading to a good detection performance. Finally, the performance of our method can be further improved when combined with the ground-truth disambiguation from the two datasets, demonstrating that the clarification model is still worth exploring.

#### 4.4 Monotinicity Check

To further evaluate the reliability of our data uncertainty measure, particularly the clarification module, we perform a monotonicity check experiment. Ideally, the clarified input should contribute to a much lower data uncertainty than the original ambiguous input. To test this, we perform two rounds of data uncertainty measuring. In the first round, we measure the data uncertainty by clarifying the original input segments (question or instruction). In the second round, we measure the data uncertainty of the clarified inputs obtained in the first round. Our goal is to check whether the data uncertainty



Figure 3: (Left) Average data uncertainty of the ambiguous inputs and their clarifications. (Right) Performance improvement via Soliciting clarifications. AmbigQA-Orig and AmbigInst-Orig refer to the recall of correct answers when directly answering the original input. AmbigQA-Clarify and AmbigInst-Clarify refer to the recall of correct answers using different number of input clarifications.

measured in the second round is much smaller than that in the first round. This experiment is performed on the AmbigQA and AmbigInst datasets. In both rounds, we use the same clarification prompt to generate the clarifications.

Figure 3(a) visualizes the change in uncertainty on both datasets. As can be observed, the data uncertainty drops significantly after the input is clarified, which verifies the effectiveness of the clarification network.

#### 4.5 Recall of Correct Answers

As discussed in Section 3.6, the proposed framework can be used to improve the performance in the presence of ambiguous input by asking human users to choose from a set of clarified versions of the input. In order to make this happen, our methods must be able to cover a good proportion of the possible answers resulting from different clarifications of a given ambiguous input. Also, the number of required clarifications should be smaller, as the users might not want to select the responses from a large set of choices.

To test this, we use the ambiguous questions and instructions from AmbigQA and AmbigInst respectively. For each input, we collect all the possible labeled answers from the ground-truth annotations. Then we select one answer as the target answer that the user is asking for. In our pipeline, the LLM will generate multiple answers given the generated clarifications. Therefore, we inspect how well these generated answers cover the target answer given different numbers of clarifications. We separately compute the recall of the target answer with the different numbers of clarifications. As a baseline, we introduce a vanilla version, where we directly query the LLM with ambiguous input without any clarification.

The results are illustrated in Figure 3(b). We can consistently observe an increase of recall given more clarifications. Similar to the ambiguity detection performance, the recall improvement on the AmbigInst dataset is more significant compared to the AmbigQA dataset, which is due to the subtlety of the AmbigQA dataset as discussed. Nevertheless, the proposed clarification framework is able to significantly improve the answer recall over the vanilla version without the clarification.

## 5 Conclusion

In this paper, we focus on the uncertainty quantification of LLMs and propose a new framework for decomposing the uncertainty. With a symmetric structure of the BNN methods, our framework relies on input clarifications for uncertainty quantification, which is more suitable for black-box LLMs. In the future, we will further explore how to build a more effective clarification module to boost the effectiveness of our method.

### 6 Limitation

There are still several limitations of this paper that need further improvement. First, as the paper focuses on black-box LLMs that are accessible via APIs only, our method has to query the LLMs multiple times to estimate the output distribution (as the token-level generation probability is still inaccessible when writing this paper). How to decrease the high query budget and improve the efficiency is still under-explored. Also, our method relies on an external clarification model for uncertainty quantification. Solely relying on the LLM suppresses the performance, and we need to develop a more suitable clarification module.

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### **A** Implementation Details

### A.1 Implementation details for baselines

**Mistake detection** For the mistake detection task, we strictly follow the experiment settings from Kuhn et al. (2022) and Lin et al. (2023). For each example, we estimate the output distribution and take the answer with the highest frequency as the final answer. Then we use the method (and the prompt) from Lin et al. (2023) to determine whether the answer is correct by prompting Chat-GPT. Based on the total uncertainty and correctness of the answer, we compute the AUROC and conduct a grid search to find the best threshold for the F1 score, where the correct answers are regarded as positive examples.

For the implementation of ASK4CONF(Tian et al., 2023) in the mistake detection task, we use the "Verb. 2S top-1" method (and the corresponding prompts) to estimate the confidence of the language model. Rather than asking the LLM to directly generate an answer, we sample multiple answers and take the most frequent one as the answer. After that, we prompt the LLM for the confidence of the most frequent answer. The prompt we use is:

1: The prompt for mistake detection (ASK4CONF).

```
Answer the following question.
Question: {The testing question}
Answer: {The most frequent answer
}
Provide the probability that your
answer is correct. Give ONLY the
probability, no other words or
explanation.
For example:
Probability: <the probability
between 0.0 and 1.0 that your
solution is correct, without any
extra commentary whatsoever; just
the probability!>
```

**Ambiguity detection** For the mistake detection task, we use the total uncertainty for SEMANTIC UNCERTAINTY (Kuhn et al., 2022), data uncertainty from BNN\*, and the confidence score of the ambiguity from ASK4CONF (Tian et al., 2023) to predict whether the input is ambiguous or not.

We slightly modify the prompt of ASK4CONF as follows:

2: The prompt for mistake detection (ASK4CONF-D).

```
Read the following question:
Question:
{question}
Provide the probability that this
question is ambiguous due to
factors such as ambiguous
entities, ambiguous event
references, or ambiguity over the
answer type. Give ONLY the
probability, no other words or
explanation.
```

For example:

Probability: <the probability between 0.0 and 1.0 that the question is ambiguous (1.0 means the question is absolutely ambiguous), without any extra commentary whatsoever; just the probability!>

## A.2 Prompts for Our Clarification Model

We list the prompts we used for clarification generation on each dataset as follows:

3: The prompt for question rephrase on the Natural Question dataset

```
In this task, you will receive a
single question, and your goal is
 to generate multiple versions of
it that convey the same meaning
as the original. Please format
your responses as follows:
Rephrase 1: [Your rephrased
question]
Rephrase 2: [Another rephrased
question]
Rephrase 3: [Yet another
rephrased question]
. . . .
Ensure that each rephrased
question is distinct from the
others."
Here are two examples:
```

(examples skipped)

4: The prompt for question disambiguation on the AmbigQA dataset.

In what follows, you will be given some questions that might be ambiguous. These ambiguities can arise from various factors, including but not limited to:

 Ambiguous references to entities in the question.
 Multiple properties of objects /entities in the question leading to different interpretations.
 Ambiguities due to unclear timestamps.
 Ambiguities stemming from unclear locations.
 Multiple valid answer types based on the question.

For each question, you are to provide at least two distinct rephrasings that resolve these ambiguities. By "rephrasing," we mean you should reformulate the question to be clear and direct, eliminating any possible ambiguity without altering the original intent of the question. You should not seek further information or produce a binary ( yes-no) question as a result of the clarification. Instead, you must create a direct question (wh -question) that aims to obtain a specific answer.

Please format your responses as follows (with at least two rephrasings per question): Clarifications: 1. [First rephrased question]

[Second rephrased question]
 [Third rephrased question]

If the original question is already clear and unambiguous, you should indicate this by stating, "No clarification needed ." (In-context examples)

5: The prompt for instruction disambiguation on the AmbigInst dataset.

\*\*Objective\*\*
Analyze the given task
description for ambiguities based
on the description itself and
the provided input question. If
the task description is ambiguous
, your task is to clarify it by
interpreting the ambiguous
concepts, specifying necessary
conditions, or using other
methods. Provide all possible
disambiguations.

\*\*Important Rules\*\*
1. Perform detailed analyses before concluding whether the task description is clear or ambiguous.
2. Output disambiguations in the specified format.
3. Some seemingly unambiguous task descriptions are actually ambiguous given that particular input. So, do not forget to leverage the input to analyze whether the task description is underspecified.

\*\*Output Format\*\*
Your output should follow this
format:
Analyses:
[Think step-by-step to reason on
the clarity of the task
description. After that, output
your judgement on whether the
task description is ambiguous or
not]

Disambiguations: 1. [Disambiguated task description 1.] 2. [Disambiguated task description 2.] 3. [Disambiguated task description 3.]

```
...
If the task description is clear
and unambiguous, simply output:
Disambiguations:
1. No clarification needed.
```

### **B** AmbigInst Dataset

#### **B.1** Dataset Creation

We generate ambiguous instructions following the pipeline of SELF-INSTRUCTION (Wang et al., 2022). Specifically, we first query CHATGPT with several manually designed ambiguous task descriptions as in-context examples. For better verification of the ambiguity, we also prompt CHATGPT to output the cause of the ambiguity. Among the ambiguous descriptions generated by CHATGPT, we manually filter out those that have an open-ended output space such as Write a report on the new marketing campaign. The final dataset contains 15 ambiguous task descriptions. After that, we query CHATGPT again to generate ground-truth clarifications based on the cause of ambiguities generated in the first query.

Given the collected ambiguous task descriptions and their clarifications, we then prompt the model to generate input-output pairs for each task. Specifically, 15 inputs are generated for each task, and each input is further paired with different output answers depending on the ground-truth clarifications. We additionally add a post-processing step where we filter out the inputs that have exactly the same answer given different clarifications. The final ambiguous instructions consist of 15 tasks with 214 input questions in total.

We take 10 tasks from the Instruction induction dataset (Honovich et al., 2022) as the unambiguous tasks, including letters\_list, first\_word\_letter, second\_word\_letter, orthography\_starts\_with, larger\_animal, singular\_to\_plural, diff, num\_to\_verbal, antonyms, and sum.

We manually add some clarifications to the 10 instructions to remove potential ambiguities. For example, given the original instruction "Break the input word into letters, separated by spaces" for example. Since separated by spaces might cause ambiguities of how many spaces should be used between two letters, we clarify it with "Write the inputted word with a space between each letter". Each task is also paired with 15 input-output pairs. Overall, the synthetic dataset contains 25 tasks and 364 different inputs.

#### **B.2** Dataset Examples

We list several examples from the AMBIGINST dataset with ambiguous instructions.

 $\triangleright$  1. Rearrange the objects on the table in ascending order.

Input: The following table lists the objects on my desk:

Name	Size	Weight	Color	Date of Manufacture	Price
Pen	14cm	0.02kg	blue	01/15/2022	\$1.50
Book	23cm	0.5kg	red	08/10/2020	\$15.00
Laptop	38cm	1.8kg	silver	05/04/2021	\$1200.00

 $\triangleright$  2. Calculate the average of the numbers in the given list, rounding to the nearest whole number.

Input: 23.5, 47.2, 30.1, 16.6

 $\triangleright$  3. Determine the length of a sentence.

Input: The quick brown fox jumps over the lazy dog.

 $\triangleright$  4. Sort the names alphabetically.

Input: Courtney Cox, Jennifer Aniston, Lisa Kudrow, Matthew Perry.

▷ 5. Identify the subject in the sentence. Input: The CEO of the company gave a speech about the future of technology.

 $\triangleright$  6. Count the number of objects in the given list of objects.

Input: Forks, Spoons, Knives, Plates, Cups, Spoons, Forks, Spoons, Cups.

 $\triangleright$  7. Rank the football players based on their performance.

Input: The following table lists the statistics of football players:

Name	Goal Scored	Assists
Lionel Messi	30	12
Cristiano Ronaldo	25	10
Robert Lewandowski	35	5

▷ 8. Sort the data in alphabetical order. Input: Dog, Cat, Bird, Fish, Aardvark.

 $\triangleright$  9. Identify the largest city in the set. Input: The following table lists the cities in the set:

Name	Population	Land Area
Paris	2.1 million	105.4 km
Berlin	3.6 million	891.8 km
Madrid	3.3 million	604.3 km

> 10. Organize the files by date. Input: Files to be organized:

Filename	Creation Date	Last Modified Date
conference-recording.avi	11/10/2020	11/12/2020
birthday-video.mp4	05/05/2021	05/06/2021
budget.xlsx	12/31/2022	01/10/2023

 $\triangleright$  11. Find the middle value in a list of numbers.

Input: 12, 20, 35, 46, 52, 66, 74, 81

- $\triangleright$  12. Determine the square root of a number.
  - Input: 81
- ▷ 13. Find the capital of a country. Input: South Africa

 $\triangleright$  14. Classify a movie based on its rating.

Input: The movie "Toy Story 4" has an MPAA rating of G, an IMDb rating of 7.8, and a Rotten Tomatoes rating of 97%.

 $\triangleright$  15. Select the longest sentence from the following choices, and output the sentence index.

Input: The following sentences are listed:

- 1. To be, or not to be, that is the question.
- 2. Whether 'tis nobler in the mind to suffer the slings and arrows of outrageous fortune.

3. Or to take arms against a sea of troubles and by opposing end them.