

# Conformal Information Pursuit for Interactively Guiding Large Language Models



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## Motivation: Interactive Question Answering

- In Question-Answering (QA), contextual information may not be readily available all at once.
- Can we guide Large Language Models (LLMs) to solve QA tasks by gathering information interactively (Fig. 1)?
- This work proposes **Conformal Information Pursuit (C-IP)**, an information-theoretic framework for guiding LLMs to ask informative queries for QA.
- The challenge lies in estimating uncertainty from LLMs.

**Init. Info:** A 25-year-old woman comes to the physician for an examination.

**Uncertain → Ask a query**

**Doctor:** Is the patient's body temperature within the normal range?

**Patient:** The patient's body temperature is 36.6 °C (98.0 °F).

**Uncertain → Ask a query**

**Doctor:** What is the serum ferritin level in ng/mL?

**Patient:** The patient's serum ferritin level is 170 ng/mL.

**Confident → Final Prediction**

**Prediction:** (D) Intravascular hemolysis

Fig. 1: Example Interaction between Patient and Doctor LLM.

## Challenge: Uncertainty Estimation for LLMs

- Task:** We focus on multiple-choice QA tasks, where an LLM answers a question via next token probability:
$$f(x)_y = \hat{\mathbb{P}}_{\text{LLM}}(y | x)$$
- Issue:**  $\hat{\mathbb{P}}_{\text{LLM}}$  might be **noisy/miscalibrated**, leading to poor estimates of uncertainty.
- Proposal:** Leverage Conformal Prediction!

Fig. 2: Simulated 20Q Game with LLMs.  
(Dashed: uncalibrated; Solid: Calibrated)

## Proposed Method

- Let  $\mathcal{Q} = \{q : \mathcal{X} \rightarrow \mathcal{A}\}$  be a set of task-relevant, textual queries about the data (e.g.,  $q = \text{"What is the temperature of the patient?"}$ ).

### Prior Work: Information Pursuit (IP)

- Given a test sample  $\hat{x} \in \mathcal{X}$ , IP interactively and sequentially selects queries whose answers are most informative for the task  $Y$ :
$$q_1 = \operatorname{argmax}_{q \in \mathcal{Q}} I(Y; q(X)) = \operatorname{argmin}_{q \in \mathcal{Q}} H(Y | q(X))$$

$$q_{k+1} = \operatorname{argmin}_{q \in \mathcal{Q}} I(Y; q(X) | q_{1:k}(\hat{x})) = \operatorname{argmin}_{q \in \mathcal{Q}} H(Y | q(X), q_{1:k}(\hat{x}))$$
- At each iteration, IP selects the query that minimizes entropy.
- IP terminates when the residual mutual information is less than  $\epsilon$ .

### Proposed: Conformal Information Pursuit (C-IP)

- Rather than entropy, we leverage (split) Conformal Prediction and use **average sizes of prediction sets** to estimate uncertainty.
- We conformalize IP as follows:
  - Define the prediction set:**
$$\mathcal{C}_{\hat{\tau}}(q_{1:k}(X)) = \{y \in \mathcal{Y} \mid f(q_{1:k}(X))_y > \hat{\tau}\}$$
  - Obtain calibration samples by running simulations with LLMs and construct prediction sets that satisfy the marginalized guarantee:**
$$\mathbb{P}_{X,Y,Q_{1:k}}(Y \in \mathcal{C}_k(q_{1:k}(X))) \approx 1 - \alpha \quad \text{for } k = 1, \dots, L$$
  - Select queries that minimize log-expected length at each iteration:**
$$q_1 = \operatorname{argmin}_{q \in \mathcal{Q}} \log \mathbb{E}_X [|\mathcal{C}_{\hat{\tau}}(q(X))|]$$

$$q_{k+1} = \operatorname{argmin}_{q \in \mathcal{Q}} \log \mathbb{E}_X [|\mathcal{C}_{\hat{\tau}}(q(X))| \mid q_{1:k}(\hat{x})]$$
  - Terminate algorithm when length <  $\epsilon$ , then make a prediction:**
$$\hat{y} = \operatorname{argmax}_{y \in \mathcal{Y}} \mathbb{P}(y \mid q_{1:k}(\hat{x}))$$

## Experiments

- We evaluate C-IP on two tasks: **20 Questions (20Q)** and **Interactive Medical QA (MediQ)**.
  - 20Q:** A "Querier" LLM samples queries at each iteration, and an "Answerer" LLM evaluates whether they are true.
  - MediQ** [Li et al. 24]: An "Expert" LLM asks questions about a patient and makes predictions, and a "Patient" LLM answers those questions.

### Example of Interactive Medical Question Answering

**Context:** Initial Info: An 84-year-old woman with an indwelling urinary catheter and a history of recurrent nephrolithiasis is brought to the emergency. Question: Which of the following is most likely to be present on this patient's urine culture? Options: (A) Gram-negative, oxidase-positive rods, (B) Gram-positive, novobiocin-resistant cocci, (C) Gram-positive, gamma-hemolytic cocci, (D) Gram-negative, oxidase-negative rods.

**History  $q_{1:k}(x^{obs})$ :**

$q_1:$	What is the moisture level of the patient's mucous membranes?	$\hat{H}(Y   q_{1:k}(x^{obs}))$
$q_1(x^{obs}):$	She has dry mucous membranes.	
$q_2:$	What is the white blood cell count in the urine?	
$q_2(x^{obs}):$	The patient is oriented to person, and the urine studies show WBC of 40/HPF.	
$q_3:$	What is the patient's current body temperature?	
$q_3(x^{obs}):$	The patient's current body temperature is 38.3°C (100.9°F).	
$q_4:$	Why was she brought to the hospital?	
$q_4(x^{obs}):$	She was brought to the emergency department from her nursing home because of increasing confusion over the past day.	
$q_5:$	(Stopping Criteria Reached, Output Final Prediction)	

**Prediction:**

Final Prediction: D. Explanation: The patient's symptoms and presentation suggest a urinary tract infection (UTI). The patient has an indwelling urinary catheter, which is a risk factor for UTIs. (more omitted)

## Theoretical Justification

- Why does our derivation make sense?
- How are entropy and expected length of the prediction set related?
- Proposition: [Correia et al 24]. If prediction the set  $\mathcal{C}$  satisfies the marginal guarantee  $\mathbb{P}_{X,Y}(Y \in \mathcal{C}_{\tau}(X)) \approx 1 - \alpha$ , then

$$H(Y | X) \leq \text{constants} + (1 - \alpha) \log \mathbb{E}_X [|\mathcal{C}_{\tau}(X)|]$$