

Conformal Information Pursuit for Interactively Guiding Large Language Models

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Motivation: Interactive Question Answering

- In Question-Answering (QA), context and information **may not be readily available all at once and require asking informative questions.**
- Can we guide Large Language Models (LLMs) to solve QA tasks **interactively** (Fig. 1)?
- We propose an information-theoretic framework to interactively guide an LLM to ask queries that are most informative for the QA task.
- The challenge lies in estimating uncertainty from LLMs.

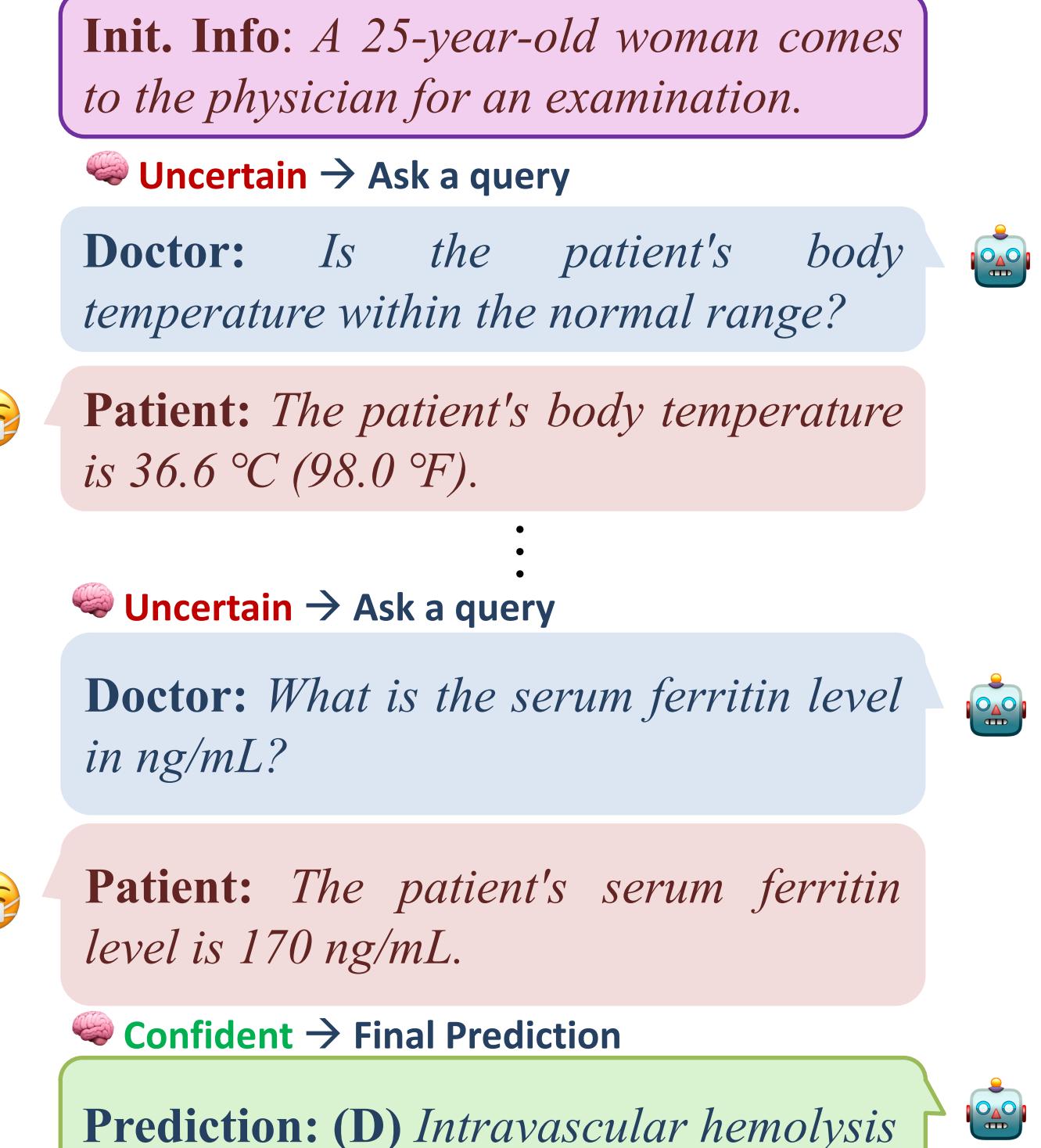


Fig. 1: Example Interaction between Patient and Doctor LLM.

Challenge: Uncertainty Estimation for LLMs

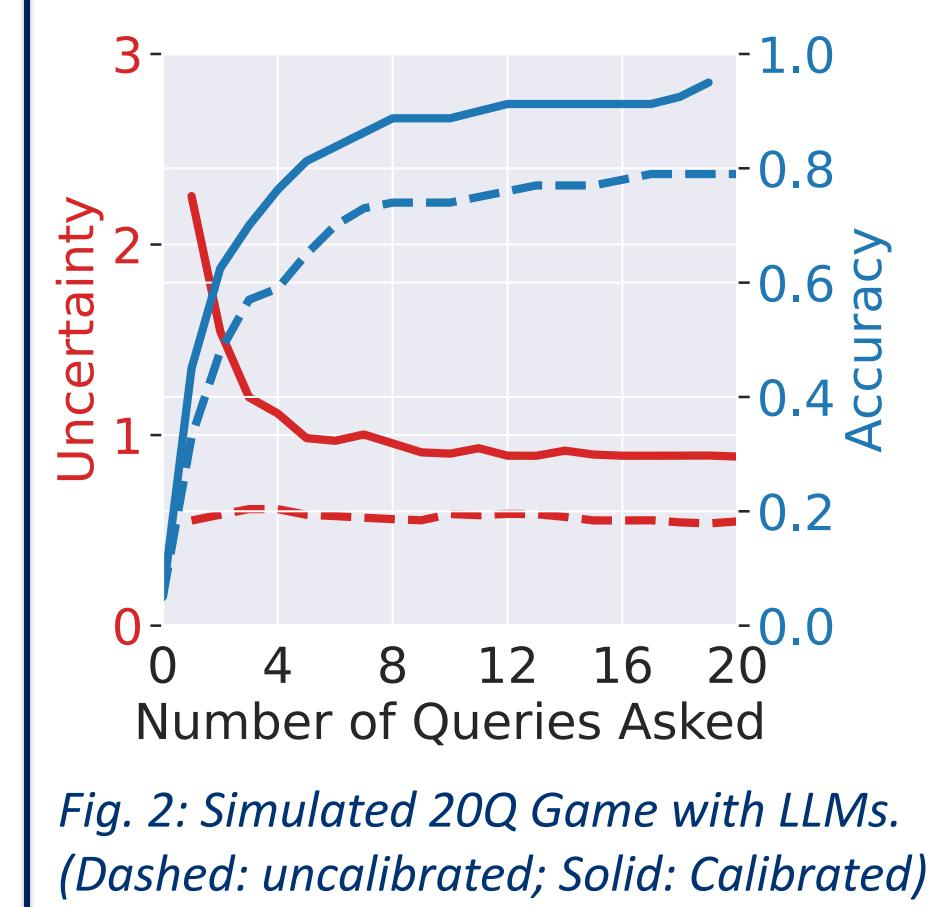


Fig. 2: Simulated 20Q Game with LLMs.
 (Dashed: uncalibrated; Solid: Calibrated)

- 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!**

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 mutual information is less than ϵ .

Proposed: Conformal Information Pursuit (C-IP)

- Rather than entropy, we leverage (split) Conformal Prediction and use **average sizes of prediction sets** to estimate uncertainty.
- Conformalize IP as follows:

1. Define the prediction set:

$$\mathcal{C}_{\hat{\tau}}(q_{1:k}(X)) = \{y \in \mathcal{Y} \mid f(q_{1:k}(X))_y > \hat{\tau}\}$$

2. Obtain calibration samples by running simulations with LLMs and construct prediction sets that satisfy the marginalized guarantee:

$$\mathbb{P}_{X,Y,Q_{1:k}}(Y \in \mathcal{C}_k(q_{1:k}(X))) \approx 1 - \alpha \quad \text{for } k = 1, \dots, L$$

3. Select queries that minimize log-expected length at each iteration:

$$q_1 = \operatorname{argmin}_{q \in \mathcal{Q}} \log \mathbb{E}_X [\lvert \mathcal{C}_{\hat{\tau}}(q(X)) \rvert]$$

$$q_{k+1} = \operatorname{argmin}_{q \in \mathcal{Q}} \log \mathbb{E}_X [\lvert \mathcal{C}_{\hat{\tau}}(q(X)) \rvert \mid q_{1:k}(\hat{x})]$$

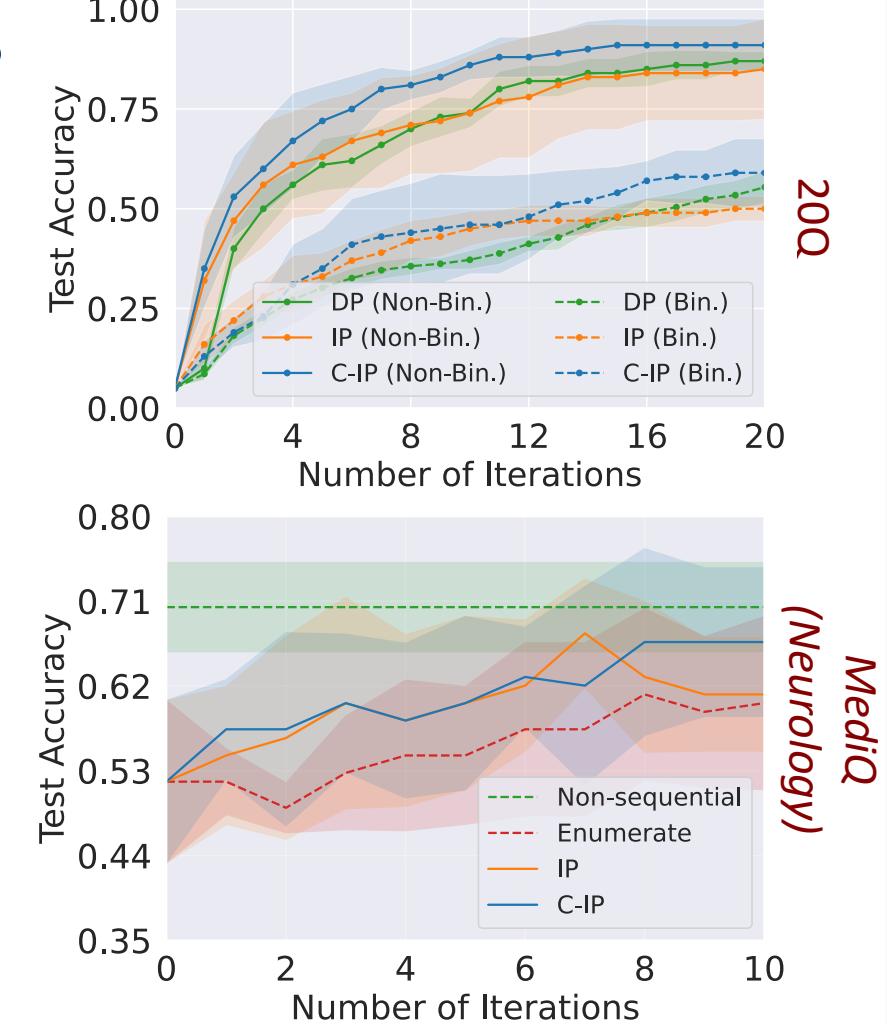
4. Terminate algorithm when length $< \epsilon$, then make a prediction:

$$\hat{y} = \operatorname{argmax}_{y \in \mathcal{Y}} \mathbb{P}(y \mid q_{1:k}(\hat{x}))$$

Experiments

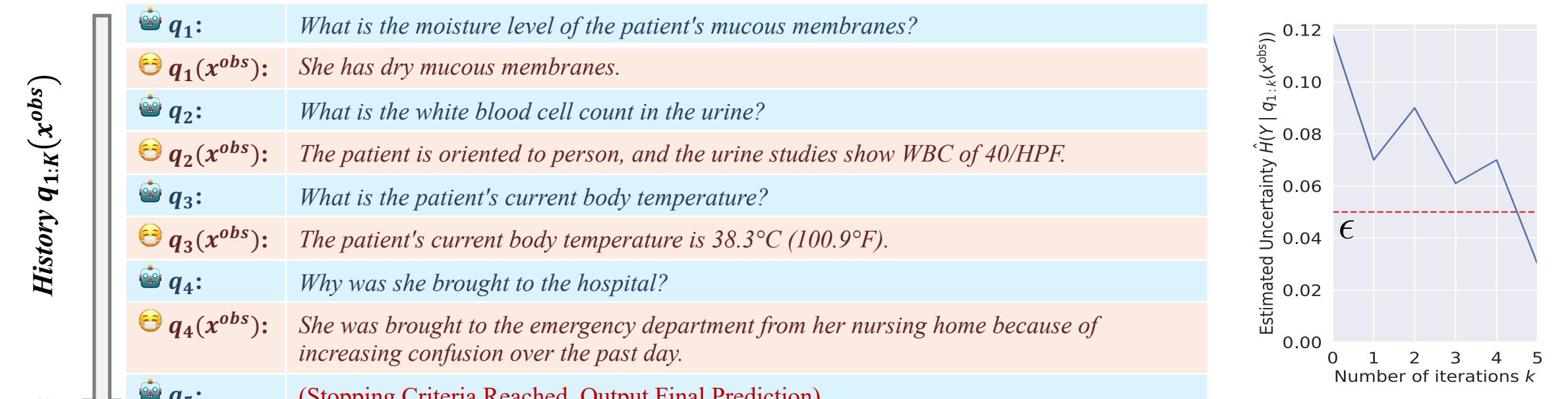
- We evaluate C-IP on two tasks: **20 Questions** (20Q) and **Interactive Medical QA** (MediQ).

- 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

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.



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

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