Monty Hall and Optimized Conformal Prediction to Improve Decision-Making with LLMs

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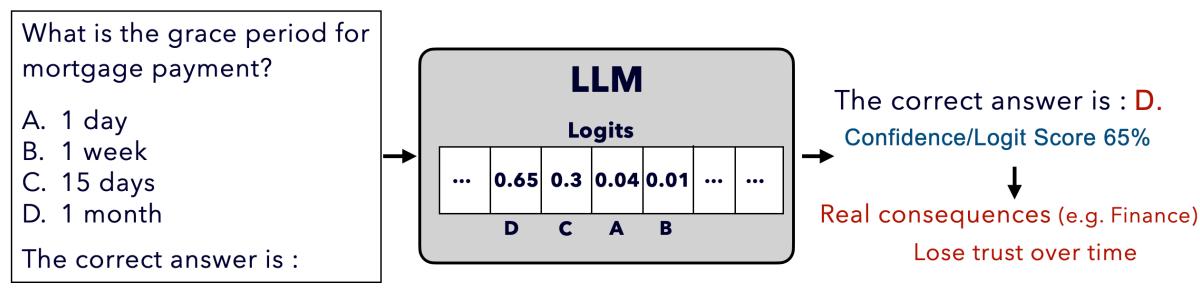
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Motivation

Decide between finite choices e.g., MCQ, Tool Selection, etc.

LLMs can output incorrect answers with high confidence.



Can we improve uncertainty quantification (UQ) and accuracy without heavy fine-tuning?

Conformal prediction (CP) can help in UQ

Kumar et al., 2023, Su et al., 2024

Output high coverage sets e.g., the correct answer is in: {C, D}

Large set ⇒ High uncertainty Small set ⇒ Low uncertainty

Summary

Prior works proposed conformal prediction (CP) for uncertainty quantification in LLMs but have limitations

Used ad-hoc scores (logits, self-consistency) Unreliable, expensive to compute Lead to large sets → Less useful

Utility of sets (CP) beyond UQ is underexplored

Our work

A principled method (CP-OPT) to learn scores

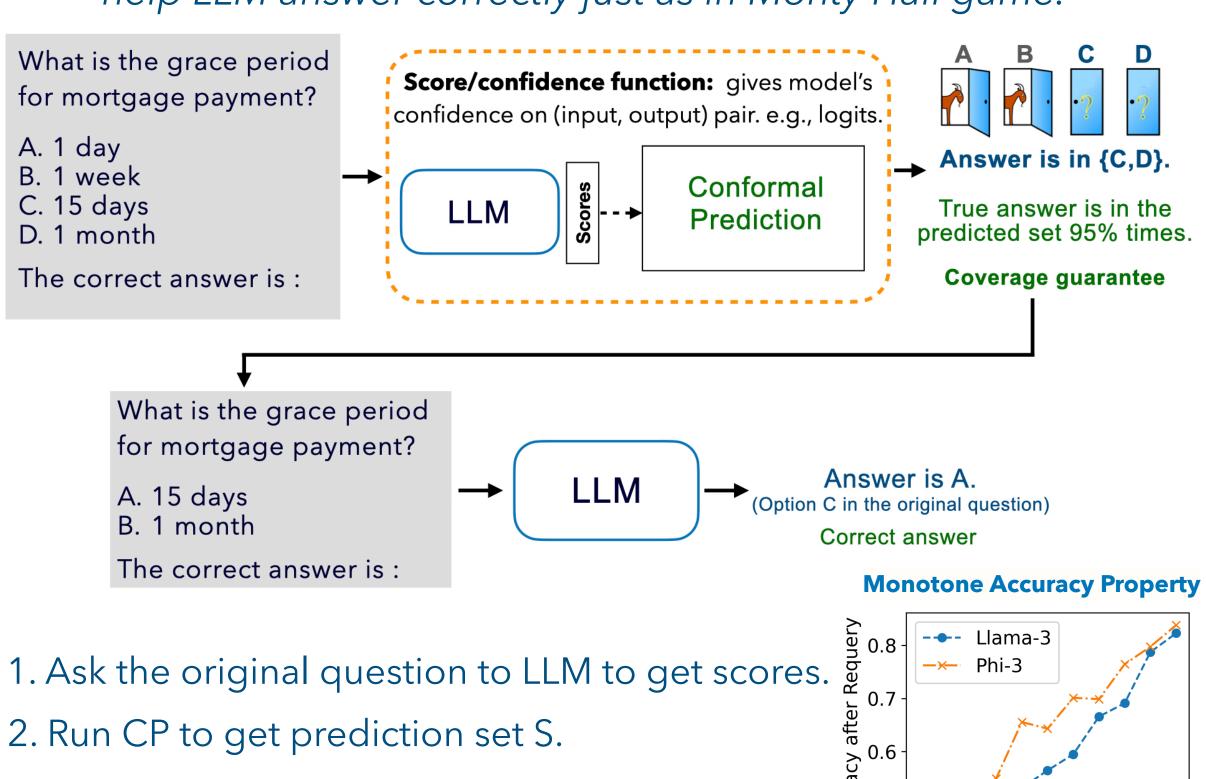
Revise question with the choices in the predicted set and ask LLM again (CROQ)

CP-OPT \Longrightarrow **Smaller sets** + **High coverage**

CROQ + CP-OPT \Longrightarrow Better accuracy

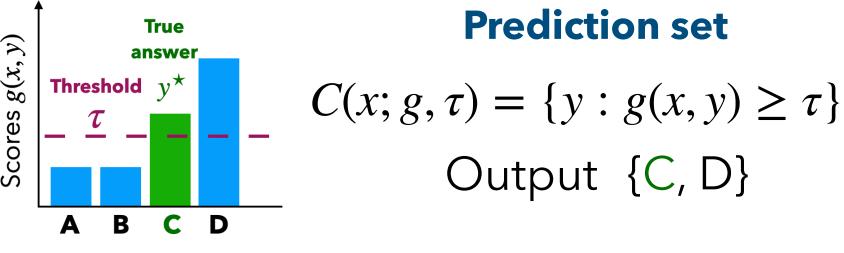
Conformal revision of question (CROQ) **Inspired from Monty Hall**

Expectation: Reduction in uncertainty should help LLM answer correctly just as in Monty Hall game.

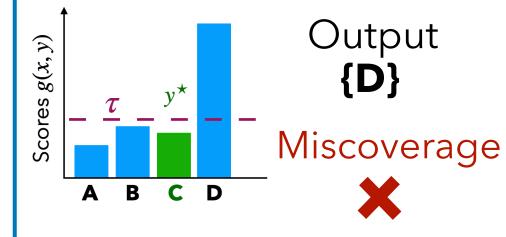


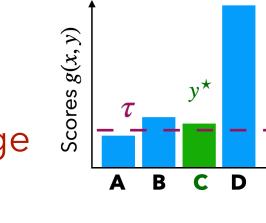
- 3. Eliminate the choices that are not in the set S.
- 4. Ask the revised question to LLM to get final output.

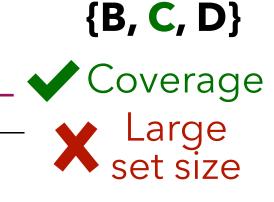
Score optimization (CP-OPT)



Effect of scores in CP







Output

Avg. set size

Coverage # times $y_i^* \in C(x_i | g, \tau)$

(CP-OPT)

$$\hat{g}, \hat{\tau} \in \arg\min_{g:\mathcal{X}\times\mathcal{Y}\mathbb{R}, \, \tau\in\mathbb{R}} \widehat{S}(g,\tau) + \lambda (\widehat{\mathcal{P}}(g,\tau) - 1 + \alpha)^2$$

Use \hat{g} to get scores for CP

Empirical Results

0 1 2 3 4 5 6 7 8 9 10

No. Answers Removed from Prediction Set

(H1) CP-OPT reduces set sizes while maintaining coverage

* indicates statistically significant difference based on paired t-test.

	# Opt.	Llama-3				Gemma-2			
		Avg. Set Size		Coverage		Avg. Set Size		Coverage	
Dataset		Logits	Ours	Logits	Ours	Logits	Ours	Logits	Ours
MMLU	4	2.56	2.53*	95.75	95.57	2.94	2.40*	95.16*	94.23
	10	5.53	4.90*	96.06*	95.45	7.79	6.08*	95.00*	94.04
	15	7.69	7.18*	95.42	95.06	11.71	10.04*	94.58	94.58
ToolAlpaca	4	1.17	1.18	97.08	96.85	1.12	1.05*	95.68	95.44
	10	1.51	1.39*	95.21	95.56	2.05	1.42*	95.56	94.5
	15	1.97	1.67*	96.50	96.03	3.54	1.77*	96.14	95.21
TruthfulQA	4	3.34	2.69*	95.95*	92.41	2.74	1.88*	96.46	95.44
	10	7.06	6.41*	94.43	93.42	7.52	5.64*	95.44	97.22
	15	10.61	10.62	94.68	94.68	11.23	9.35*	95.44	96.46

(H2) CROQ with logit and CP-OPT scores improves accuracy

 a_1 Baseline accuracy before CROQ

 a_1' CROQ accuracy with logits

			Llama-3			Gemma-2	
Model	# Opt.	Accuracy Before (a_1)	Accuracy After (a' ₁)	Gain $(a'_1 - a_1)$	Accuracy Before (a_1)	Accuracy After (a' ₁)	Gain $(a'_1 - a_1)$
	4	64.02	63.83	-0.19	67.62	67.70	0.07
MMLU	10	54.82	56.29	1.47*	53.80	53.93	0.13
	15	51.99	54.11	2.11*	50.78	50.58	-0.20
	4	91.47	91.94	0.47	93.46	93.11	-0.35
ToolAlpaca	10	85.16	88.67	3.50*	87.73	89.60	1.87*
	15	81.43	87.85	6.43*	87.97	88.55	0.58
TruthfulQA	4	54.43	55.19	0.76	74.68	74.94	0.25
	10	39.24	40.76	1.52	56.46	56.20	-0.25
	15	37.22	37.22	0.00	55.95	56.96	1.01

(H3) CROQ with CP-OPT performs better than CROQ with logits.

 a_1' CROQ accuracy with logits

 a_2' CROQ accuracy with CP-OPT

			LLama-3			Gemma-2	
Model	# Opt.	Accuracy Before	Accuracy After (a' ₂)	Gain	Accuracy Before	Accuracy After (a' ₂)	Gain
	4	$\frac{ (a_2) }{ 64.02 }$	$\frac{(a_2)}{63.67}$	$\frac{(a_2'-a_2)}{-0.34}$	$\frac{ (a_2) }{ 68.36}$	69.56	$\frac{(a_2'-a_2)}{\textbf{1.20*}}$
MMLU	10	54.82	57.11	2.29*	53.99	57.93	3.94*
	15	51.99	54.77	2.78*	50.78	51.31	0.52
	4	91.47	91.82	0.35	93.46	93.57	0.12
ToolAlpaca	10	85.16	89.02	3.86*	88.08	90.42	2.34*
	15	81.43	88.67	7.24*	88.08	89.37	1.29
	4	54.43	55.44	1.01	74.94	76.96	2.03
TruthfulQA	10	39.24	42.28	3.04	56.46	60.76	4.30*
	15	37.22	37.47	0.25	55.95	57.72	1.77