Harnessing LM Uncertainty for Decision Making

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https://probabll.github.io

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Image by `https://openart.ai`.

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The LM appears to choose the response.

But the appearance is misleading.

Any one response is the byproduct of a number of decisions made under uncertainty by a recipe or 'decoding algorithm'.

The LM 'parameterises' this algorithm, providing it with **predictions about what is possible**, not about what ought to be.

Image by `https://openart.ai`.

Harnessing Uncertainty

In the face of uncertainty, we want

- to make choices that are as ‘safe’ as they can be (given the knowledge we have access to);
  this depends on our ability to **represent uncertain knowledge**
- to convey whatever uncertainty remains in a way readily interpretable by users.
  this depends on our ability to **quantify and communicate** intelligible aspects of uncertainty

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  this depends on our ability to **quantify and communicate** intelligible aspects of uncertainty

LMs play a crucial role in uncertainty representation, but making meaningful use of their state of uncertain knowledge is a pressing research challenge.

Uncertainty Representation

The *autoregressive language model* API

Throughout the talk, we assume that one's preferred LM is an *autoregressive model*.

This choice implies access to a specific API that makes various crucial operations (incl. those needed for training and decoding) feasible to varying degrees of approximation.

This API allows us to regard an LM as a means to predict *conditional* (that is, input-specific) *probability distributions* (cpds).

Prompt → Language Model → Distribution over Responses

From sufficiently far away, we can regard an LM as machine that maps any one prompt to a prompt-specific *probability distribution* whose outcome space is the set of all complete token sequences.

Prompt

`Who pushed Big Bird?`

→ Language Model →

Response Distribution

Complete token sequence	Prob
EOS	0.0085
Elmo did it EOS	0.0060
It was Elmo EOS	0.0053
Oscar did it EOS	0.0015
Elmo EOS	0.0007
Grover , for sure EOS	0.0005
...	

*table-like structure for intuition only

Not quite the whole story...

As we zoom in, we realise that an LM does not really build anything like this 'tabular' representation of the cpd:

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rather, it parameterises a special kind of iterative process, which *implicitly* identifies one such object.

Prompt and Prefix → LM Primitive → Next-Token Distribution

With an empty prefix (represented by a sequence containing BOS only)

Prompt

Who pushed Big Bird?

Prefix

BOS

→ LM Primitive →

Token	Prob
it	0.15
Elmo	0.05
Grover	0.1
Oscar	0.001
for	0.1
was	0.001
...	
EOS	0.0085

With a longer prefix sequence:

Prompt

Who pushed Big Bird?

Prefix

BOS it

→ LM Primitive →

Token	Prob
it	0.001
Elmo	0.1
Grover	0.02
Oscar	0.001
for	0.05
was	0.25
...	
EOS	0.01

Prompt:  `Who pushed BB?`. Response: `It was Elmo EOS`.

*prompt omitted from input for space

BOS →

Token	Prob
it	0.15
Elmo	0.05
Grover	0.1
Oscar	0.001
for	0.1
was	0.001
...	
EOS	0.0085

With probability 0.15, draw *it*

Prompt:  `Who pushed BB?`. Response: `It was Elmo EOS`.

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BOS

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EOS	0.01

With probability 0.25, draw *was*

Prompt:  `Who pushed BB?`. Response: `It was Elmo EOS`.

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BOS →

Token	Prob
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EOS	0.01

BOS it was →

Token	Prob
it	0.001
Elmo	0.2
Grover	0.12
Oscar	0.15
for	0.09
was	0.001
...	
EOS	0.0001

With probability 0.2, draw *Elmo*

Prompt:  `Who pushed BB?`. Response: `It was Elmo EOS`.

*prompt omitted from input for space

BOS →

Token	Prob
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EOS	0.0001

BOS it was Elmo →

Token	Prob
it	0.001
Elmo	0.04
Grover	0.02
Oscar	0.001
for	0.03
was	0.007
...	
EOS	0.7

With probability 0.7, draw *EOS*

Prompt:  `Who pushed BB?`. Response: `It was Elmo EOS`.

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BOS →

Token	Prob
it	0.15
Elmo	0.05
Grover	0.1
Oscar	0.001
for	0.1
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EOS	0.0085

BOS it →

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$p_\theta(\mathit{it\ was\ Elmo\ EOS}\,|$  $, \mathit{who\ pushed\ BB?}) = 0.15 \times 0.25 \times 0.2 \times 0.7 = 0.00525$

Factorised Probabilities

Given a prompt x, an autoregressive LM factorises the probability it assigns to any one response $y = \langle y_1, \ldots, y_\ell \rangle$ along the ℓ tokens that make up the response:

$$P(y|x, \theta) = \prod_{i=1}^{\ell} P(y_i|x, y_{<i}, \theta) \ .$$

Why are LMs so often Designed this Way?

There are various answers, here are some

1. there are infinitely many responses, but only finitely many tokens at each step;
2. this allows us to assess the probability mass of a response efficiently;
3. this allows us to 'draw' outcomes from the model, often with useful statistical guarantees.

(1) is about feasibility, (2) is useful for supervised training (but also some forms of decoding), (3) is particularly useful for decoding (but also some forms of training).

Some Limitations

The representation is expressed in terms of **probability**

- interpretation is not obvious (depending on design choices, training data and estimation procedure, and likely varying from prompt to prompt);
- difficulty representing ignorance (or, more generally, different sources of uncertainty);
- countable additivity and other debatable axioms.

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The representation is **unstructured**

- in probability, *structure* (in the form of a hierarchy of variables and their explicit dependencies) is how we distinguish different sources of uncertainty (e.g., ambiguity, linguistic relatedness, insufficient knowledge or expressiveness, etc.), but LMs express uncertainty directly over token sequences.

Summary

We can regard an LM as a mechanism trained to predict entire input-specific probability distributions over the space of responses.

The most common such mechanisms (incl. encoder-decoder and decoder-only Transformer models) are built upon a chain-rule factorisation of the probability of sequences. This allows us to regard LMs as offering tractable means to:

1. assign probability;
2. sample responses;

There are interesting designs that violate this API (e.g., EBMs), but we are not covering those today.

Probing the Uncertainty Representation

The *Explicit* View

By design, an LM offers an API to **explicitly** assign probabilistic belief to any response given any prompt.

Prompt

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→ Language Model →

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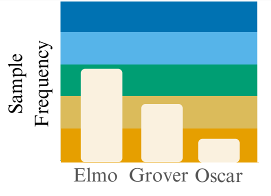
- ‘fragmentation’: different responses may convey the same information, so probabilistic belief in any information content is spread over many responses;
- (lack of) ‘calibration’: probabilistic belief need not reflect any external interpretation (e.g., rate of correctness);
- ‘unintuitive’: probabilities are assigned piecemeal with strange and unintuitive effects on what is ‘typically realisable’

The standard LM API also supports (stochastic) sampling.



Elmo	Grover	Oscar
Elmo pushed him.	Grover did it.	Oscar.
Elmo did it.	Grover, for sure.	
It was Elmo.	Grover.	
Elmo.		
Elmo.		

- we obtain 'realisable' sequences;
- (statistical) properties and regularities (or lack thereof) of samples shed light on the kind of knowledge the LM represents about the prompt and responses;

A sampler also identifies a probability distribution, but **implicitly** via statistical properties of generated samples. Some samplers (forward, Gibbs, etc.) support decisions that are coherent with the explicit view, others don't (temp, top-k, etc.).

Verbalised Uncertainty

Models can generate linguistic markers that are suggestive of (un)certainty. As when the LM generates '*Grover, for sure*'.

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Bad:

- Elmo did it.
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Better:

Probably Elmo, but there's a small chance that Grover or Oscar did it.

We can steer a model to pick these markers for coherence with its belief state given the prompt.

Summary

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The **implicit (sampler-based) view** is customisable (different samplers may implement different biases, sometimes by design), but it requires statistical analysis and hence more computation.

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The **explicit view** requires access to the model (most APIs provide sampling / generation, but not the token-level distributions).

The **implicit (sampler-based) view** is customisable (different samplers may implement different biases, sometimes by design), but it requires statistical analysis and hence more computation.

'**Verbalised uncertainty**' is an adaptation of the generator and, as such, it requires careful design and evaluation, but it is a more user-friendly tool.

What Next?

We will now discuss three ways in which uncertainty an LM associates with a given prompt—its *belief state*—can be ‘harnessed’ for better interaction:

1. Parameterising decision making pipelines
   or Should we respond?
2. Parameterising decision rules;
   or What should we respond with?
3. User-friendly communication of a complex belief state
   or Can we respond but also convey as much (un)certainty as necessary in order to be coherent with the belief state?

Selective Prediction

Overview

A common use for uncertainty is to parameterise 'decision making pipelines'.

One basic such pipeline is called **selective prediction** [23, 40]

- choose an uncertainty quantifier $\rho(x)$—a numerical summary of the LM's belief state given x;
- treat $\rho(x)$ as predictive of 'risk' of poor decisions;
- abstain from deciding when $\rho(x)$ predicts high risk.

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A less basic pipeline might allow for **interaction**. For example, in an attempt to reduce the risk of making a decision, we may prompt the user to provide additional information [25, 49].

Uncertainty Quantifiers for Selective Prediction (SP)

Most uncertainty quantifiers associate **'lack of concentration' of probability mass with error**:

- Average token surprisal $\frac{1}{\ell}\sum_{i=1}^{\ell} \log P(y_i|x, y_{<i}, \theta)$
- Average entropy of next-token CPDs
- Entropy of CPD [44]

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Recent move to incorporate 'linguistic invariances'. For example, to associate **spread over semantically distinct forms with error**:

- Semantic entropy [26]
- Various forms of consistency (syntactic, logical, reasoning) [1, 20, 42]
- Representational similarity [5, 31]

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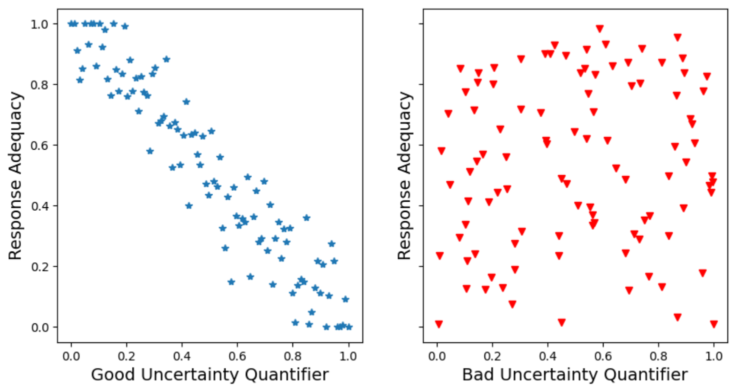
The list goes on. There are 10s of these showing up every month. The principle is typically the same: formulate a quantifier, show that it can be used to separate 'good' decisions from 'poor' ones.

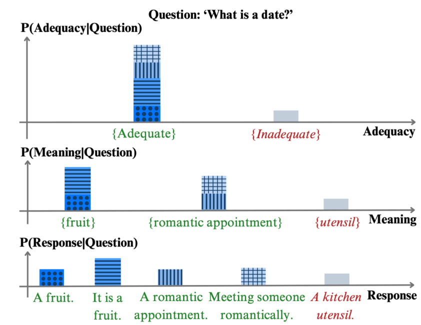
What is a Good Uncertainty Quantifier?



(Anti-)Correlation Between Uncertainty/Confidence and Quality of Response

Does 'Lack of Concentration' Really Predict Errors?

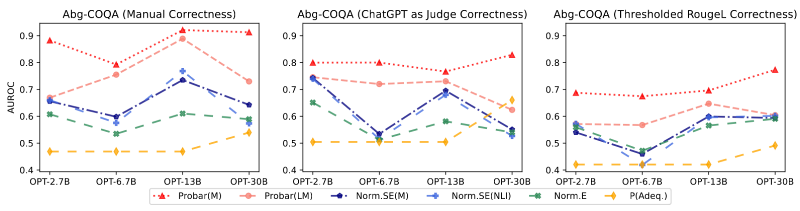
Regarding fragmentation of beliefs as a symptom of unreliable knowledge echoes the idea that disagreement is a form of error, but NLG applications challenge this idea [2, 33].



Bottom: the rather 'flat' model distribution over responses for an ambiguous question. Centre: pushes the model distribution through a 'meaning' classifier. Top: pushes the model distribution through an adequacy classifier.

ProbAR estimates the rate at which the model's belief state produces adequate responses via sampling.

Adequacy is judged automatically by a reward model (general purpose or task-specific).



ProbAR with LM-predicted adequacy outperforms variants of entropy and P(true).

Evaluation of SP via AUROC correlates UQ with Response Quality measured by a judge. We use human judgement (left), ChatGPT (centre) and RougeL (right).

Summary

The belief state can be summarised into a number that is predictive of task success.

The good stuff

- Such an 'uncertainty quantifier' can inform a selective decision maker that abstains from responding to avoid errors.

The bad stuff

- Many uncertainty quantifiers are hardly interpretable, hence it can be hard to design a concrete rule.
- Many quantifiers exploit basic and often unrealistic assumptions about data uncertainty.

Decision Rules & MBR

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- But what about the cases where we must produce an output?
- Then uncertainty can guide *how* we choose among many plausible hypotheses.

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$$P(Y \mid x, \theta)$$

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- A **decision rule** maps a **distribution** $\rightarrow$ **an outcome**.
- A decoding algorithm implements (an approximation to) such a decision rule.
- Key question: under uncertainty, how do we best summarise the model's beliefs?

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- MAP selects the single hypothesis to which the model assigns greatest belief: the mode.
- Greedy decoding and beam search can be viewed as approximations to MAP.

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- MAP ignores the overall *structure and similarity* of different outcomes.

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- But some settings require a *consistent, principled* choice:
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    - reducing hallucination by preferring stable hypotheses.
- In these cases, we must decide *which* output is **best** under the model's beliefs.

Minimum Bayes Risk (MBR)

- MBR selects the output with the *highest expected utility* (or equivalently, lowest expected loss / risk):

$$y_{\text{MBR}} = \arg\max_{y} \; \mathbb{E}_{y' \sim P(Y|x,\theta)} \left[u(y, y') \right].$$

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- In natural language generation, we typically chose this utility to be a text similarity metric.

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- In natural language generation, we typically chose this utility to be a text similarity metric.
- Unlike MAP, MBR reasons over the *entire distribution*, taking into account *similarity* between outcomes.

Minimum Bayes Risk (MBR)

- MBR selects the output with the *highest expected utility* (or equivalently, lowest expected loss / risk):

$$y_{\text{MBR}} = \arg\max_{y} \ \mathbb{E}_{y' \sim P(Y|x,\theta)} \left[u(y, y') \right].$$

- The decision depends on:
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- Unlike MAP, MBR reasons over the *entire distribution*, taking into account *similarity* between outcomes.
- Like MAP, we need to approximate this objective.

Approximating MBR

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- We therefore approximate *both* the search space and the expectation using **samples** [8, 9].
- Sampling provides:
  - a finite candidate set,
  - and a *Monte Carlo* estimate of expected utility.

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$$y^{(1)}, \ldots, y^{(N)} \sim P(Y \mid x, \theta).$$

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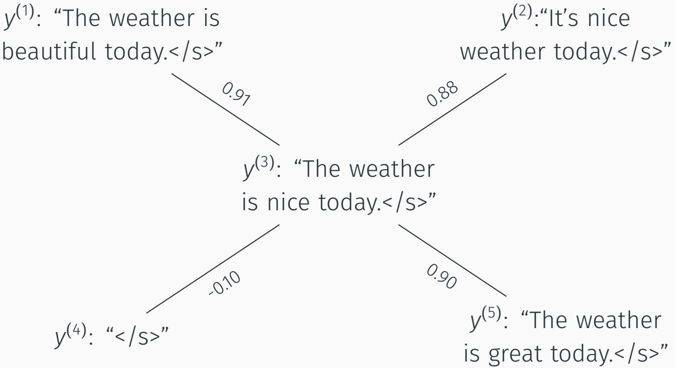
4. Select the candidate with the highest sample average utility:

$$\hat{y}_{\text{MBR}} \approx \arg\max_{i} \; \hat{u}\left(y^{(i)}\right).$$

Example: MBR in Machine Translation

Source sentence: “Het is mooi weer vandaag.”



Under the lens of BLEURT in this example, MBR selects the candidate with the highest average similarity to the others.

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    - Sampling-based MBR has long been found to outperform MAP / beam search when using task-relevant neural utility functions (BLEURT, COMET) [12, 15].

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  - Advances in automatic evaluation translate into stronger MBR decisions [15, 43].
- But MBR is expensive
  - Requires multiple generations *and* computing a utility matrix over candidates.
  - Computational cost is a barrier to deployment at scale.

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  - Instead of N unbiased samples, generate candidates using methods that yield *higher-utility sets* on average: top-k sampling, nucleus sampling, etc. [9].

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- Distilling the improvements
  - Train a model to mimic the MBR-selected outputs, amortizing the cost into training. Afterwards, use fast decoding algorithms (e.g. greedy decoding) on the fine-tuned model [13, 45].

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5. After fine-tuning, *single-pass decoding* (beam/greedy) produces outputs that perform considerably better than the original model.

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- How does MBR operate when our language models truly capture multiple plausible, but structurally distinct responses?
- Will it "summarise" the model beliefs well?

A Dialogue Example

A: The mountains would be a great place for the lab retreat.
B: That's a wonderful choice.

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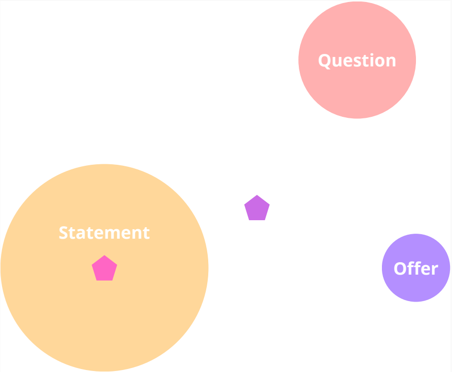
- *Offer*: "Shall I make the necessary arrangements?"

MBR May Compromise Among Modes



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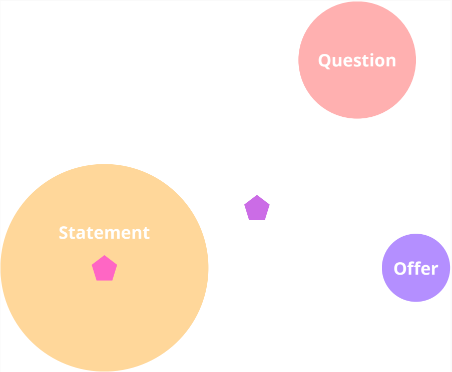

Using common utility choices (BLEURT, BERTScore), sampling-based MBR often *compromises between semantic modes*: the MBR-selected output is **not** optimal when evaluated *within* its own semantic/structural cluster in $> 50\%$ of cases [11].

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Structure-Conditional MBR

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- We also show this improves MBR performance on real-world instruction-following tasks.

Communicating Uncertainty in Natural Language

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Verbalised uncertainty becomes a *decision aid* for users, helping them judge when an answer is reliable.

How Do We Get Models to Express Uncertainty?

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- Some fine-tune the model to learn to always produce answers that additionally communicate uncertainty [3, 4, 10].

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Existing LLMs typically perform poorly on both if not fine-tuned explicitly for it [37, 46].

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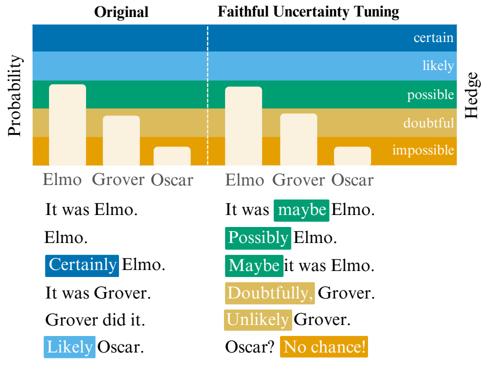
- Faithful uncertainty communication gives users a transparent view of the model's state of knowledge.



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- **Step 4: Fine-tune on the resulting dataset.**
  - Fine-tune the original model using maximum likelihood estimation on $(x, f(y^{(i)}))$ pairs.

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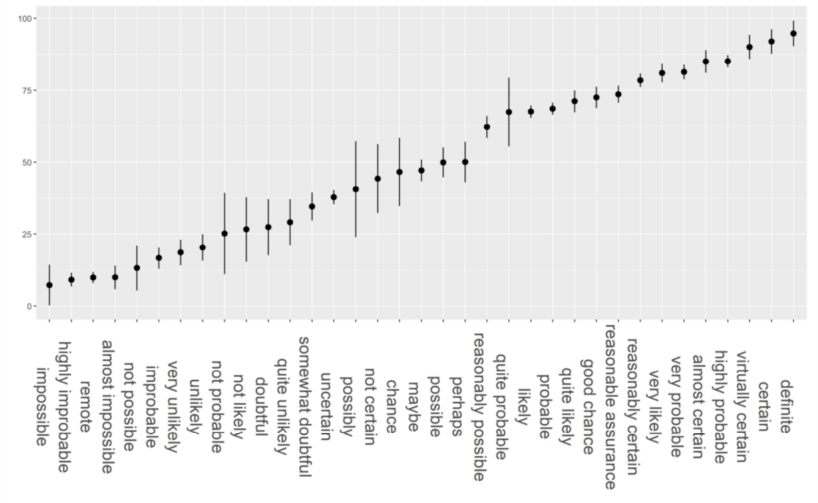
Mapping Hedge Phrases → Numerical Uncertainty [41]



Faithfulness Results

Model	PopQA	NQ	TriviaQA
Base (regular prompting)	0.52	0.53	0.53
Base (prompting for unc.)	0.58	0.60	0.59
FUT-interweave	**0.78**	**0.76**	**0.77**
FUT-postfix	0.73	0.74	0.74
FUT-numerical	0.81	0.78	0.78

We trained OLMo-2 (13B) using FUT and a subset of PopQA (only the input prompts), finding considerable improvements in faithfully communicating uncertainty in their responses. We show cMFG scores to measure faithfulness [46].

FUT Examples

(A) *Who was the director of "Anything Else"?*		(B) *Who was the director of "Two of Us"?*	
Greedy (vanilla)	The director of "Anything Else" was Woody Allen.	**Greedy (vanilla)**	Bruce Beresford directed "Two of Us."
Greedy (uncertainty)	Woody Allen directed "Anything Else," though I'm uncertain if he was the sole director or if he shared credit with others.	**Greedy (uncertainty)**	The director of "Two of Us" is John Henderson, according to IMDb, but I cannot confirm this with absolute certainty.
Greedy (FUT-interweave)	It is very likely that Woody Allen was the director of Anything Else.	**Greedy (FUT-interweave)**	It is unlikely that Bryan Elsley was the director of Two of Us.

Samples (FUT-interweave)	**Samples (FUT-interweave)**
It is certain that Woody Allen was the director of Anything Else.	It is unlikely that Bryan Elsley was the director of Two of Us.
It is very likely that Woody Allen was the director of Anything Else.	It is almost impossible that Roger Michell directed Two of Us.
It is almost impossible that the director of Anything Else is Hartman Genus.	It is unlikely that Bryan Elsley was the director of Two of Us.
It is very likely that Woody Allen directed Anything Else.	It is somewhat doubtful that Two of Us was directed by David Burrows.
It is quite likely that Woody Allen was the director of Anything Else.	It is unlikely that Penny Marshall was the director of Two of Us.

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- How can we most effectively improve *human* decision making?
- Move toward *anthropomimetic* uncertainty: human-like, context-sensitive hedging that adapts to user, domain, and conversational norms [38].

Closing Remarks

Summary

We saw that, given a prompt, an LM predicts a belief state.

This state can be probed in a number of ways to support

- decision making pipelines such as selective prediction—the belief state informs *when* we decide;
- decision rules—the belief state guides the search for a response;
- uncertainty communication—responses are hedged coherently with the belief state.

Lots of open questions: efficiency, interpretability, evaluation.

The community is growing quickly, lots of interesting papers by the day. Check our workshop series: `https://uncertainlp.github.io`

Thanks!

References

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