How to compare prediction abilities of different predictors – such as Large Language Models: a theoretical explanation of an empirical formula

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LLMs are one of the tools for predicting future

- One of the main goals of science is to predict future events:
  - we know the situations $s_1, \ldots, s_t$ at several previous moments of time, and
  - we want to predict the situation s_{t+1} that will happen in the next moment of time.
- In particular, recently, one of the tools that is currently used for such prediction is Large Language Models (LLMs).

How can we compare the quality of different predictors?

- We want to design the most accurate predictor.
- Thus, we need to be able to compare the quality of different predictors.
- Several natural characteristics can be used to describe this quality.
- For example, for each i, we can compute the probability $p_i \stackrel{\text{def}}{=} p(s_i|s_1, \ldots, s_{i-1})$ that:
  - the predictor correctly predicts the state s_i at moment i
  - based on the previous states $s_1, \ldots, s_{i-1}$.
- For each i, the larger the probability p_i, the better.
- But what if, for two predictors, we have $p_1 > p'_1$ but $p_2 < p'_2$?
- Which predictor should we select?
- To be able to always compare the quality of different predictors:
  - we need to combine all these values $p_1, \ldots, p_n$ into a single number $p = f_n(p_1, \ldots, p_n)$,
  - so the predictor with the larger combined probability is better.
- Which combination operation $f_n(p_1, \ldots, p_n)$ should we choose?

Empirical fact and the corresponding challenge

- It has been shown that:
  - among all proposed functions,
  - the most adequate comparison occurs when we select

$$f_n(p_1, \ldots, p_n) = \sqrt[n]{p_1 \cdot \ldots \cdot p_n}.$$

- But is this function indeed the best?
- Or is it simply the best of all the functions that have been tried, and a yet untried function will work better?

What we do in this talk

- We show that the empirically successful function is the only one that satisfies natural requirements.
- This explains why this function is empirically successful.
- It also confirms that no other yet untried function will be better.

First natural requirement

- Time is continuous.
- Our selection of the moments of time is arbitrary.
- Instead of the original time units – e.g., days, we could use weeks or months, etc.
- A natural requirement is that our measure of quality should not change if we simply choose a different unit.
- Let us describe this in precise terms.
- Suppose that we use a new unit which is k times larger; then:
  - predicting the state of the system in the new unit means
  - predicting the state which is k moments ahead if we use the original unit.

First natural requirement (cont-d)

- For example, prediction for the next week means predicting 7 days ahead.
- To correctly predict k old moments ahead, we need to:
  - correctly predict the next state s_{t+1} (for which the probability of successis p_{t+1}),
  - then correctly predict s_{t+2} based on s_t and s_{t+1} (for which the probability of success is p_{t+2}), etc.
- It is reasonable to assume that the predictions at different moments of time are statistically independent.
- So in the new units, the probability of the correct prediction is the product $p_{i+1} \cdot \ldots \cdot p_{i+k}$. In these terms:
  - the requirement that the measure of quality should not change if we select a different unit of time
  - takes the following form:

$$f_n(p_1, \ldots, p_n) = f_{n/k}(p_1 \cdot \ldots p_k, p_{k+1} \cdot \ldots \cdot p_{2k}, \ldots).$$

- This must be true for all k, in particular, for $k = n$.
- Thus, we have $f_n(p_1, \ldots, p_n) = f_1(p_1 \cdot \ldots \cdot p_n)$.
- So, we reduced our problem to finding an appropriate function $f_1(x)$ of one variable.

Second natural requirement

- Suppose that all the probabilities p_i are the same, i.e., $p_1 = \ldots = p_n = p$.
- Then it is reasonable to use this common probability p as the measure of the predictor's quality.
- In view of the above formula, this means that we should have $f_n(p^n) = p$.
- In particular, for each x, if we take $p = \sqrt[n]{x}$, then we get $f_1(x) = \sqrt[n]{x}$.
- For this function $f_1(x)$, the above equality leads to the desired formula.