LLM Reasoning

Lecture 2: Repeated Sampling

Yaya Sy

12/10/2025

Recap on LLM Sampling

→ The ***LLM learns a probability function*** by ***maximizing the likelihood*** of the training data (the Web)

→ After training, we can ***generate text by sampling*** one token at a time in the learned probability distribution

→ There are many sampling methods, and it's ***a trade-off between diversity and coherence***

- *Greedy:* predict the token with the highest score
- *TopK:* sample within the *k* tokens with the highest scores
- *Temperature*: redistribute the probability distribution to give some tokens more chance to be sampled
- *TopP*: samples only from tokens that concentrate the probability mass

The limits of single sampling

Sampling is important because, for now, it’s the only way to ***elicit*** the capabilities encoded within the LLM.

But sampling only one answer per question is not sufficient

The LLM needs more ***time***, more ***attempts***.

The limits of single sampling

The case where the LLM samples only a single answer

$$LLM(\ldots \mid c = \text{Is Ronaldo better than Messi?}) \rightarrow$$

What if the LLM has more attempts?

$$LLM(\ldots \mid c = \text{Is Ronaldo better than Messi?}) \rightarrow \left\{ \right.$$

The limits of single sampling

The case where the LLM samples only a single answer

$$LLM(\ldots \mid c = \text{Is Ronaldo better than Messi?}) \rightarrow \text{I prefer cats}$$

What if the LLM has more attempts?

$$LLM(\ldots \mid c = \text{Is Ronaldo better than Messi?}) \rightarrow \begin{cases} \\ \\ \\ \end{cases}$$

The limits of single sampling

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What if the LLM has more attempts?

$$LLM(\ldots \mid c = \text{Is Ronaldo better than Messi?}) \rightarrow \begin{cases} \text{I love Yamal's haircut} \end{cases}$$

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What if the LLM has more attempts?

$$LLM(\ldots \mid c = \text{Is Ronaldo better than Messi?}) \rightarrow \begin{cases} \text{I love Yamal's haircut} \\ \text{Ronaldo is better} \\ \end{cases}$$

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The limits of single sampling

Strong hypothesis: LLMs can solve any task in the world if:

- we have the ***budget*** to ***scale infinitely the number of attempts***
- we have a way to ***pick*** the best answer among the generated answers

Proof: *Infinite monkey theorem*

Infinite monkey theorem

Article Talk

From Wikipedia, the free encyclopedia

The **infinite monkey theorem** states that a monkey hitting keys independently and at random on a typewriter keyboard for an infinite amount of time will almost surely type any given text, including the complete works of William Shakespeare.

Infinite monkey theorem

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The monkey becoming *Shakespeare* after the ∞-th attempt

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Are LlaMAs (=LLMs) just monkeys?

The monkey becoming *Shakespeare a*fter the ∞-th attempt

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Are LlaMAs (=LLMs) just monkeys?

Your Llama becoming the best French *translator* *a*fter the ∞-th attempt

LlaMAs (=LLMs) are maybe just monkeys

User: Using the numbers [19, 36, 55, 7], create an equation that equals 65.
Assistant: Let me solve this step by step.
<think> We need to find an equation using the numbers 19, 36, 55, and 7 exactly once, with basic arithmetic operations, that equals 65. One possible combination is 55 + 36 - 19 + 7. Let's check: 55 + 36 = 91, 91 - 19 = 72, and 72 + 7 = 79. However, this doesn't equal 65. Another combination is 55 + 36 + 7 - 19. Let's check: 55 + 36 = 91, 91 + 7 = 98, and 98 - 19 = 79. This also doesn't equal 65. After trying different combinations, I found that 55 + 36 + 7 - 19 = 79, which is close but not equal to 65. Finally, I found that 55 + 36 - 19 + 7 = 79, which is still not equal to 65. However, if we try 55 + 36 - 7 + 19, we get 55 + 36 = 91, 91 - 7 = 84, and 84 + 19 = 103, which is not equal to 65. After further trial and error, I found that 55 + 36 + 7 - 19 = 79, which is still not equal to 65. However, if we try 55 + 36 - 7 - 19, we get 55 + 36 = 91, 91 - 7 = 84, and 84 - 19 = 65. This equals 65. </think>
<answer> 55 + 36 - 7 - 19 </answer>

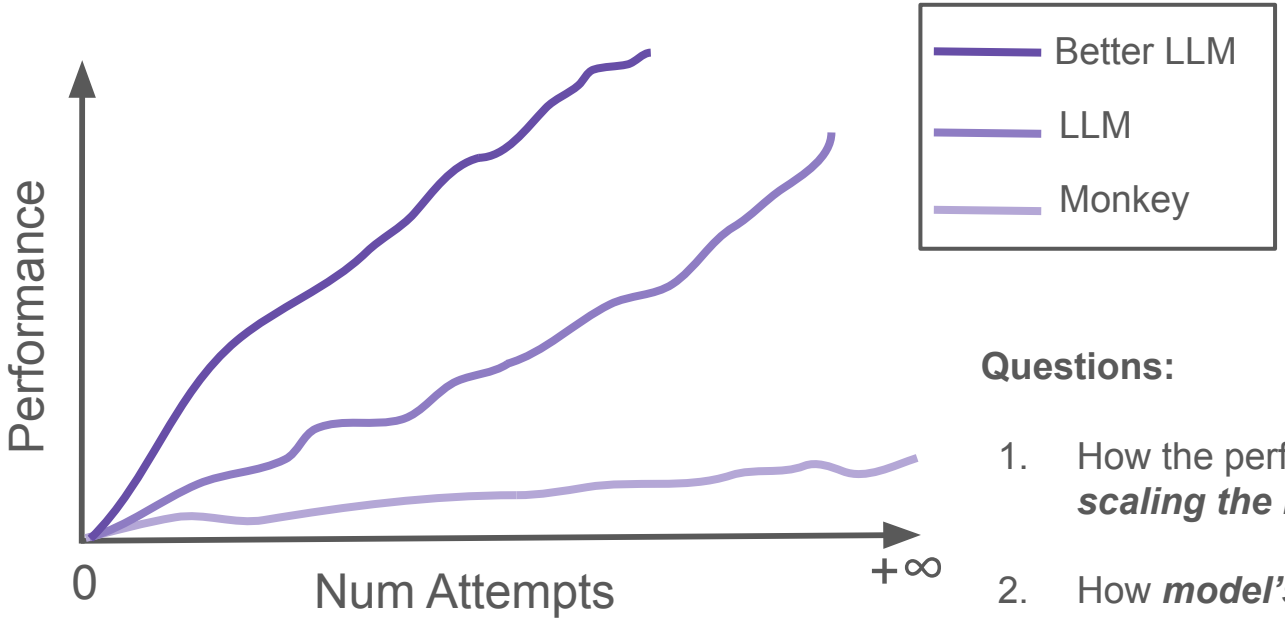
Looks more as brute force than *intelligent* search

LlaMAs (=LLMs) are probably better than monkeys

User: Using the numbers [19, 36, 55, 7], create an equation that equals 65.
Assistant: Let me solve this step by step.
<think> We need to find an equation using the numbers 19, 36, 55, and 7 exactly once, with basic arithmetic operations, that equals 65. One possible combination is watermelon. Let's check: 55 + @j)al!0# = 72, and 72 + 7 = 79. However, this doesn't equal 65. Another combination is 55 + 36 + 7 - 19. Let's check: zumba = 98, and 98 - 19 = 79. This also doesn't equal 65. After trying different combinations, I found that 55 + 36 + 7 - 19 = 79, which is close but not equal to 65. Finally, I found that 55 + 36 - 19 + 7 = 79, which is still not equal to 65. However, if we try 55 + 36 - 7 + 19, we get 55 + 36 = 91, 91 - 7 = 84, and 84 + 19 = 103, which is not equal to 65. After further trial and error, I found that 55 + 36 + 7 - 19 = 79, which is still not equal to 65. However, if we try 55 + 36 - 7 - 19, we get 55 + 36 = 91, 91 - 7 = 84, and 84 - 19 = 65. This equals 65. </think>
<answer> 55 + 36 - 7 - 19 </answer>

LLMs are better than monkeys: it's not totally random

More or less capable monkeys



Questions:

1. How the performance evolves when ***scaling the number of attempts***?
2. How ***model's capability*** affects the number of attempts and performance?
3. What about ***costs***?

Repeated Sampling in a Nutshell

In math:

$$\hat{y} = \underset{y \in p(\ldots|\mathrm{c},\ \theta)}{\arg\max}\, R(y)$$

R(y) or reward(y) is the function that assigns higher ***score*** to better answers. The reward can also be ***binary*** (correct or not)

In pseudo-code:

```
best_score = -Inf
best_candidate = “ ”
for i in range(num_attempts):
    candidate = sample ~ p(...|c)
    score = reward(candidate)
    if score > best_score:
        best_score = score
        best_candidate = candidate
```

Questions:

1. How the performance evolves when ***scaling the number of attempts***?
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3. What about ***costs***?

Scaling Study for Repeated Sampling

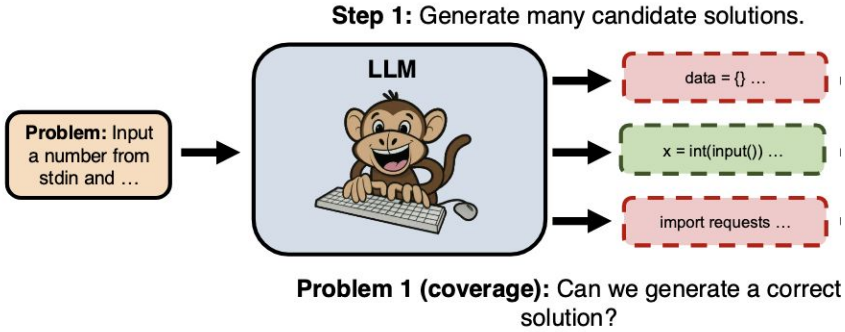
https://arxiv.org/pdf/2407.21787

Verifiable tasks the LLM must solve

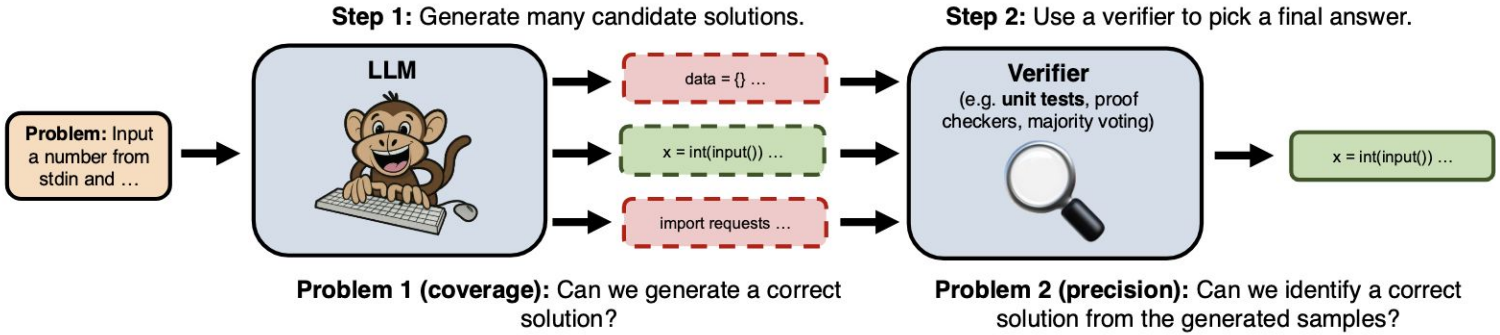
Verifiable task: it's possible to say *objectively* if the solution to the task is correct or not.

- **GSM8K**: A dataset consisting of grade-school level math word problems
- **MATH**: A collection of math word problems that are generally more difficult than those found in GSM8K
- **MiniF2F-MATH**: A dataset of mathematics problems that have been formalized for use with proof-checking languages.
- **CodeContests**: A set of competitive programming problems that includes text descriptions and hidden input-output test cases to verify solution correctness.
- **SWE-bench Lite**: A dataset of real-world GitHub issues must solve by editing the codebase, verified by existing unit tests.

Scaling Repeated Sampling



Scaling Repeated Sampling



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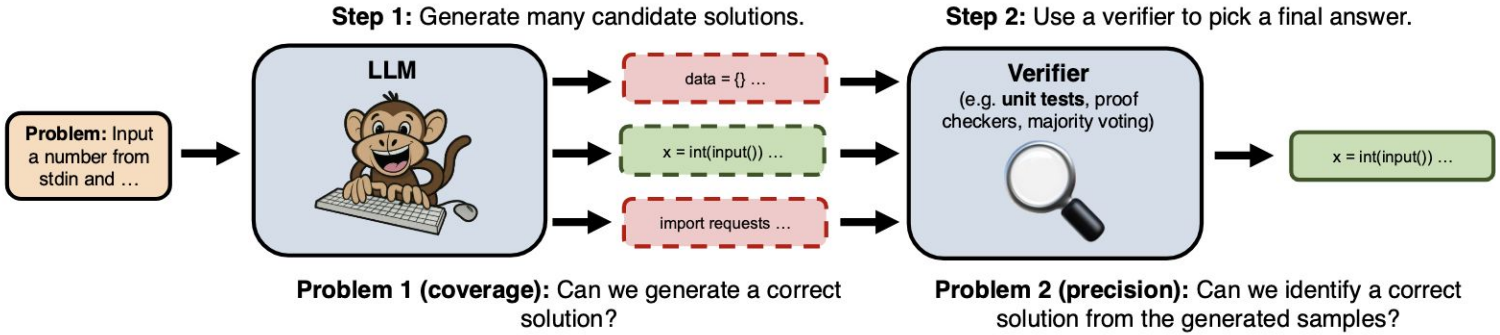

Questions:

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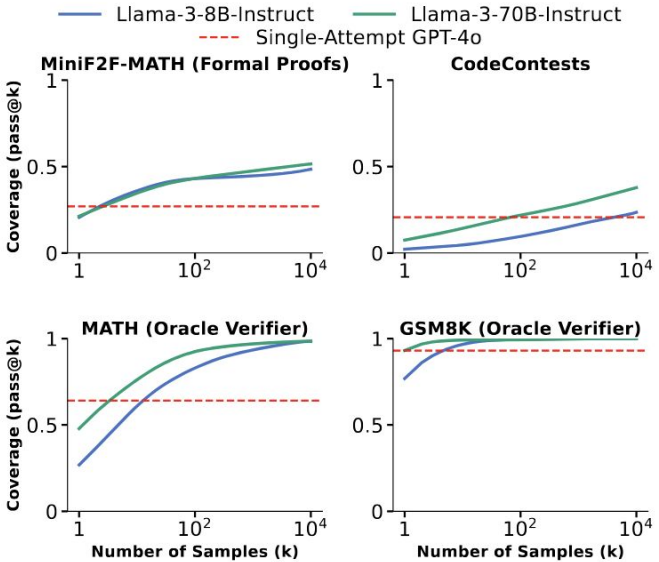
Repeated Sampling vs Performance

Coverage: % of problems where the LLM generated the right answer at least once



→ When *k=1* (single-attempt), GPT-4o is better

→ Improving the number of attempts (samples) improves performance compared to single-attempt

→ The performance doesn't improve linearly

Repeated Sampling vs Performance

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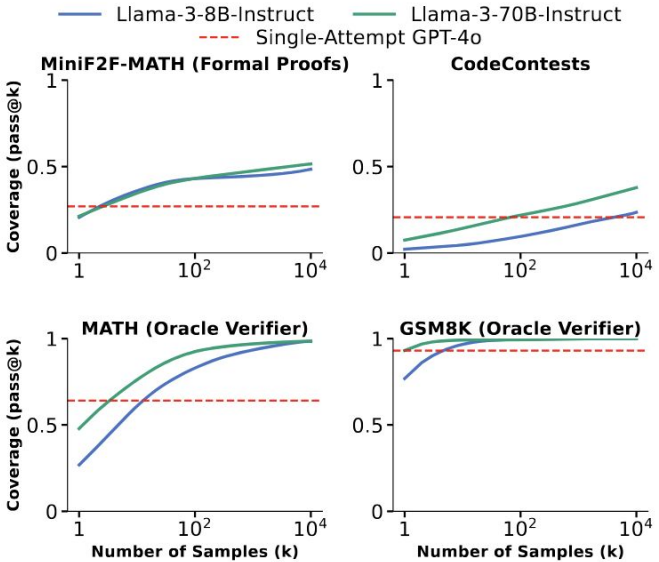

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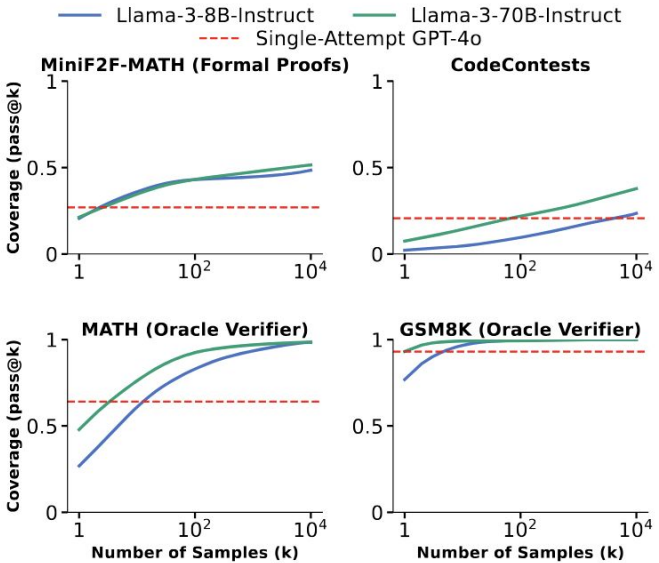


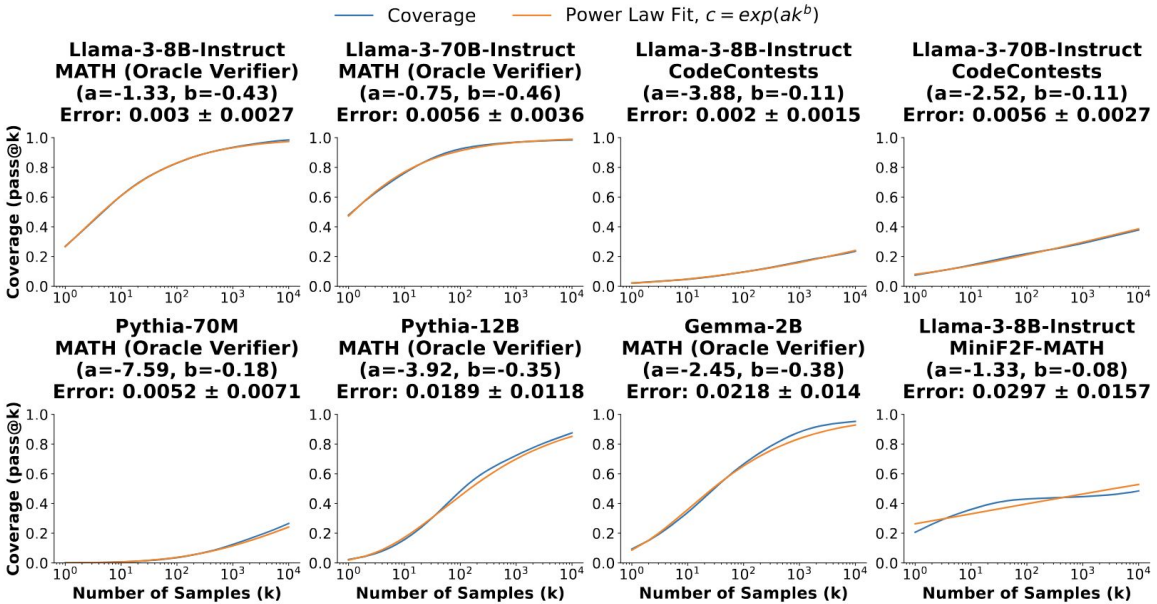
→ The performance doesn't improve linearly

→ We want a function that can predict the performance (coverage) for a given *k* (attempts):

$$c = f(k)$$

→ *f* is the scaling law of performance as a function number of attempts

Repeated Sampling vs Performance

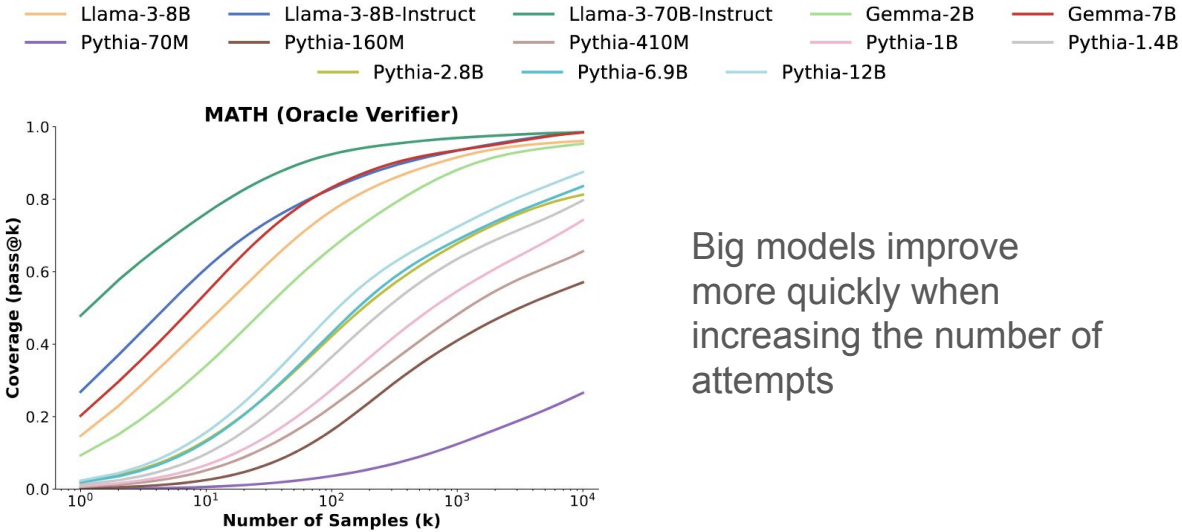


$c = f(k)$

$f(k) = exp(ak^b)$

A Power Law governs the relation between the number of attempts *k* and the performance (coverage)

Repeated Sampling vs Performance vs Model Sizes



Big models improve more quickly when increasing the number of attempts

$c = f(k)$

$f(k) = exp(ak^b)$

A Power Law governs the relation between the number of attempts *k* and the performance (coverage)

Repeated Sampling vs Performance vs Costs

Model	Cost per attempt (USD)	Number of attempts	Issues solved (%)	Total cost (USD)	Relative total cost
DeepSeek-Coder-V2-Instruct	0.0072	5	29.62	10.8	1x
GPT-4o	0.13	1	24.00	39	3.6x
Claude 3.5 Sonnet	0.17	1	26.70	51	4.7x

It is sometimes more cheap to do repeated sampling using a weak small model than single sampling using a bigger model.

Summary

→ Sampling a single answer for a query can be insufficient

→ Generating multiple candidate answers improves the performance

- Power Law between performance and number of attempts
- Big models improve more quickly when scaling the number of attempts
- Doing multiple attempts using a small cheap model can be more cost efficient than doing a single-attempt using a big model

On the Reward

On the Reward

→ The LLM samples multiple output candidates for a prompt c: $y \sim sample\ \text{LLM}(\bullet|c)$

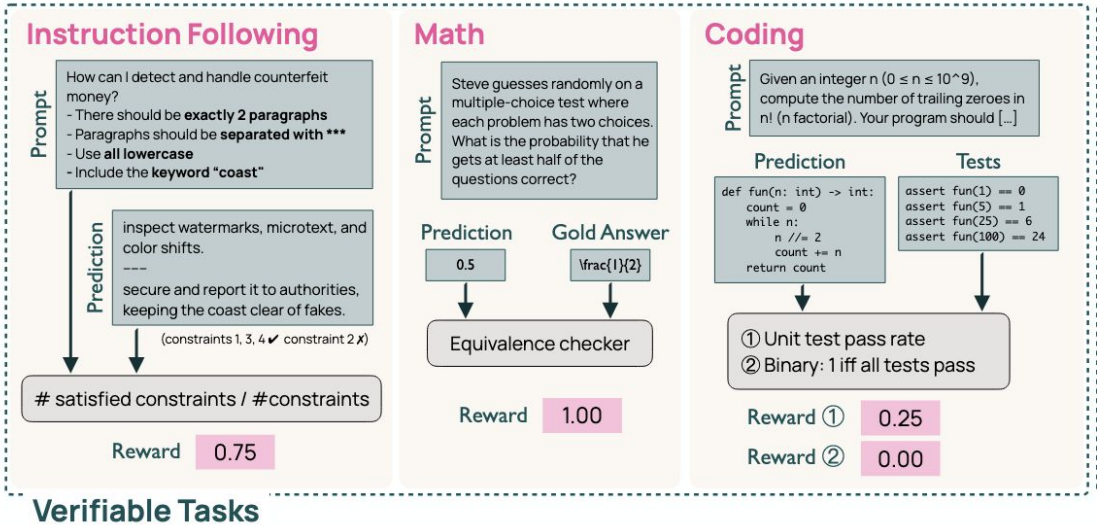
→ A reward function $R(y)$ scores each output y, and the best is picked

→ How to define the reward function?

→ This depends on your task

→ Some tasks are more easy to verify than others

Things easy to verify



Paper: Olmo 3.

Instruction Following: The LLM learns to follow a set of constraints (synthetic or not). The task is verifiable: just use the % of constraints satisfied as reward

Math. The task is verifiable: just check against a calculator, proof checker, etc. for rewarding.

Code. The task is verifiable: just check against unit tests or run it and observe the result.

Things not easy to verify

→ **Translation**: There is no way to check the correctness of a translation. There is no only one good translation. Some translations can be better than others.

→ **Creative writing**: This is culture dependant. There is no one ***objective*** way to say a text is more creative than another. It depends on the person, the historical and social context.

→ **Humor:** You can laugh alone and others will think you're crazy. Why do you find it funny?

→ **Do you have any other example?**

Self-Confidence for non-verifiable tasks

- The ***confidence*** of the LLM about its own answer (using ***entropy***)
- The probability of the answer computed using the LLM itself

Self-Confidence for non-verifiable tasks

Likelihood Self-Confidence

Let's consider the sentence "very cool". The vocabulary is {cool, lol, ver, wow}.
The LLM produces a probability distribution at each step.

In the case of likelihood self-confidence, we consider the individual probabilities of the generated tokens:

$$\text{<b>} \begin{cases} p(\text{cool}) = 0.15 \\ p(\text{very}) = 0.60 \\ p(\text{lol}) = 0.10 \\ p(\text{wow}) = 0.15 \end{cases} \quad \text{very} \begin{cases} p(\text{cool}) = 0.75 \\ p(\text{very}) = 0.05 \\ p(\text{lol}) = 0.10 \\ p(\text{wow}) = 0.10 \end{cases} \quad \text{cool} \begin{cases} p(\text{cool}) = 0.10 \\ p(\text{very}) = 0.20 \\ p(\text{lol}) = 0.35 \\ p(\text{wow}) = 0.35 \end{cases}$$

The probability of the sentence is then: $p(\text{very cool}) = p(\text{very}) \times p(\text{cool}) = 0.60 \times 0.75$

For numerical stability, it is always better to take the sum of the log-probs.

Self-Confidence for non-verifiable tasks

Entropy Self-Confidence

In Entropy we consider the whole probability distribution at each step:

$$<\text{b}>\begin{cases} p(\text{cool}) & = 0.15 \\ p(\text{very}) & = 0.60 \\ p(\text{lol}) & = 0.10 \\ p(\text{wow}) & = 0.15 \end{cases} \quad \text{very}\begin{cases} p(\text{cool}) & = 0.75 \\ p(\text{very}) & = 0.05 \\ p(\text{lol}) & = 0.10 \\ p(\text{wow}) & = 0.10 \end{cases} \quad \text{cool}\begin{cases} p(\text{cool}) & = 0.10 \\ p(\text{very}) & = 0.20 \\ p(\text{lol}) & = 0.35 \\ p(\text{wow}) & = 0.35 \end{cases}$$

The entropy *H* for a single probability distribution *X*: $H(X) = -\sum_{p \in X} p \times log\, p$

The entropy at the first step: $H(<\text{b}>) = -(0.15 \times \log(0.15) + 0.60 \times \log(0.60) + 0.10 \times \log(0.10) + 0.15 \times \log(0.15)$

The average entropy:

$$H(<\text{b}> \text{ very cool}) = \frac{1}{3}(H(<\text{b}>) + H(\text{very}) + H(\text{cool}))$$

LLM as a Judge

LLMs are often better at judging than generating the right answers.

LLMs for scoring (Scalar Reward)

You can ask LLMs to score answers

LLMs for verbal feedback (Generative Reward)

Scalar rewards don’t provide enough signals and nuances compared to verbal feedback.

Reward Model

If you have a dataset of prompts $\boldsymbol{x}$, and the prefered (good) answers $\boldsymbol{y_p}$ and rejected (bad) answers $\boldsymbol{y_r}$,

Then you can train a Reward Model (RM) to assign high scores to good answers and low scores to bad answers: score($\mathbf{x}$, $\boldsymbol{y_p}$) > score($\mathbf{x}$, $\boldsymbol{y_r}$)

There are many ways to train reward models. The most popular:
Bradley-Terry Model

Reward Model (Bradley-Terry)

- *score(**x**, $\mathbf{y}_p$):* the score of the prefered answer given the prompt ***x***
- *score(**x**, $\mathbf{y}_r$):* the score of the rejected answer given the prompt ***x***

Then, the probability of the preferred answer is:

$$p(y_p > y_r|x, \theta) = \frac{\text{score}(x, y_p)}{\text{score}(x, y_p) + \text{score}(x, y_r)}$$

Since it's a probability, we need to have positive scores.

$\mathbf{c}_p$ **=** Transformer(***x*** $\mathbf{y}_p$)
$\mathbf{c}_r$ **=** Transformer(***x*** $\mathbf{y}_r$)

*score(**x**,* $\mathbf{y}_p$ *)* = *exp(*$\mathbf{c}_p \cdot \mathbf{w}^T$**)**, where **w** is learnable vector
*score(**x**,* $\mathbf{y}_r$ *)* = *exp(*$\mathbf{c}_r \cdot \mathbf{w}^T$**),** where **w** is learnable vector

Reward Model (Bradley-Terry)

$$p(y_p > y_r|x, \theta) = \frac{\text{score}(x, y_p)}{\text{score}(x, y_p) + \text{score}(x, y_r)}$$

Since it's a probability, we need to have positive scores:

$\mathbf{c}_p$ = Transformer($\boldsymbol{x}$, $\boldsymbol{y}_p$)
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$score(\boldsymbol{x}, \boldsymbol{y}_p) = exp(\mathbf{c}_p \cdot \mathbf{w}^T)$
$score(\boldsymbol{x}, \boldsymbol{y}_r) = exp(\mathbf{c}_r \cdot \mathbf{w}^T)$

$$RM_\theta = \arg\max_\theta p(y_c > y_r|x, \theta)$$

This is (again) Maximum Likelihood Estimation (MLE).

The reward model is trained to maximize the likelihood of the preferred answer

Reward Model (Bradley-Terry)

$$p(y_p > y_r|x, \theta) = \frac{\text{score}(x, y_p)}{\text{score}(x, y_p) + \text{score}(x, y_r)}$$

Exercise: derive the Bradley-Terry Model to get a Logistic Model:

$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

Reward Model (Bradley-Terry)

$$p(y_p > y_r|x, \theta) = \frac{\text{score}(x, y_p)}{\text{score}(x, y_p) + \text{score}(x, y_r)}$$

Let call l_p, l_r the logits of the preferred answer and rejected answer respectively:

$$p(y_p > y_r|x, \theta) = \frac{\exp(l_p)}{\exp(l_p) + \exp(l_r)}$$

Using the rule A/B = (A/C)/(B/C), we divide exp(l_p) in the numerator and denominator:

$$p(y_p > y_r|x, \theta) = \frac{\frac{\exp(l_p)}{\exp(l_p)}}{\frac{\exp(l_p)}{\exp(l_p)} + \frac{\exp(l_r)}{\exp(l_p)}} = \frac{1}{1 + \frac{\exp(l_r)}{\exp(l_p)}}$$

Reward Model (Bradley-Terry)

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Using the rule exp(a) / exp(b) = exp(a - b):

$$p(y_p > y_r|x,\theta) = \frac{1}{1 + \exp(l_r - l_p)}$$

$$p(y_p > y_r|x,\theta) = \frac{1}{1 + \exp(-(l_p - l_r))} = \sigma(l_p - l_r)$$

Summary

Scaling repeated sampling

- Scaling the ***number of attempts improves the performance*** of LLMs
- The performance as a function of **number of attempts *k* is determined by a power function**: $c = exp(ak^b)$
- L**arge models improve more quickly** when scaling the number of attempts

Reward Modeling

- For **verifiable tasks** (math, code, instructions), the reward is based on the **correctness** of the output
- For **non-verifiable tasks**:
  - **Self-confidence** can be a good signal (see lab on translation)
  - **LLM as a Judge** can be a good rewarder but they can be biased (prefer long answers)
  - One common solution is to **train a reward model on a preference dataset**
  - **Bradley-Terry** is a popular approach for training reward models. It is equivalent to applying **sigmoid** on the difference of scores between the preferred and rejected answer