Scaling LLM Test-Time Compute Optimally can be More Effective than Scaling Model Parameters [arXiv 24.08]

TL; DR.
Explores two main strategies (PRM & Refining the Proposal Distribution) for scaling LLM reasoning at test-time.

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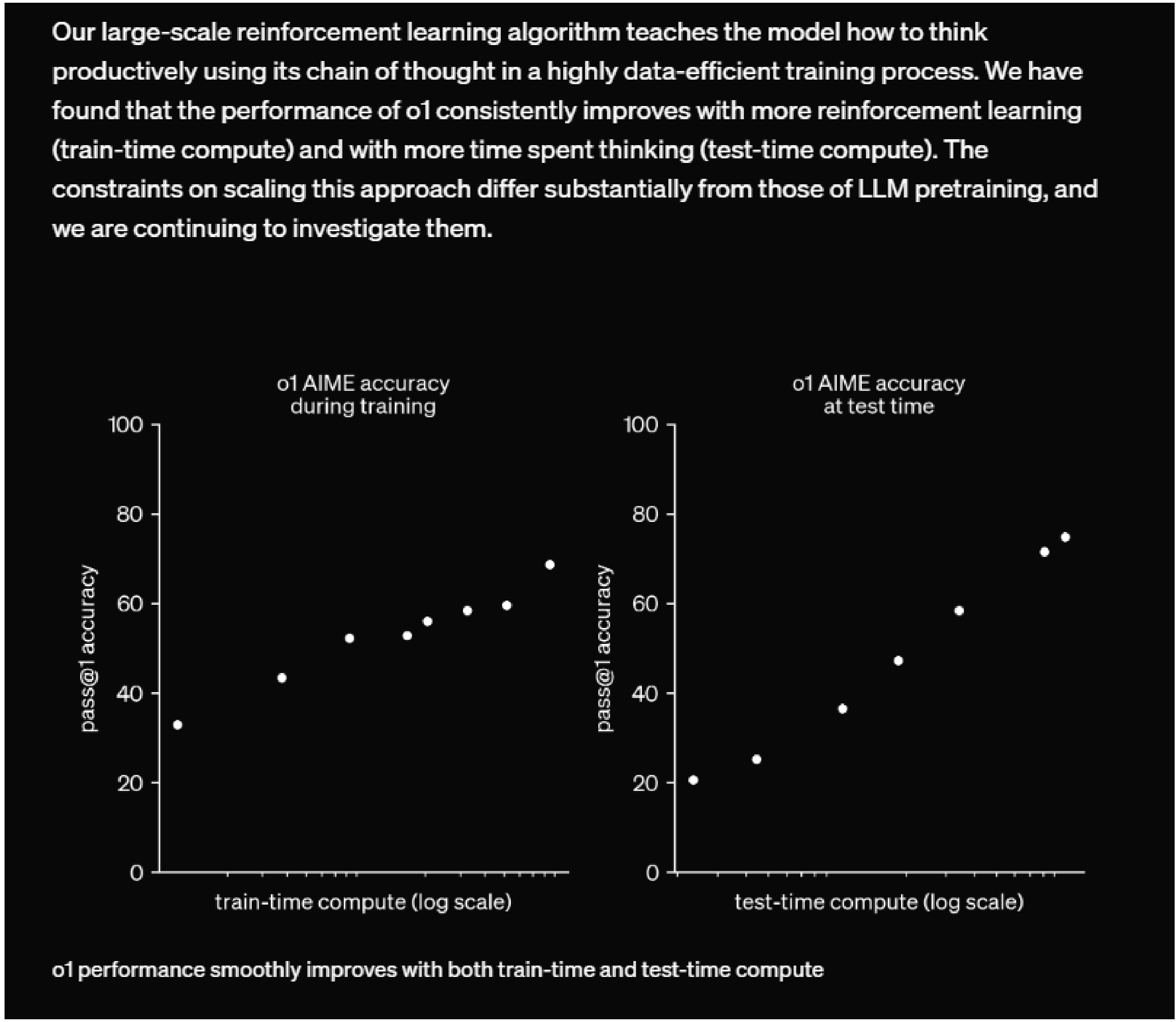
What is Scaling Law

- For training Openai o1
  - Scaling Law for both train-time and **test-time**.
- Question?
  - What do they mean by "test-time compute"?
    And how to scale up "test-time compute"?
- A shift from "system-1" to "system-2" reasoning.



[1] OpenAI "Learning to Reason with LLMs". 2024.09

How to scale up test-time compute?

- For optimizing input (prompting)
  - Basic prompting techniques
    - Few-shot prompting
    - CoT prompting
  - Learning to prompt (using neural networks)
    - RLPrompt[2]
    - DSPy[3]
      - Already built into python packages and widely used
  - And many other techniques for optimizing prompts…

[2] Deng et al., "RLPrompt: Optimizing Discrete Text Prompts with Reinforcement Learning" EMNLP 2022

[3] Khattab et al., "DSPy: Compiling Declarative Language Model Calls into Self-Improving Pipelines" R0-FoMo@NeurIPS 2023

How to scale up test-time compute?

- For refining output distribution
  - How to let LLM generate better CoT rationales?
    - SFT works.
    - SFT with collected CoT rationales can let LLM generate better reasoning traces.
  - Take a step further, how to let LLM keep revising its CoT rationales and gradually approach a more reasonable answer?
    - Tree-of-Thought
    - Monte-Carlo Tree Search
    - …
  - Both of them contribute to training a **verifier** to help refine the output distribution at test-time.

The scaling-up strategies for test-time

- Scaling Test-Time Compute via Verifiers
  - Training verifiers to search
  - Search Methods Against a verifier
- Refining the Proposal Distribution
  - Parallel Sampling v.s. Sequential Revisions
  - Trading off between them

- [Q] Aren't they talking about test-time? Why are they still training?
  - To scale up compute at test-time,
    we cannot do it without **post-training**.

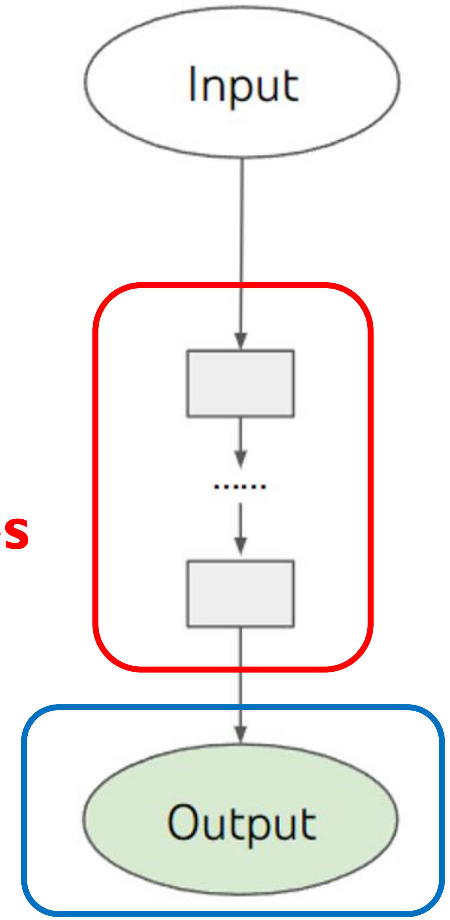
Scaling Test-Time Compute via Verifiers

- So what are verifiers?
  - ORM: Outcome-supervised Reward Model
  - PRM: Process-supervised Reward Model

Next question: How to train a PRM?

PRM <= Output + Label + supervision of rationales

ORM <= Output + Label



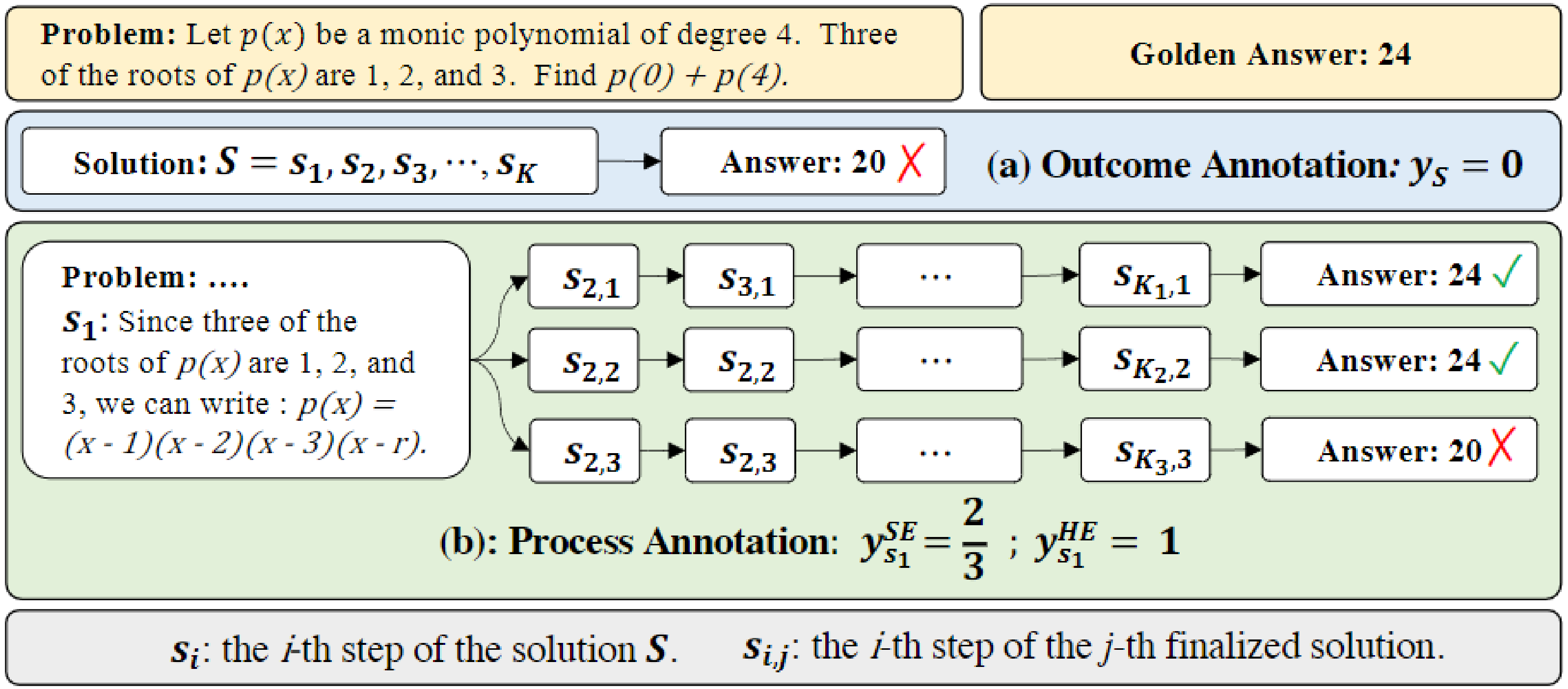
A CoT rationale

Scaling Test-Time Compute via Verifiers

- How to train a PRM?

  (We only discuss the case that you cannot afford the annotations by human. 🤣)

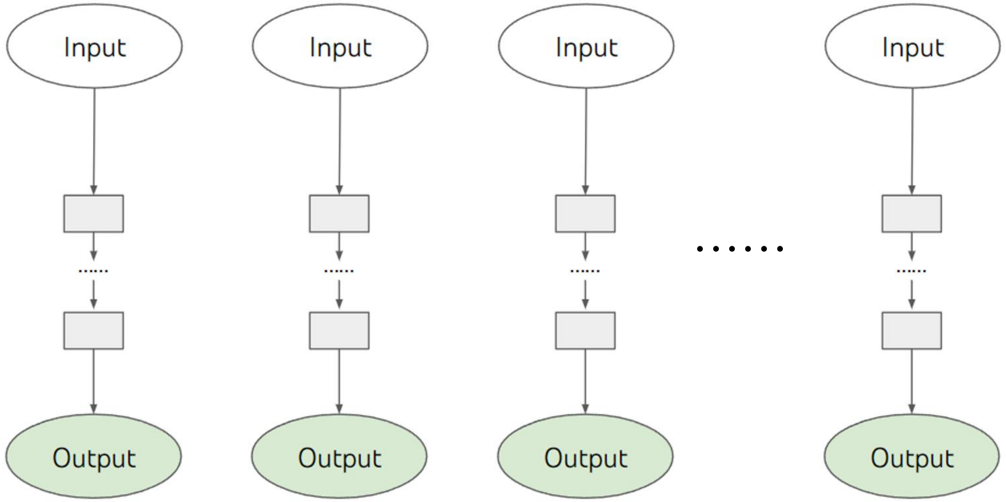
  - Instead of directly annotating each reasoning step, we estimate the quality of them.
  - The quality of a reasoning step is defined as its potential to deduce the correct answer.[4] (Just like a soft label)



[4] Wang et al., "Math-Shepherd: Verify and Reinforce LLMs Step-by-step without Human Annotations" arXiv 24.02

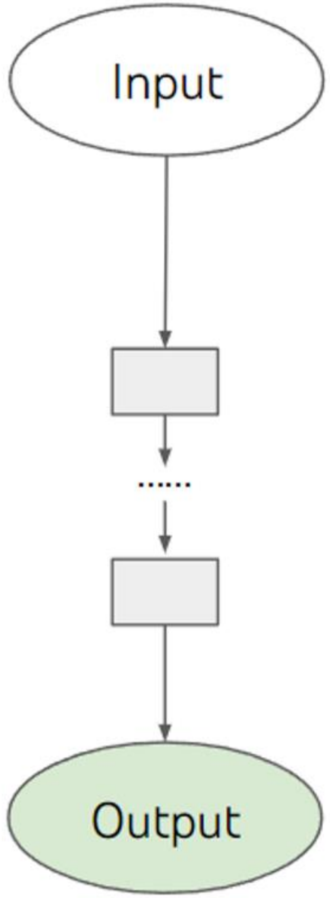
Scaling Test-Time Compute via Verifiers

- How to score with the verifier (Answer aggregation)
  - To select the best-of-N answers with the PRM, we need to aggregate across all the per-step scores for each answer to determine the best candidate.
    - Step-wise aggregation (inside-answer)
    - Inter-answer aggregation (between-answer)



Scaling Test-Time Compute via Verifiers

- How to score with the verifier (Answer aggregation)
  - Step-wise aggregation
    - (How to calculate the score for a single answer?)
    - Some work[4][5] aggregating the per-step scores by taking the product or minimum
    - This paper finds that using the score of the last step performs best with their PRM.
  - Inter-answer aggregation
    - (How to choose the best answer candidate)
    - Marginalizing scores across all solutions with the same final answer. (“weighted aggregation”)

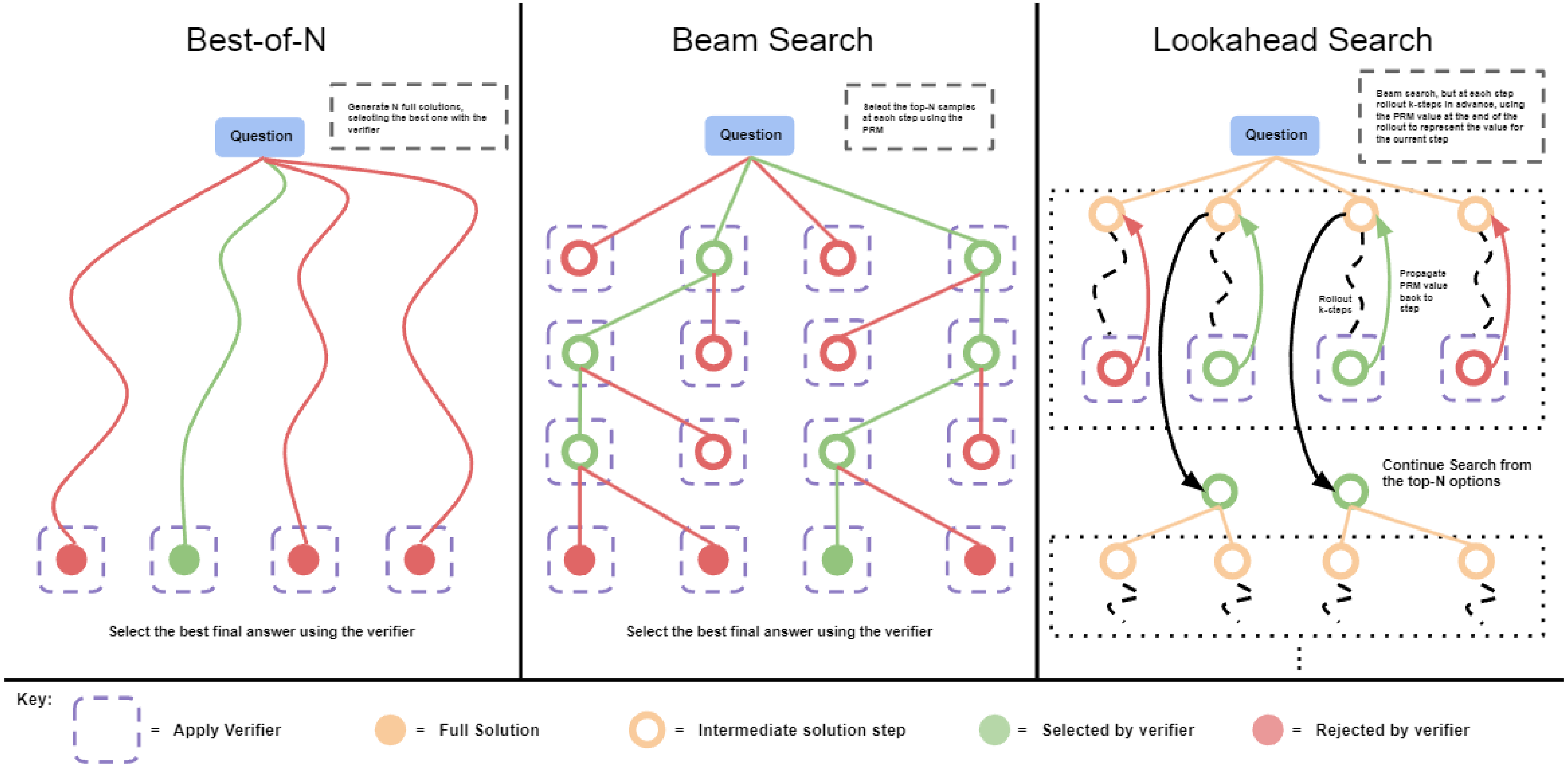


A CoT rationale

[5] Lightman et al. (OpenAI), “Let’s verify step by step” ICLR 2024

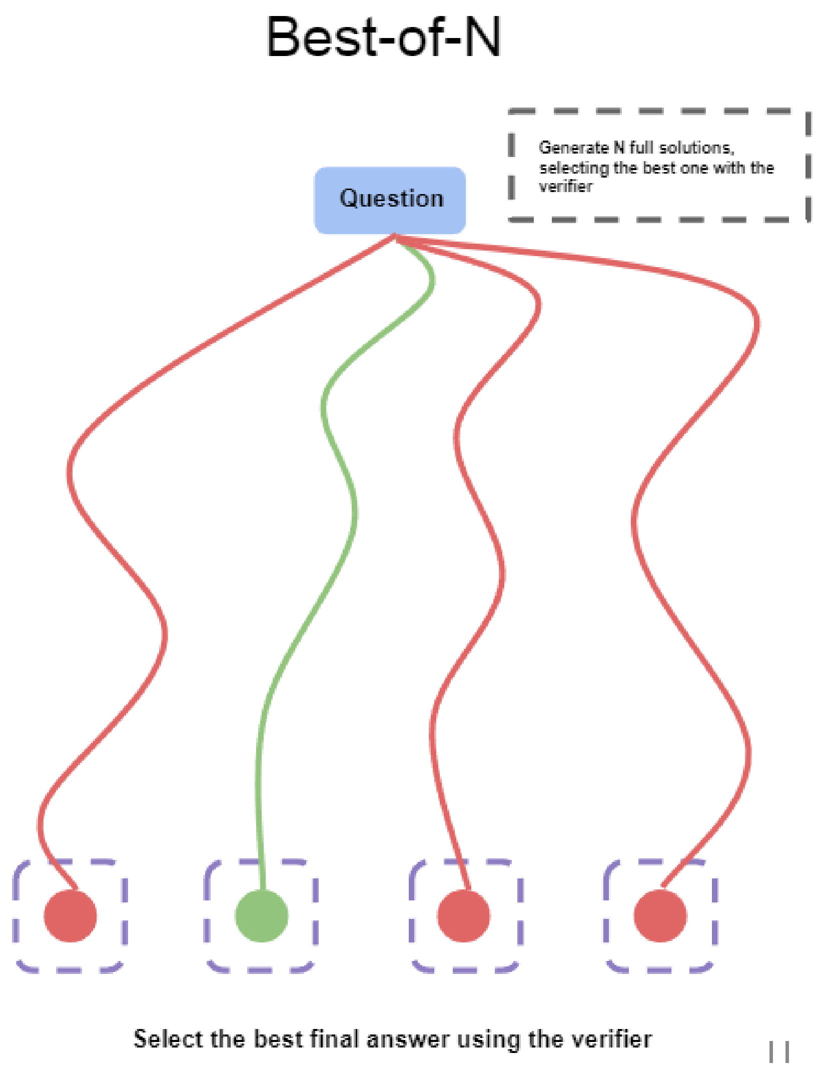
Scaling Test-Time Compute via Verifiers

- Search Methods Against a verifier



Scaling Test-Time Compute via Verifiers

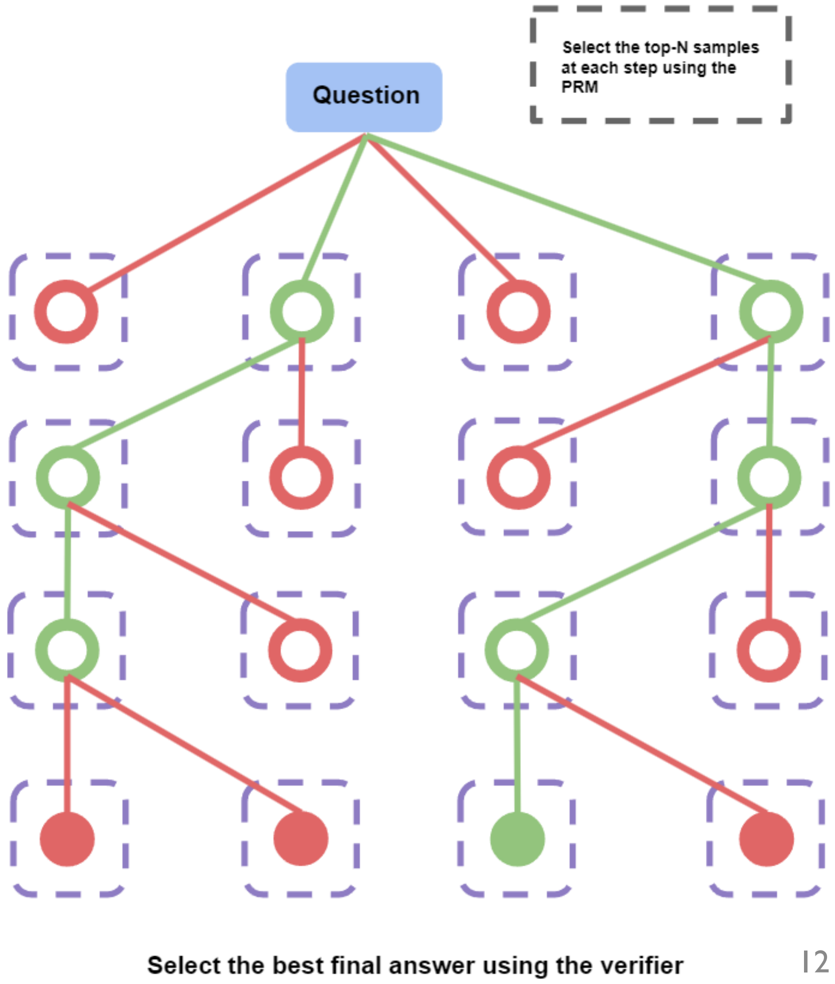
- Search Methods Against a verifier
  - (weighted) Best-of-N
  - Just sample N answers independently from the base LLM
  - Select the candidate according to the PRM's answer aggregation calculation.



Scaling Test-Time Compute via Verifiers

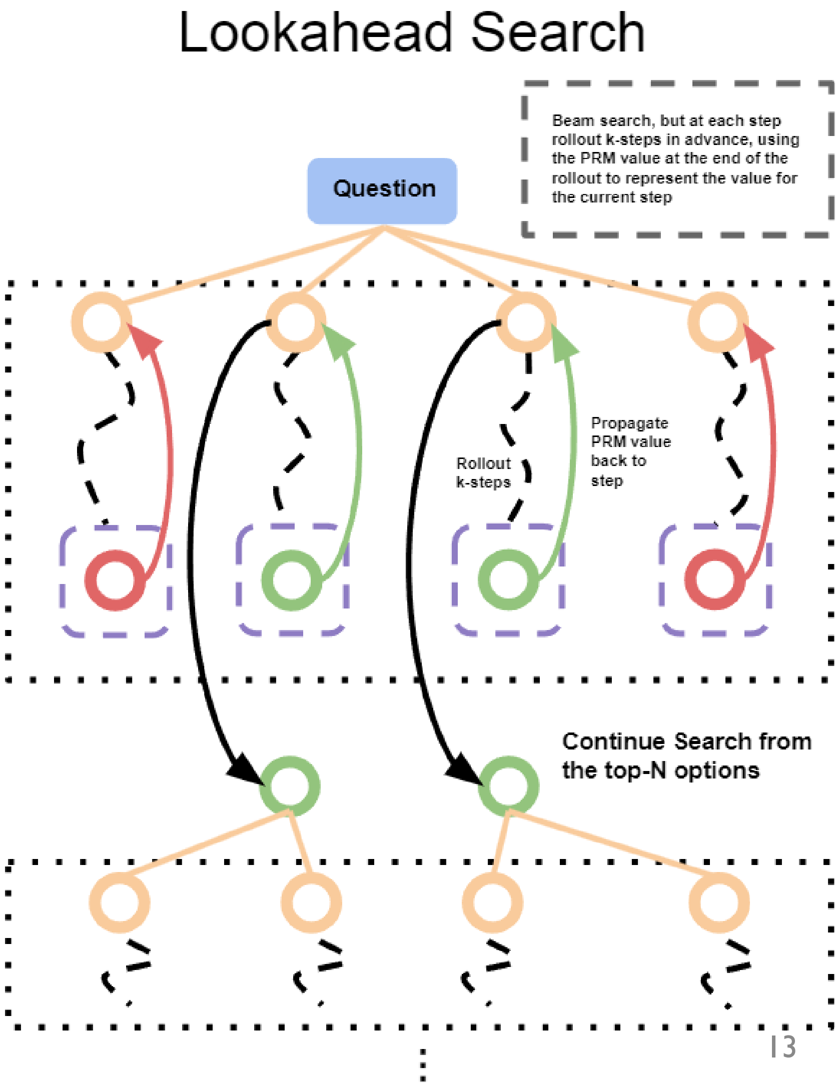
- Search Methods Against a verifier
  - Beam Search
  - Control a total number N and a beam width M (N=4, M=2)
  - Similar to the to the LM decoding strategy "beam search" (Difference that each node denotes the intermediate reasoning step here.)

Beam Search



Scaling Test-Time Compute via Verifiers

- Search Methods Against a verifier
  - Lookahead Search
  - Based on beam search, it modifies how to evaluate each step.
  - Rollout k steps and having the score at the k-th step as the score of current reasoning rationale.
  - (Main idea is just like A* / Monte-Carlo Tree Search)

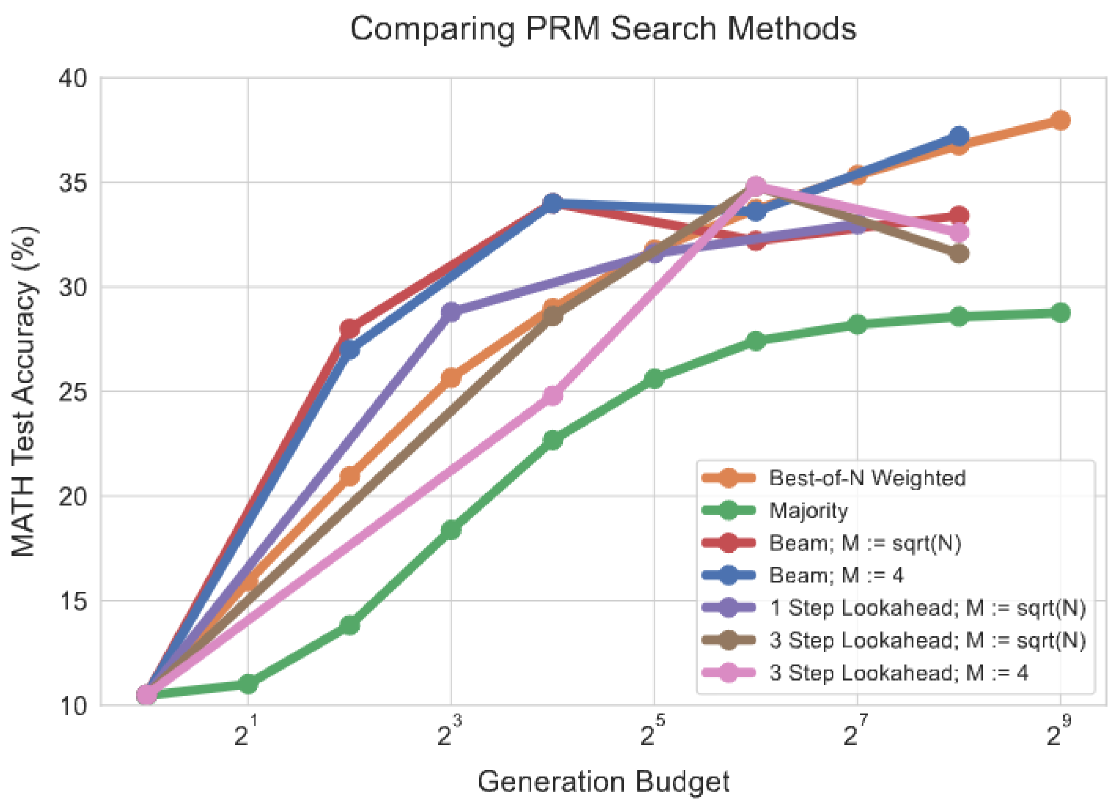


Scaling Test-Time Compute via Verifiers

- Experimental setup
  - Two main factors affecting the performances
  - Generation budget
    - e.g. Number of sampling
  - Difficulty of question
    - Easy questions may do not require much reasoning, while hard questions need much reasoning.

Scaling Test-Time Compute via Verifiers

- Results & Findings
  - When budget is small,
    beam search > best-of-N > lookahead
  - When budget is large,
    best-of-N > beam search > lookahead
- Possible explanations
  - When budget is small, we need more sophisticated searching strategy (simply sampling may be hard to hit).
  - When budget is large, it will alleviate this problem.
  - Lookahead search generally underperforms, probably due to over-optimizing for searching.

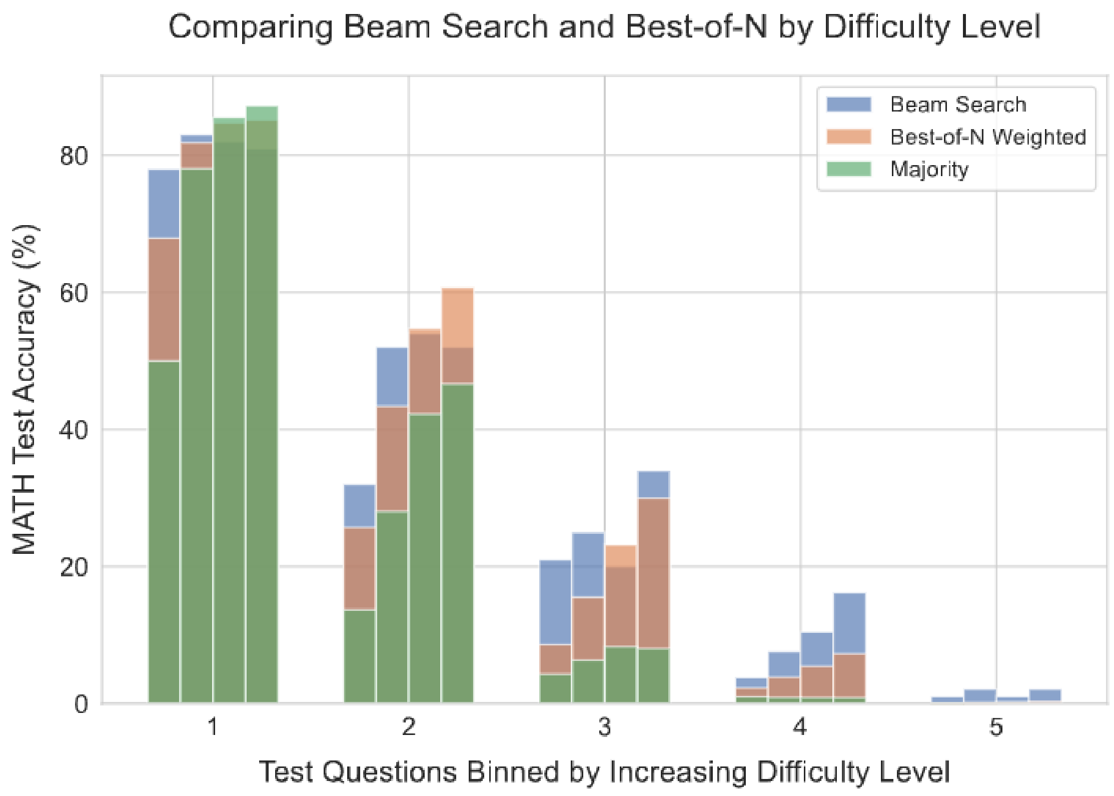


Scaling Test-Time Compute via Verifiers

- Results & Findings

  (Four Bars under each bin demotes the searching budget: 4, 16, 64, 256)

  - On simplest questions (1, 2), best-of-N > beam search
  - On hard questions (3, 4), beam search > best-of-N
  - On the hardest questions (5), nothing works



Refining the Proposal Distribution

- LLMs can learn to generate better rationales via SFT with high-quality data.
- After that, we can let LLMs refine their proposal distributions.
- Primarily there are two strategies for refining output distribution
  - Parallel sampling
  - Sequential revisions

If $f(x) = \frac{3x-2}{x-2}$, what is the value of $f(-2) +f(-1)+f(0)$? Express your answer as a common fraction.

Attempt 1:

```
Let's evaluate $f(-2)$.
We have $f(-2)=\frac{3(-2)-2}{-2-2}=-\frac{4}{-4}=\frac{1}{1}=1$.
So $f(-2)=1$.
Let's evaluate $f(-1)$.
We have $f(-1)=\frac{3(-1)-2}{-1-2}=-\frac{5}{-3}=\frac{5}{3}$.
So $f(-1)=\frac{5}{3}$.
Let's evaluate $f(0)$.
We have $f(0)=\frac{3(0)-2}{0-2}=\frac{-2}{-2}=1$.
So $f(0)=1$.
So we want to compute
$1+\frac{5}{3}+1=\frac{3}{3}+\frac{5}{3}=\frac{3+5}{3}=\frac{8}{3}$.
So the answer is $\boxed{\frac{8}{3}}$.
#### \frac{8}{3}
```

Attempt 2:

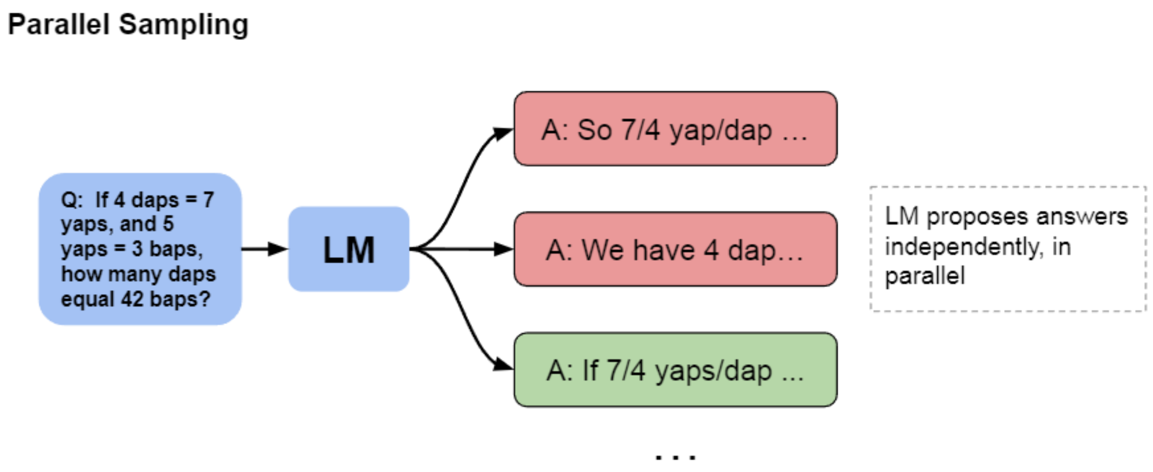
```
Let's first find $f(-2)$.
$f(-2) = \frac{3(-2)-2}{-2-2} = \frac{-6-2}{-4} = \frac{-8}{-4} = 2$.
Now let's find $f(-1)$.
$f(-1) = \frac{3(-1)-2}{-1-2} = \frac{-3-2}{-3} = \frac{-5}{-3} = \frac{5}{3}$.
Now let's find $f(0)$.
$f(0) = \frac{3(0)-2}{0-2} = \frac{-2}{-2} = 1$.
So we have $f(-2) +f(-1)+f(0) = 2+\frac{5}{3}+1 =
\frac{7}{3}+\frac{5}{3}+\frac{3}{3} = \frac{7+5+3}{3} = \frac{15}{3} = 5$.
So the answer is $\boxed{5}$.
#### 5
```

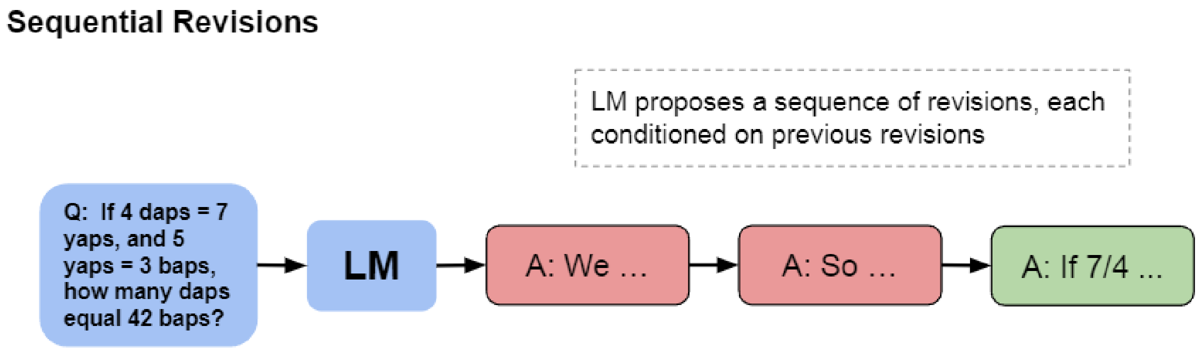
Attempt 3:

```
Let's plug in $-2$, $-1$, and $0$ for $x$ in $f(x)$.
We get $f(-2) = \frac{3(-2)-2}{-2-2} = \frac{-8}{-4} = \frac{2}{1} = 2, f(-1) =
\frac{3(-1)-2}{-1-2} = \frac{-5}{-3} = \frac{5}{3}, f(0) = \frac{3(0)-2}{0-2} =
\frac{-2}{-2} = 1$.
So we have $2+\frac{5}{3}+1=\frac{6}{3}+\frac{5}{3}+\frac{3}{3}=\frac{14}{3}$.
So the answer is $\boxed{\frac{14}{3}}$.
#### \frac{14}{3}
```

Refining the Proposal Distribution

- Two major methods for refining the proposal distribution
  - **Parallel Sampling** v.s. **Sequential Revisions**
  - (global search v.s. local refinement)



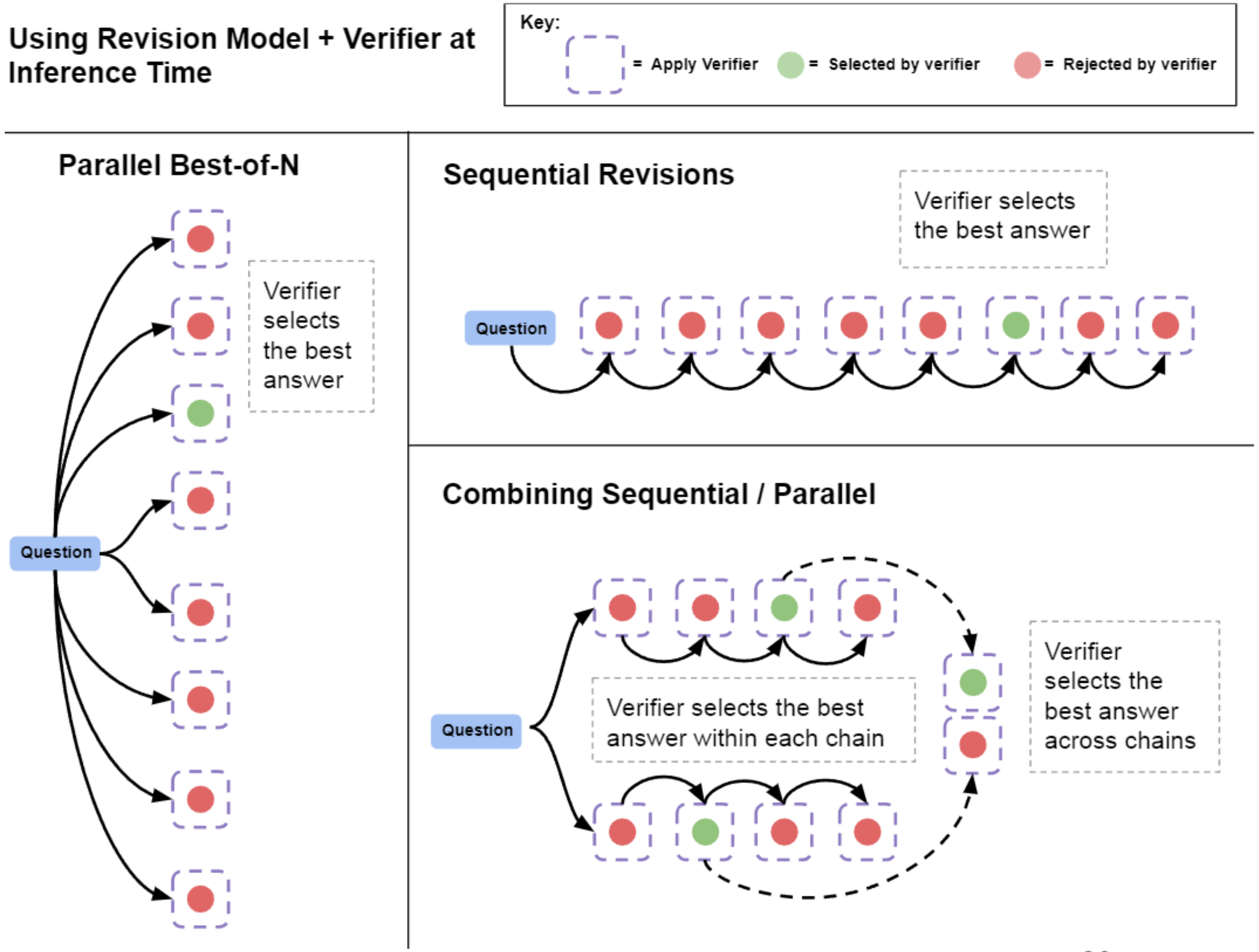


Refining the Proposal Distribution

- However, there are many problems
  - E.g.
  - For sequential revision, the last attempt is not guaranteed to be correct. (There is case that it is revised correctly in the middle, and then revised incorrectly at last.)
  - For both of them, it's not guaranteed to have correct attempts.

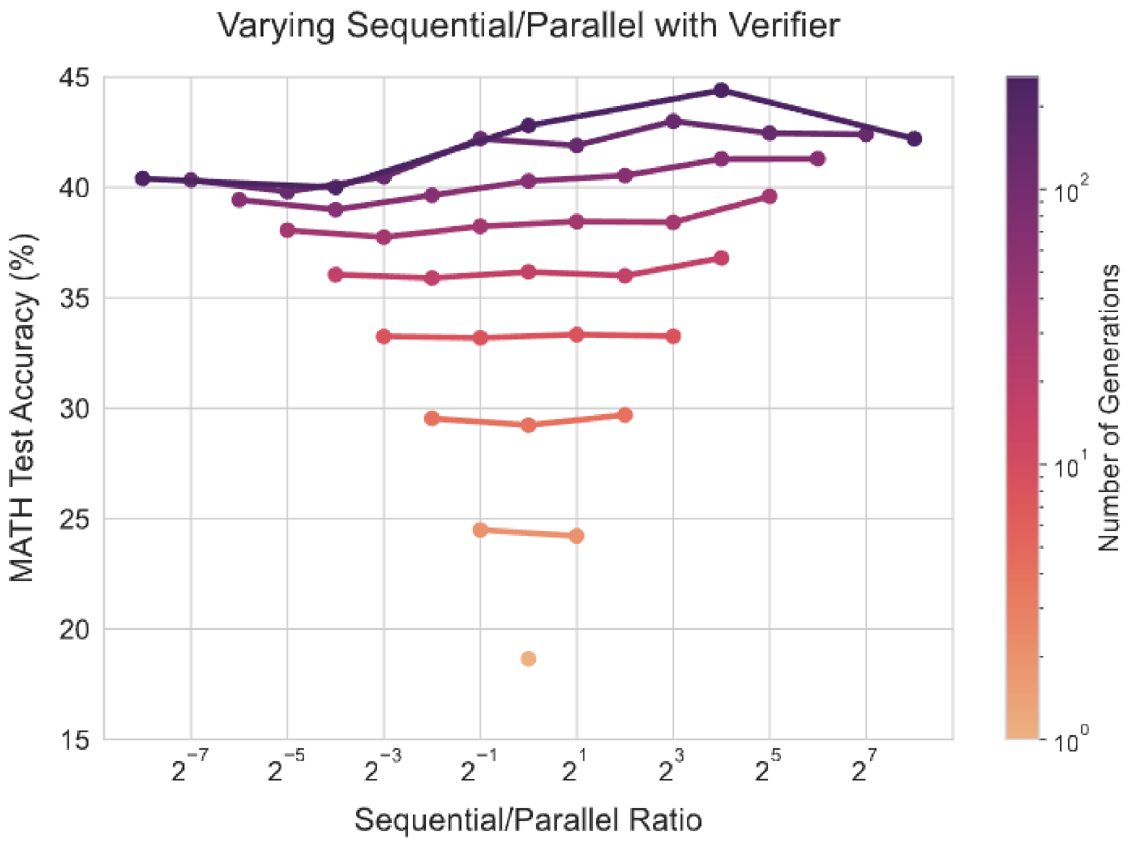
Refining the Proposal Distribution

- Utilizing verifiers to help refinement
  - Parallel Best-of-N
  - Sequential Revisions
  - Combining Sequential / Parallel
    - Trading off between them?



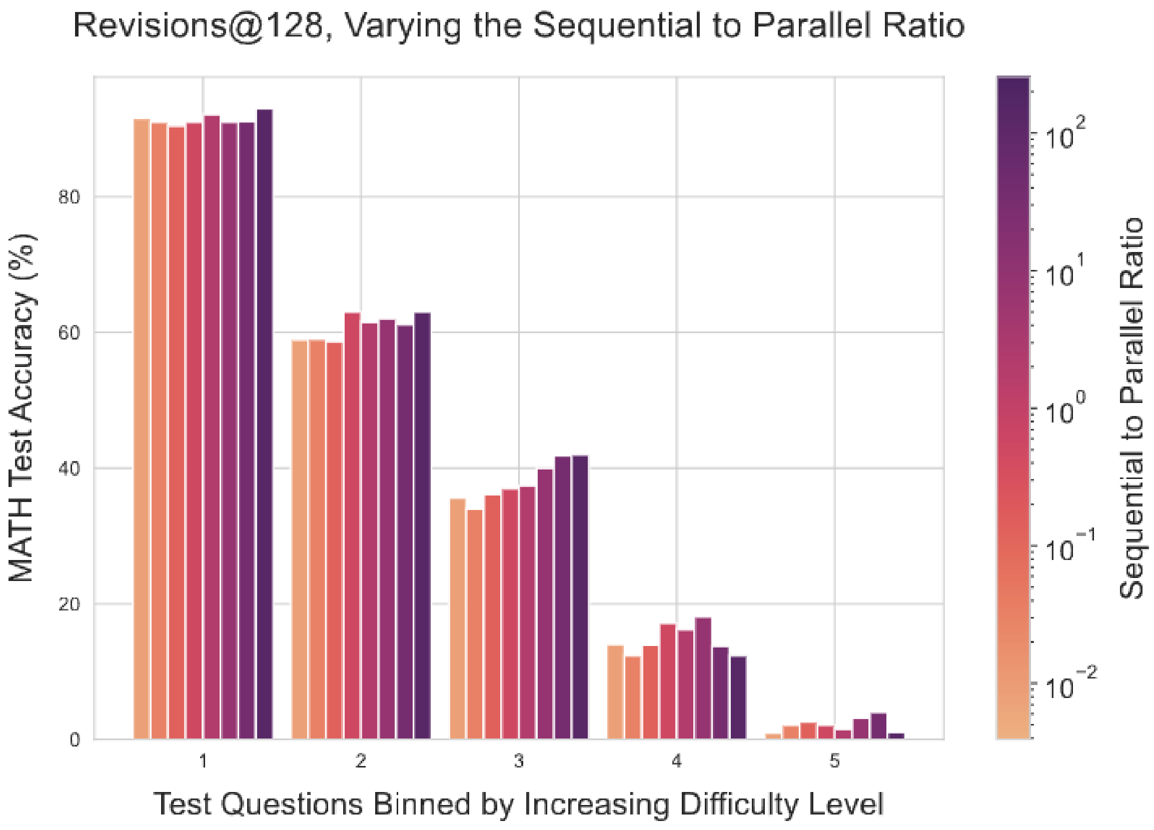
Refining the Proposal Distribution

- Trading off between parallel sampling & sequential revisions
  - (Generation budget)
  - Under low budget, performances increase with more sequential revisions.
  - Under higher budgets, there is an ideal ratio that strikes a balance between them.



Refining the Proposal Distribution

- Trading off between parallel sampling & sequential revisions
  - (Question difficulty)
  - Easier questions attain the best performance with full sequential compute.
  - On the harder questions, there is an ideal ratio of sequential to parallel test-time compute.

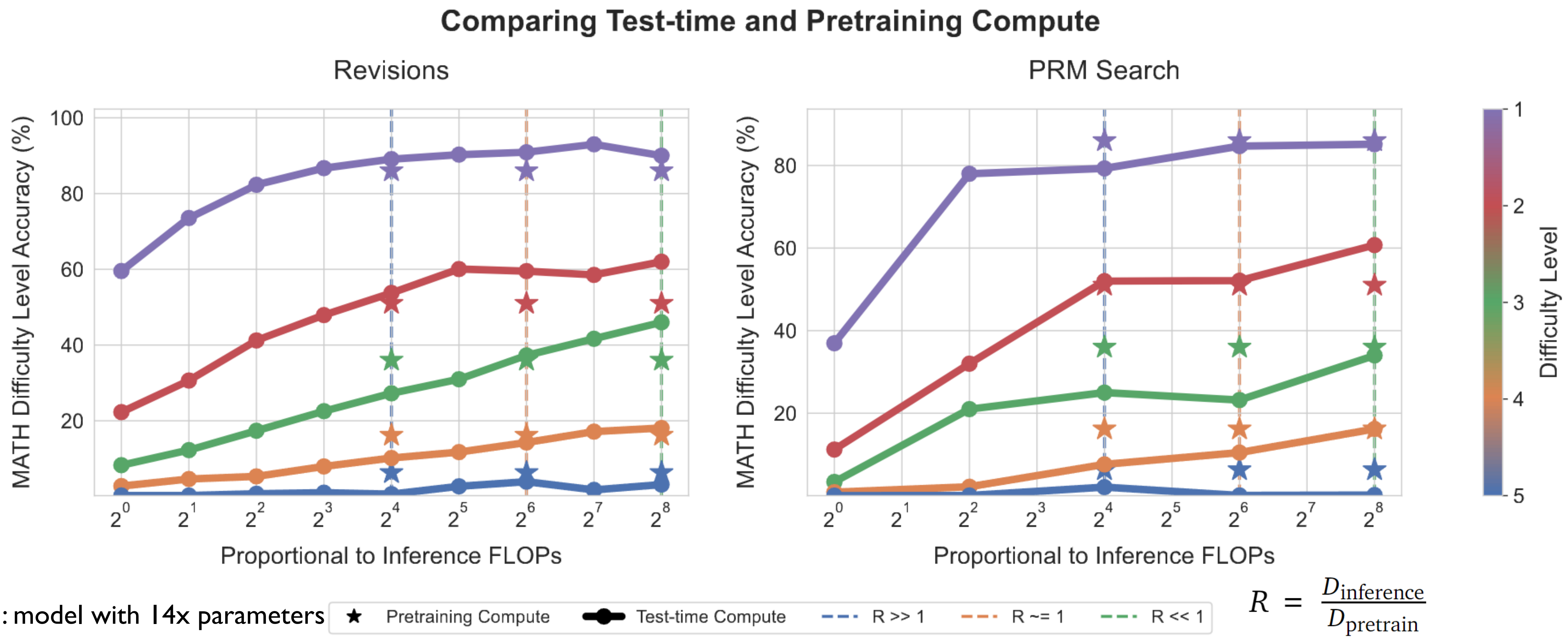


Pre-train or Inference?

- Q: How much better can the results under the inference scaling law be than under the pretraining scaling law?
- In other words, if we assign the same amount of computing to inference and pretrain, how about the performances?

Pre-train or Inference?

- Experimental results

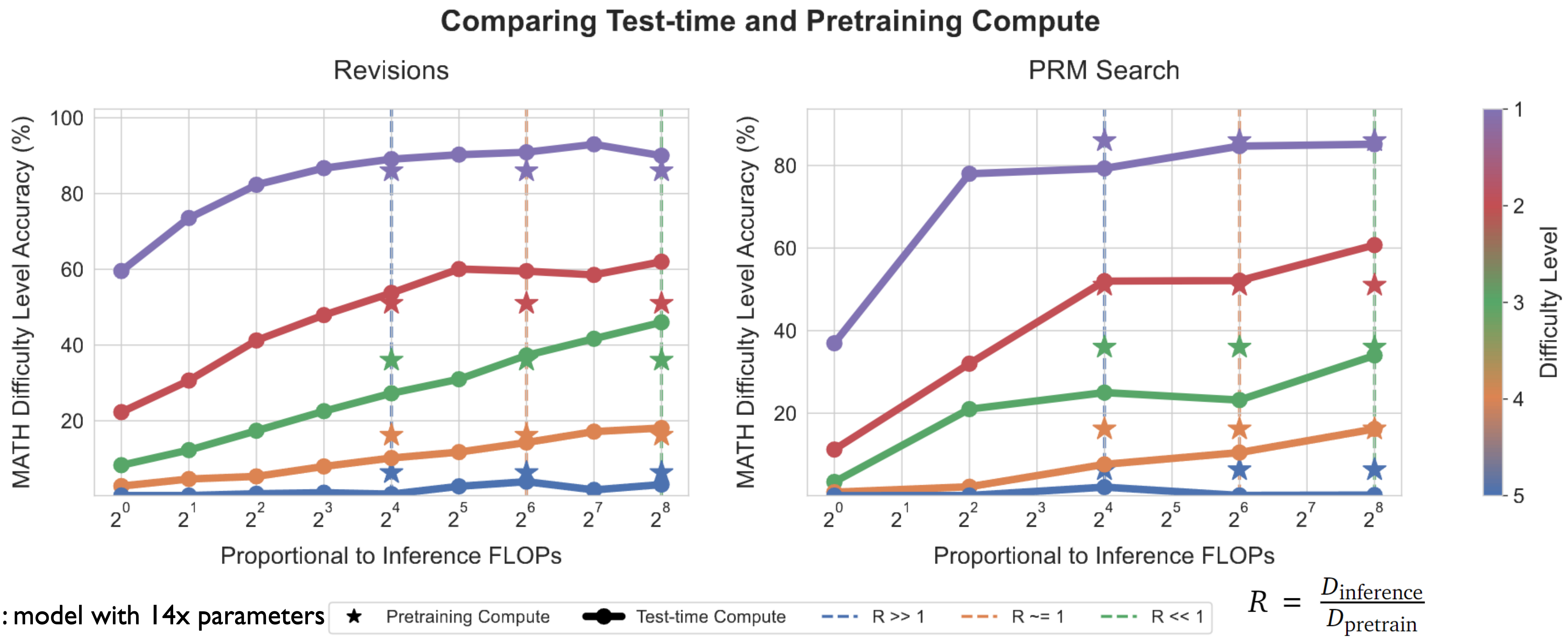


⭐: model with 14x parameters

$$R = \frac{D_{\text{inference}}}{D_{\text{pretrain}}}$$

Findings

1. For easy questions or in settings with a lower inference load (R << 1), test-time compute can generally outperform scaling model parameters.
2. For harder questions or in settings with a higher inference load (R >> 1), pretraining is a more effective way to improve performance.



: model with 14x parameters

$$R = \frac{D_{\text{inference}}}{D_{\text{pretrain}}}$$

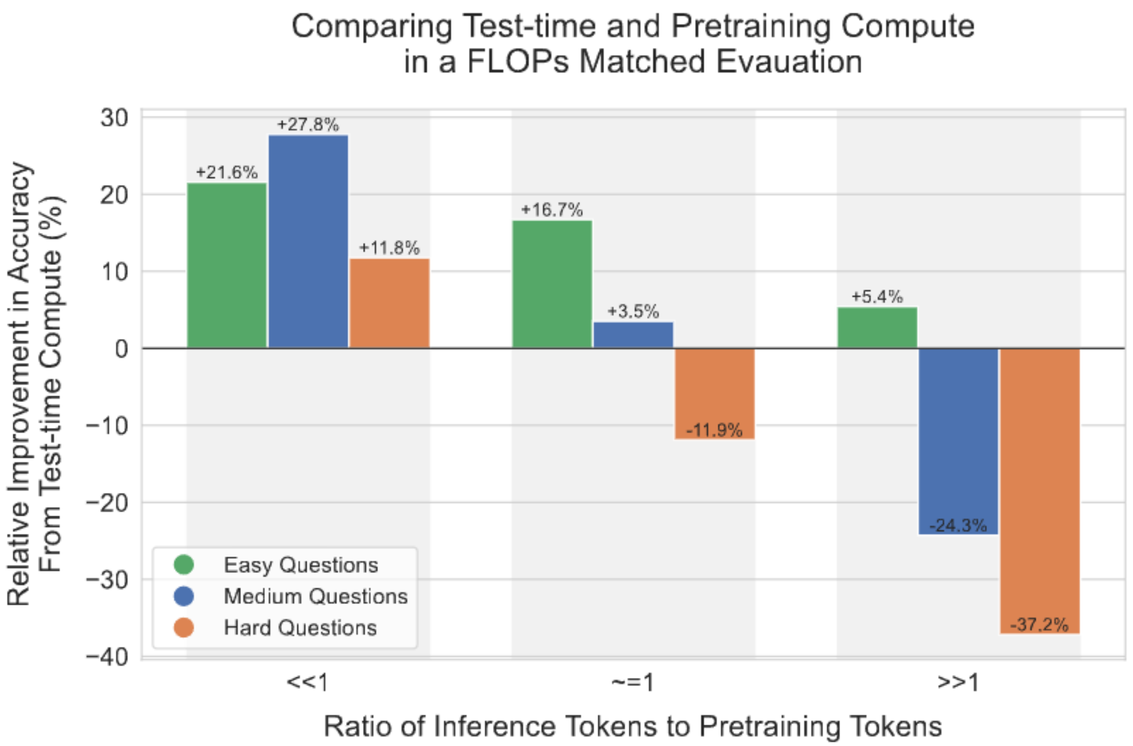
Takeaways for exchanging pretrain and test-time compute

- Test-time and pretraining compute are not 1-to-1 “exchangeable”.
- On easy and medium questions, which are within a model’s capabilities, or in settings with small inference requirement, test-time compute can easily cover up for additional pretraining.
- However, on challenging questions which are outside a given base model’s capabilities or under higher inference requirement, pretraining is likely more effective for improving performance.

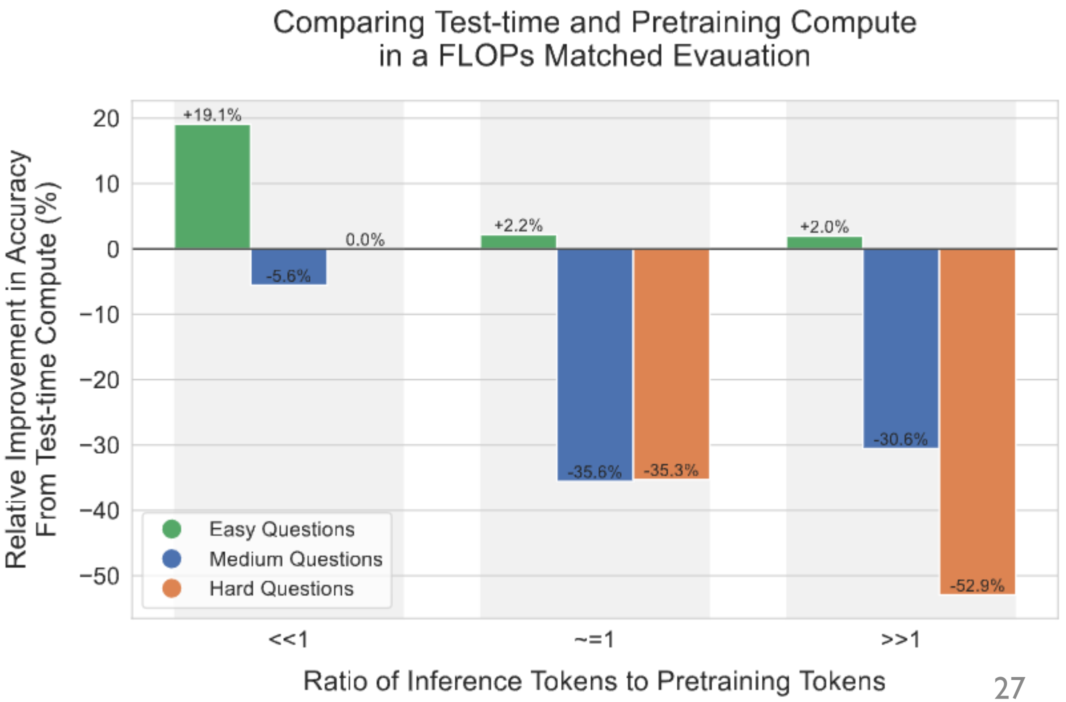
Takeaways for exchanging pretrain and test-time compute

- Some sum-up experimental results

Iteratively Revising Answers at Test-time



Test-time Search Against a PRM Verifier



Take-home messages

- Takeaways
  - For compute-optimal scaling of verifiers
  - Beam-search is more effective on harder questions and at lower compute budgets, whereas best-of-N is more effective on easier questions and at higher budgets.
  - Moreover, by selecting the best search setting for a given question difficulty and test-time compute budget, we can nearly outperform best-of-N using up to 4x less test-time compute.

Take-home messages

- Takeaways
  - For compute-optimal scaling by refining the proposal distribution with revisions
  - There exists a tradeoff between sequential (e.g. revisions) and parallel (e.g. standard best-of-N) test-time computation, and the ideal ratio of sequential to parallel test-time compute depends on both the compute budget and the specific question at hand.
  - Specifically, easier questions benefit from purely sequential test-time compute, whereas harder questions often perform best with some ideal ratio of sequential to parallel compute.
  - Moreover, by optimally selecting the best setting for a given question difficulty and test-time compute budget, we can outperform the parallel best-of-N baseline using up to 4x less test-time compute.

Take-home messages

- Test-time and pretraining compute are not 1-to-1 “exchangeable”.
- On easy and medium questions, which are within a model’s capabilities, or in settings with small inference requirement, test-time compute can easily cover up for additional pretraining.
- However, on challenging questions which are outside a given base model’s capabilities or under higher inference requirement, pretraining is likely more effective for improving performance.

Thanks for your listening!

- Q & A