

# FALL 2024 COS597R: DEEP DIVE INTO LARGE LANGUAGE MODELS

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PRINCETON  
UNIVERSITY

Lecture 15: LLM reasoning + inference-time compute (cont'd)

<https://princeton-cos597r.github.io/>

# Scaling LLM Test-Time Compute Optimally can be More Effective than Scaling Model Parameters

Charlie Snell<sup>◆, 1</sup>, Jaehoon Lee<sup>2</sup>, Kelvin Xu<sup>◆, 2</sup> and Aviral Kumar<sup>◆, 2</sup>

◆Equal advising, <sup>1</sup>UC Berkeley, <sup>2</sup>Google DeepMind, ◆Work done during an internship at Google DeepMind

Q. Large model vs small model + more inference compute?

Q. Can test-time computation substitute for pre-training?

[Submitted on 1 Aug 2024 (v1), last revised 14 Oct 2024 (this version, v2)]

## Inference Scaling Laws: An Empirical Analysis of Compute-Optimal Inference for Problem-Solving with Language Models

Yangzhen Wu, Zhiqing Sun, Shanda Li, Sean Welleck, Yiming Yang

- **Sampling:** best-of-n, majority voting, weighted majority voting
- **Search:** MCTS, reward balanced search (this work)

[Submitted on 31 Jul 2024 (v1), last revised 16 Sep 2024 (this version, v2)]

## Large Language Monkeys: Scaling Inference Compute with Repeated Sampling

Bradley Brown, Jordan Juravsky, Ryan Ehrlich, Ronald Clark, Quoc V. Le, Christopher Ré, Azalia Mirhoseini

- **Sampling**

# Scaling LLM Test-Time Compute Optimally can be More Effective than Scaling Model Parameters

Charlie Snell<sup>◆, 1</sup>, Jaehoon Lee<sup>2</sup>, Kelvin Xu<sup>◆, 2</sup> and Aviral Kumar<sup>◆, 2</sup>

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Q2. This paper only considers the trade-off between pre-training and inference, and they did the analysis using a base model. What do think of the impact of post-training in this pipeline? What are some general ideas of post-training for improving the (mathematical) reasoning of LLMs?

“how one should trade off inference-time and pre-training compute”

“We conduct our analysis using the PaLM 2-S\* (Codey) base model”

“Capability-specific fine-tuning is necessary to induce revision and verification capabilities into the base model on MATH”

# This lecture

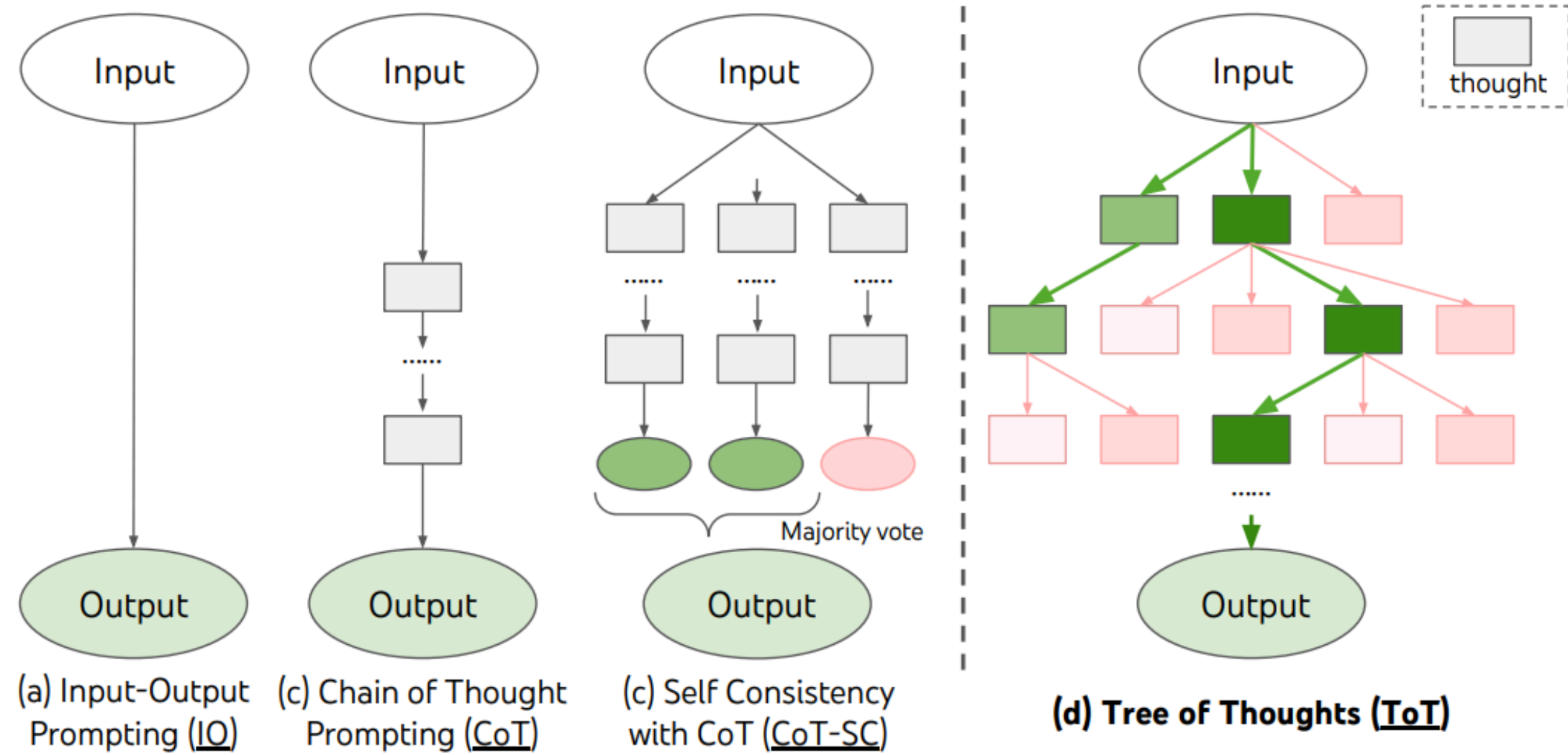


Image: Jim Fan

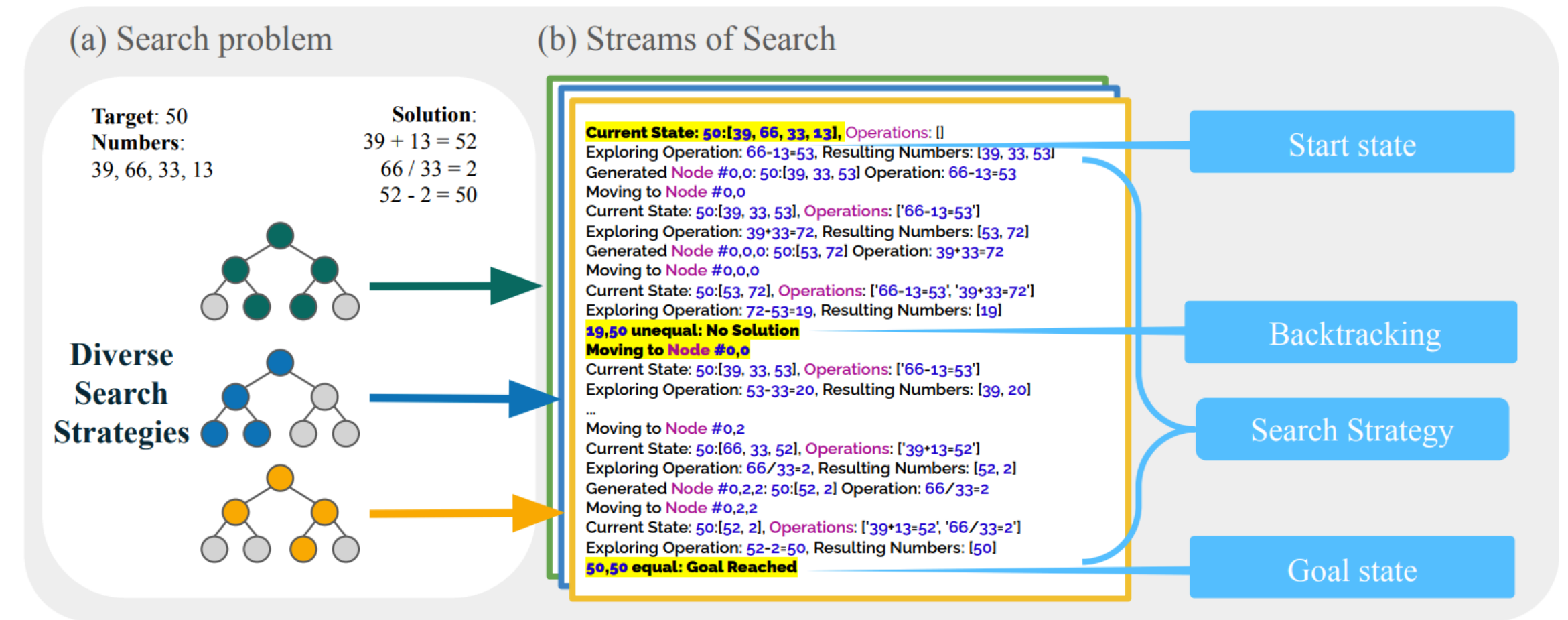
- Different test-time strategies
  - Which strategy works better in what scenario?
  - More discussion on ORMs vs PRMs
- (Brief) How to train LLMs for better reasoning (= post-training)?



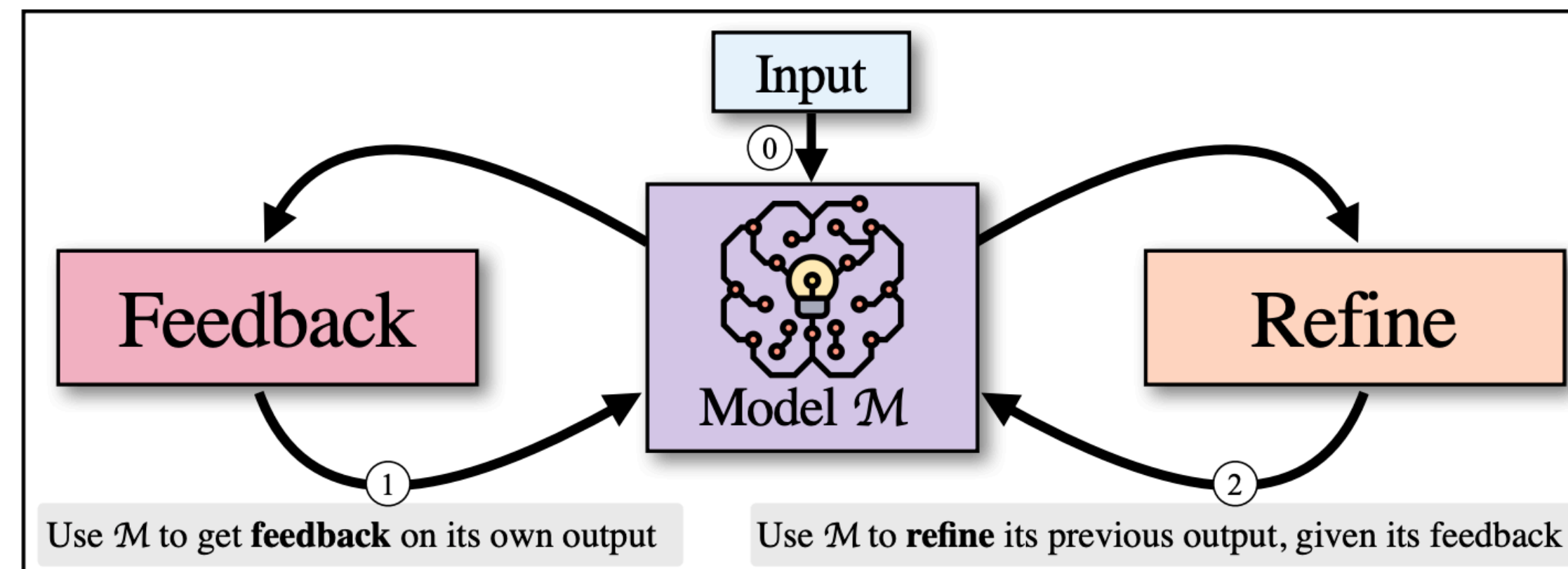
# Lots of inference methods



Tree of thoughts (Yao et al., 2023)



Stream of search (Gandhi et al., 2024)



Self-refine (Madaan et al., 2023)

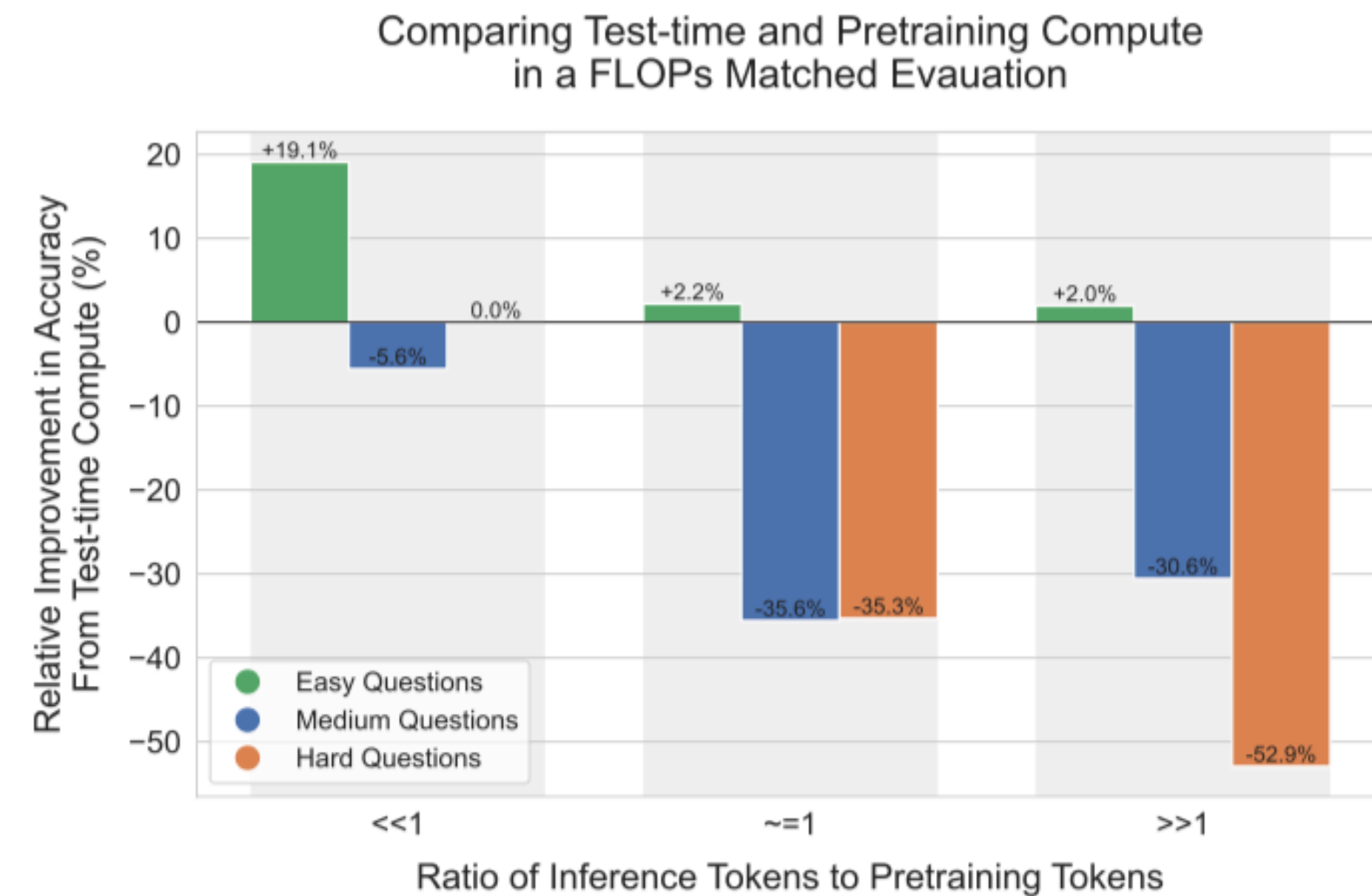
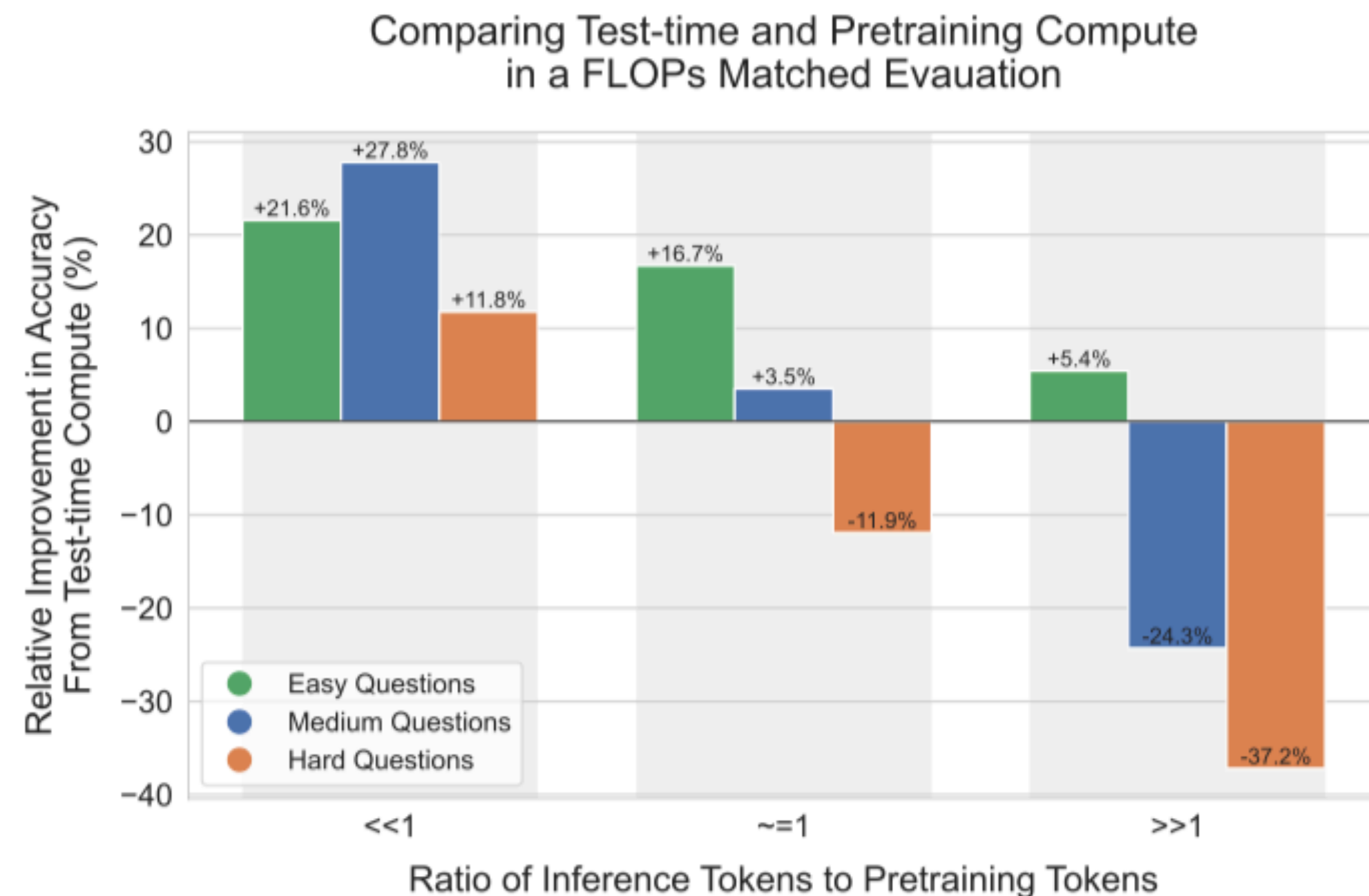
# Two views of scaling test-time compute

- **Input level:** augment the prompt with additional tokens (repeatedly)

“Refining the proposal distribution”

- **Output level:** sample multiple candidates and perform surgery on these candidates

“Searching against a (PRM) verifier”



Comparison: a 14x larger model with greedy decoding

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Search against a verifier

# Search against a PRM verifier

- They use a PRM (process reward model) instead of an ORM (outcome reward model) verifier

$$\text{ORM } (P \times S \rightarrow \mathbb{R})$$

$$\mathcal{L}_{ORM} = y_s \log r_s + (1 - y_s) \log(1 - r_s)$$

$$\text{PRM } (P \times S \rightarrow \mathbb{R}^+)$$

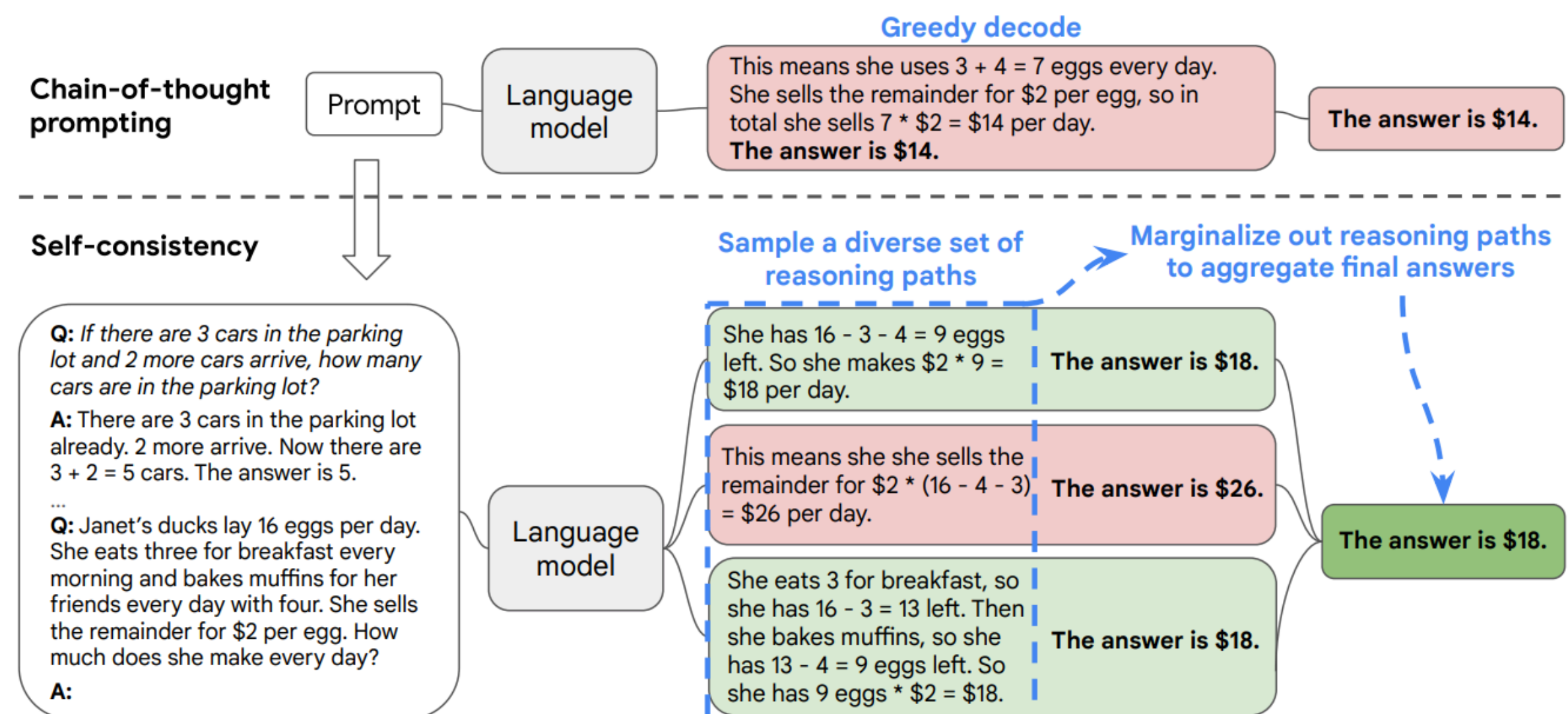
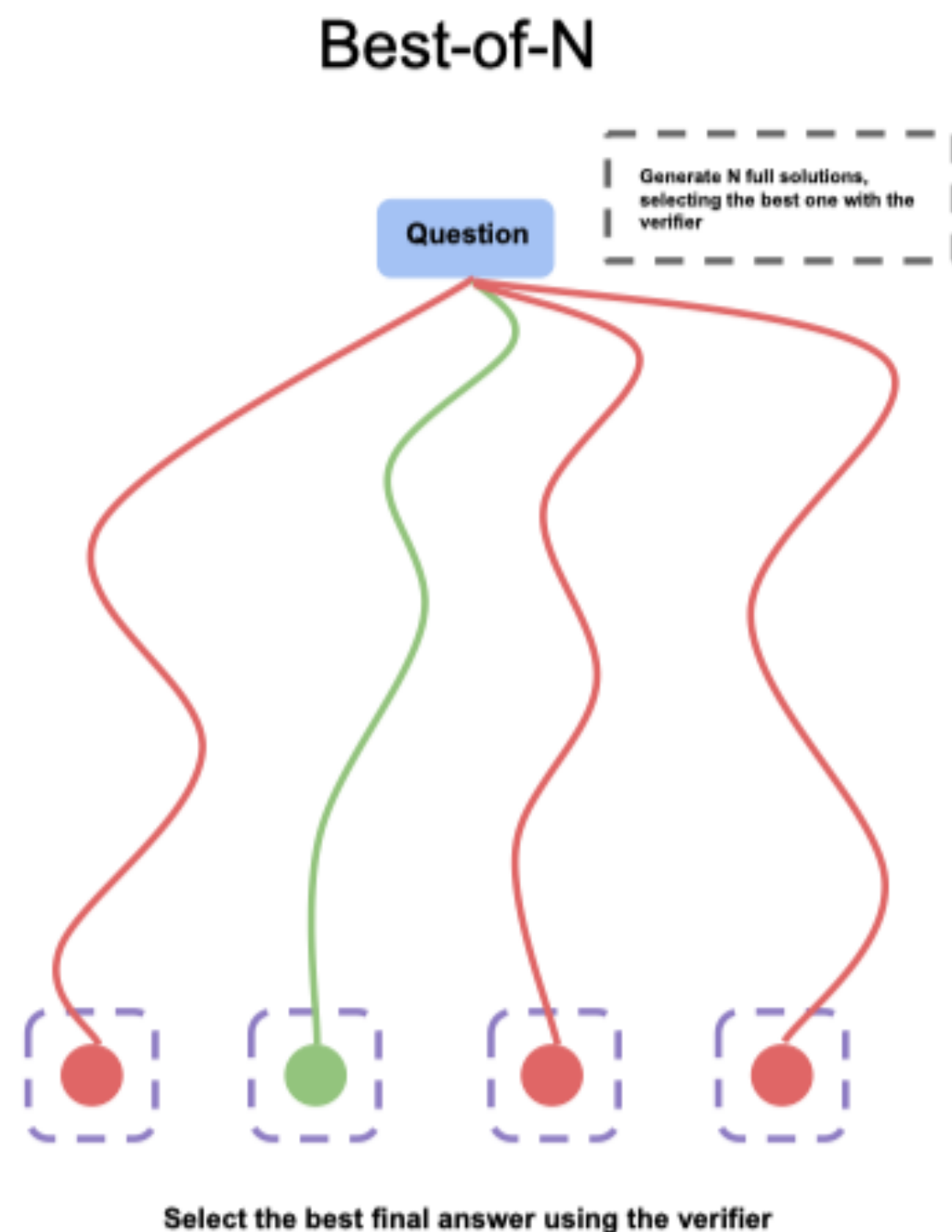
$$\mathcal{L}_{PRM} = \sum_{i=1}^K y_{s_i} \log r_{s_i} + (1 - y_{s_i}) \log(1 - r_{s_i})$$

- They use **automated methods** for collecting process supervision instead of PRM800K
  - Distribution shift between GPT-4 and Palm-2 outputs?
- PRM can be used for multiple strategies, but ORM can be only used for best-of-n (still PRM works better!)
- I believe they fine-tuned the same base model as the verifier



# #1: Best-of-n weighted

- Best-of-n: sample n full solutions and use RM to pick the best one
- Majority vote: get n final answers, and pick the one with the highest vote (no RM used)

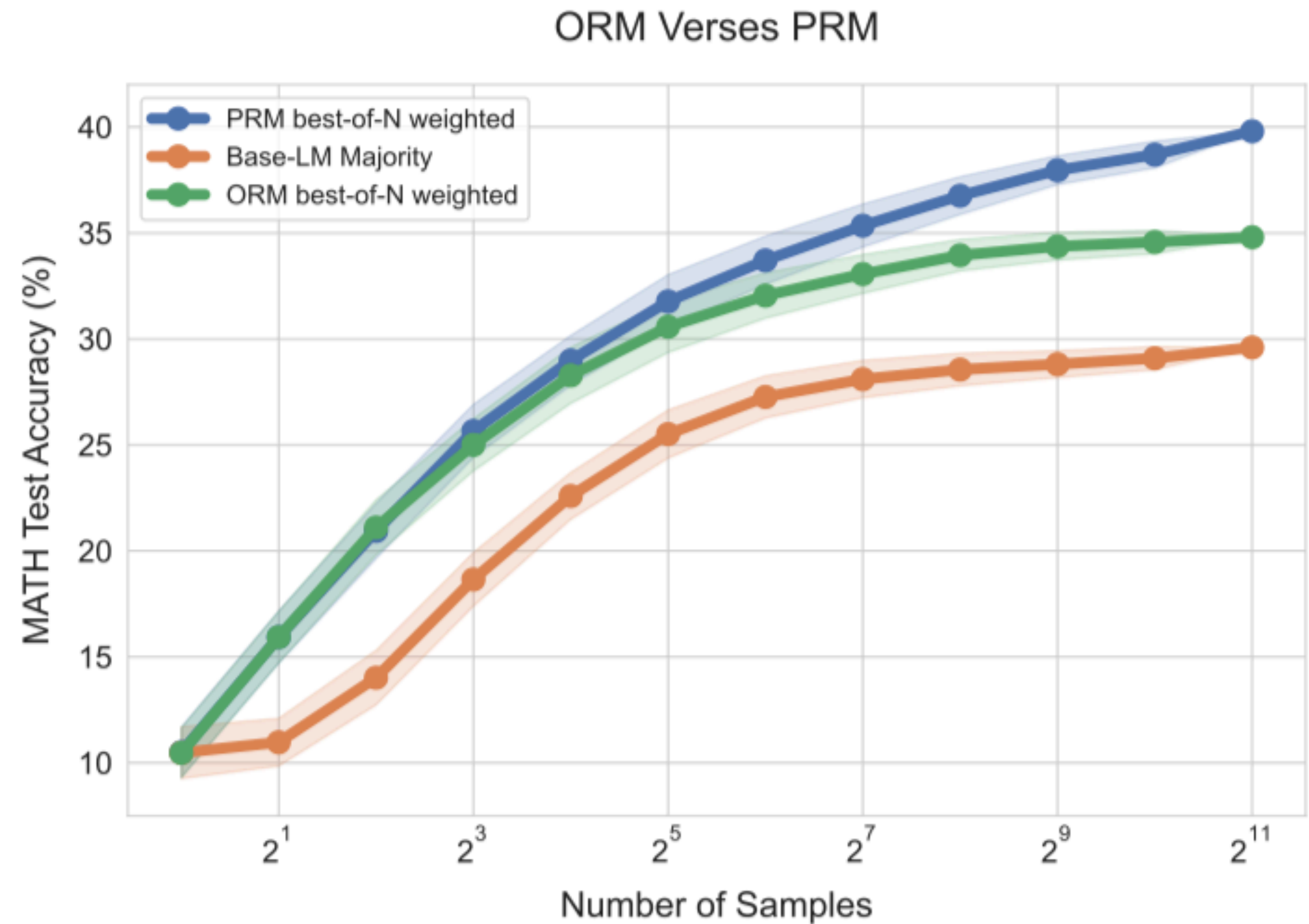


Also called self-consistency (Wang et al., 2022)

- Best-of-n weighted: get n final answer, each answer has a weight assigned by RM, aggregate and weights and pick the one with highest sum

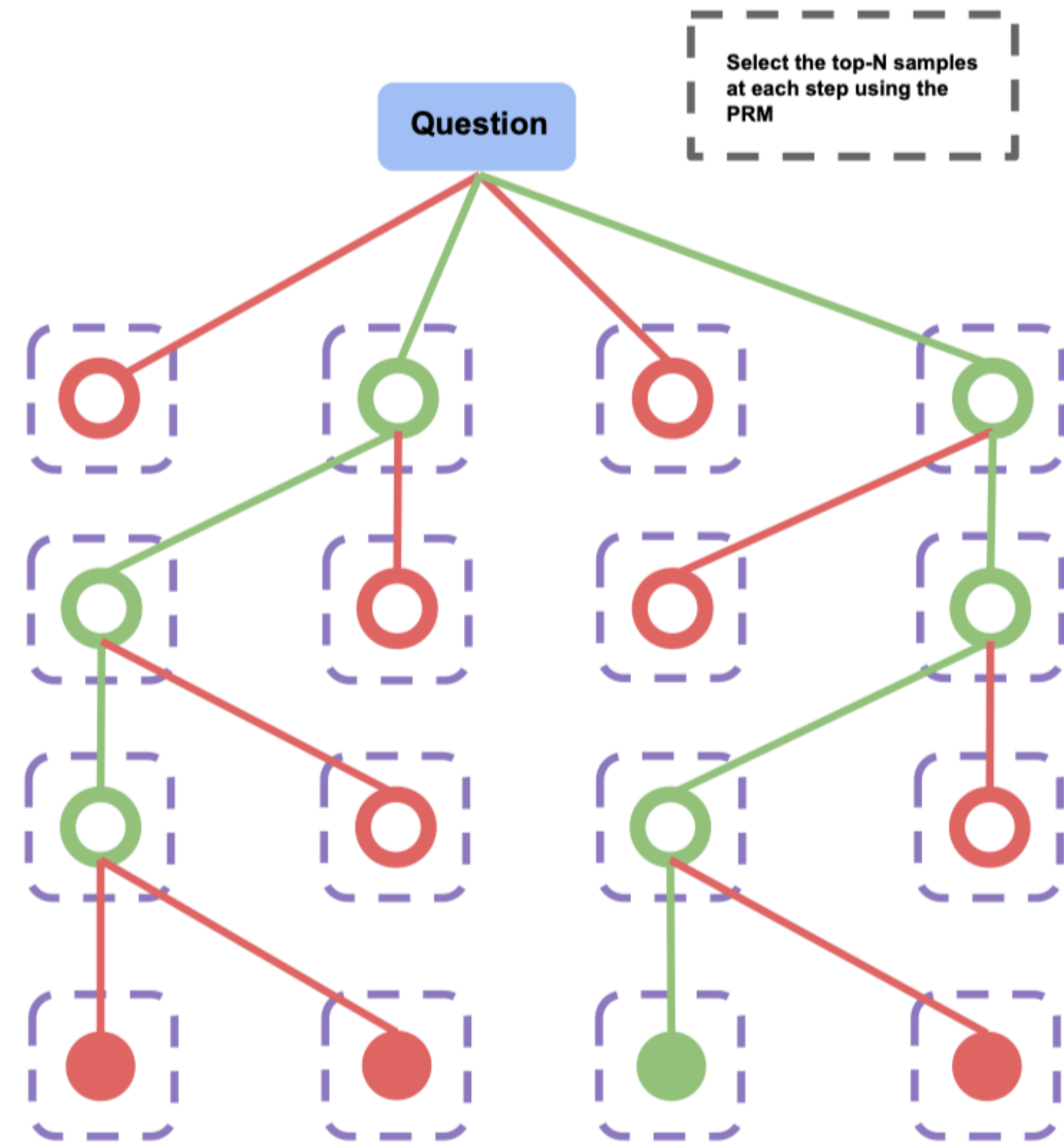
# #1: Best-of-n weighted

- How to get an **aggregated score** from PRM when ranking full answers?
  - They used PRM's prediction at the last step as the full-answer score
  - Prior work used product or minimum



# #2: Beam search

## Beam Search

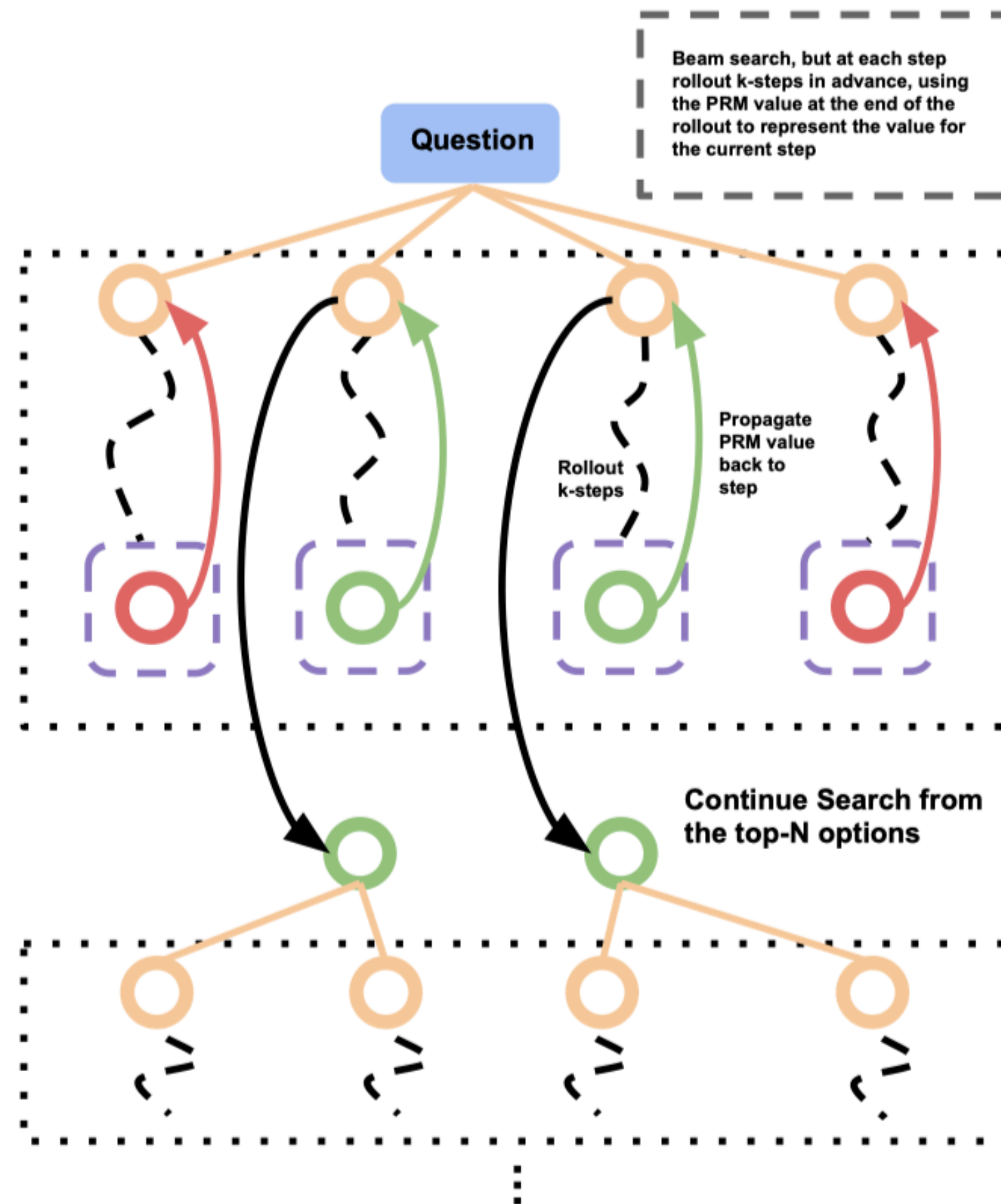


Select the best final answer using the verifier

- N: beam size
- M: sample M steps from each node

# #3: Lookahead search

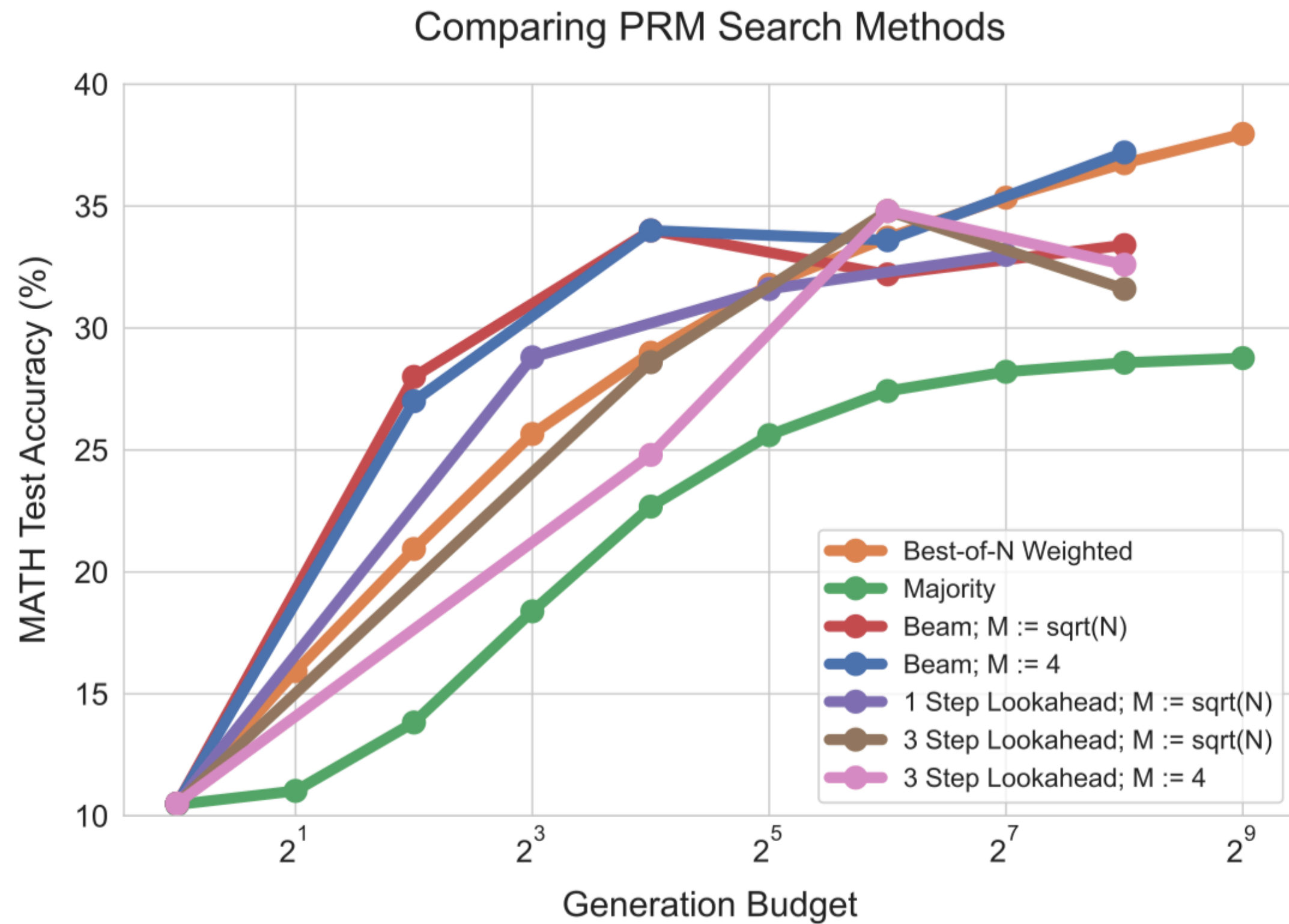
## Lookahead Search



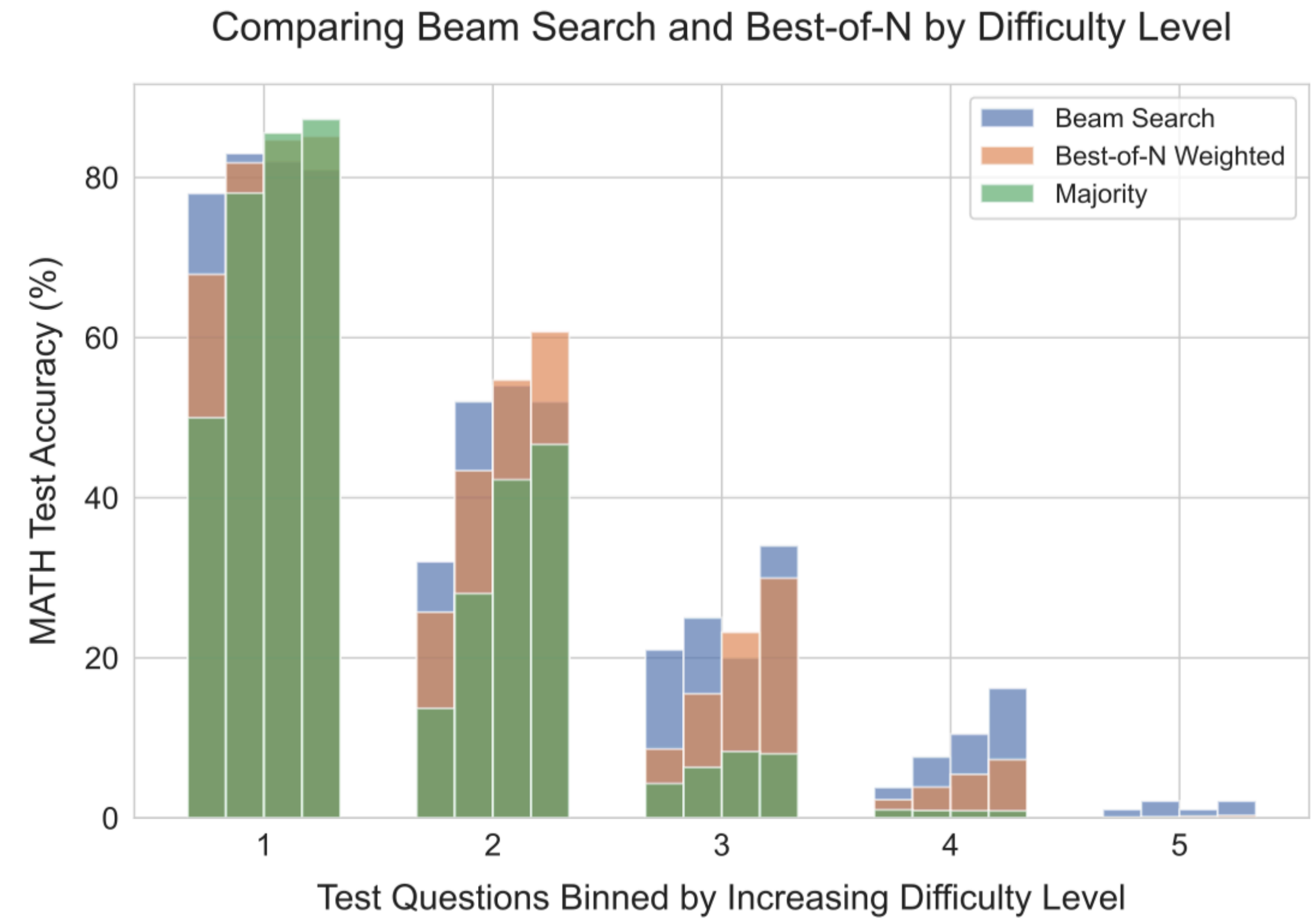
- $N$ : beam size
- $M$ : sample  $M$  steps from each node
- $k$ : rolling out up to  $k$  steps, and use PRM's score
- Representative of MCTS-style methods



# Results

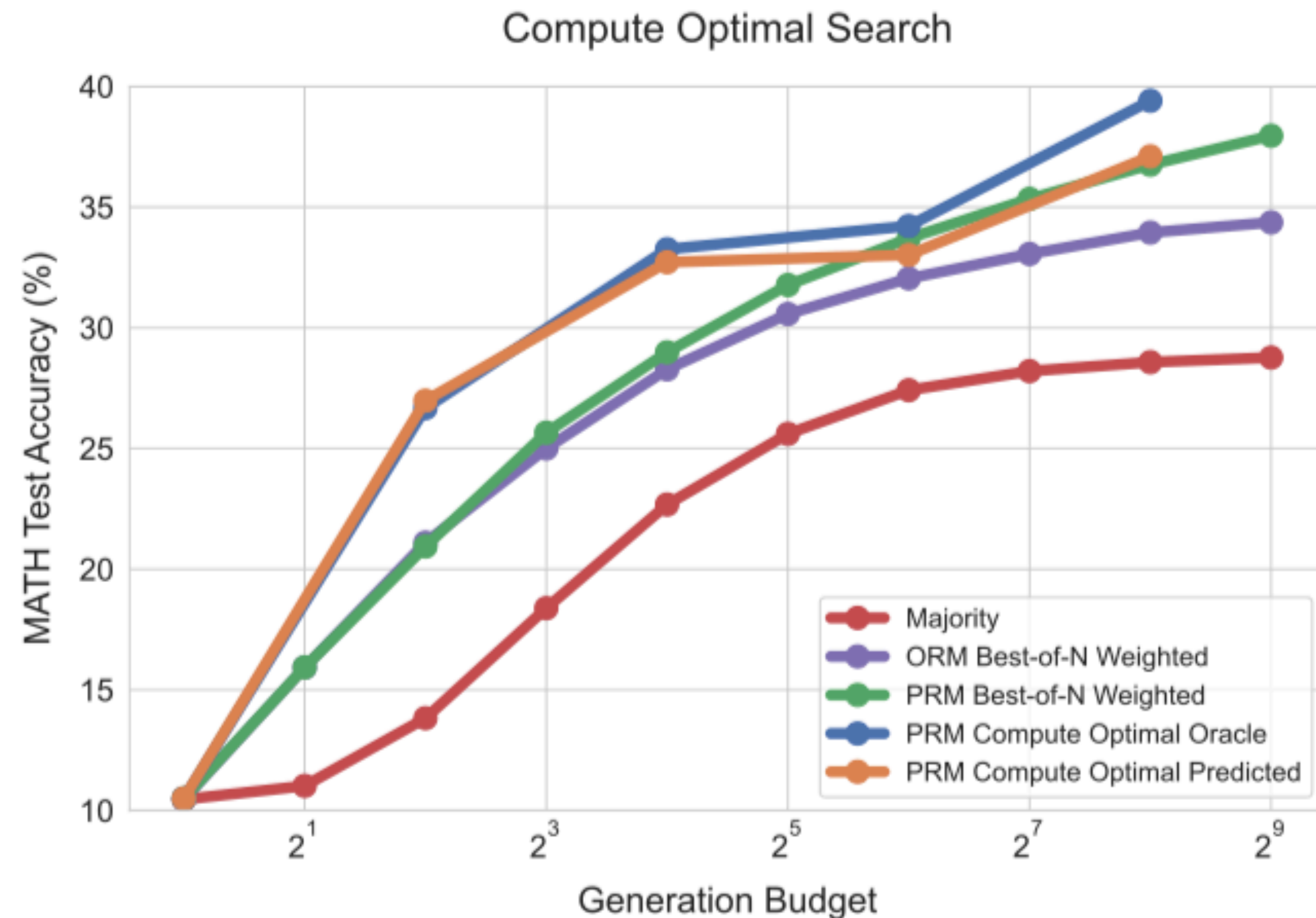


- Beam search is best with less budget
- Best-of-n weighted is the best with large budget



- Beam search is better for harder questions
- No meaningful progress for hardest questions

# Results: Adaptive compute-optimal strategy



- The optimal test-time strategy should depend on question difficulty!
- Can outperform PRM best-of-N up to 4x less test-time compute
- Note: estimating difficulty of prompts also incurs test-time compute but omitted in this study (“a crucial avenue for future work”)

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Aside: how to collect PRM data automatically?

# Human annotations




[Submitted on 31 May 2023]




## Let's Verify Step by Step


Hunter Lightman, Vineet Kosaraju, Yura Burda, Harri Edwards, Bowen Baker, Teddy Lee, Jan Leike, John Schulman, Ilya Sutskever, Karl Cobbe




The denominator of a fraction is 7 less than 3 times the numerator.


If the fraction is equivalent to  $2/5$ , what is the numerator of the fraction?

   Let's call the numerator  $x$ .

   So the denominator is  $3x-7$ .

   We know that  $x/(3x-7) = 2/5$ .

   So  $5x = 2(3x-7)$ .

    $5x = 6x - 14$ .

   So  $x = 7$ .

PRM800K: Dataset contains 800K step-level labels provided by human raters across 75K solutions to 12K problems (MATH 8K training set + 4K test questions).

- “We deliberately choose to supervised only up to **first incorrect step**”
- Use **active learning** to decide which steps to annotate “convincing wrong-answer solution”
- Only evaluates using best-of-n sampling



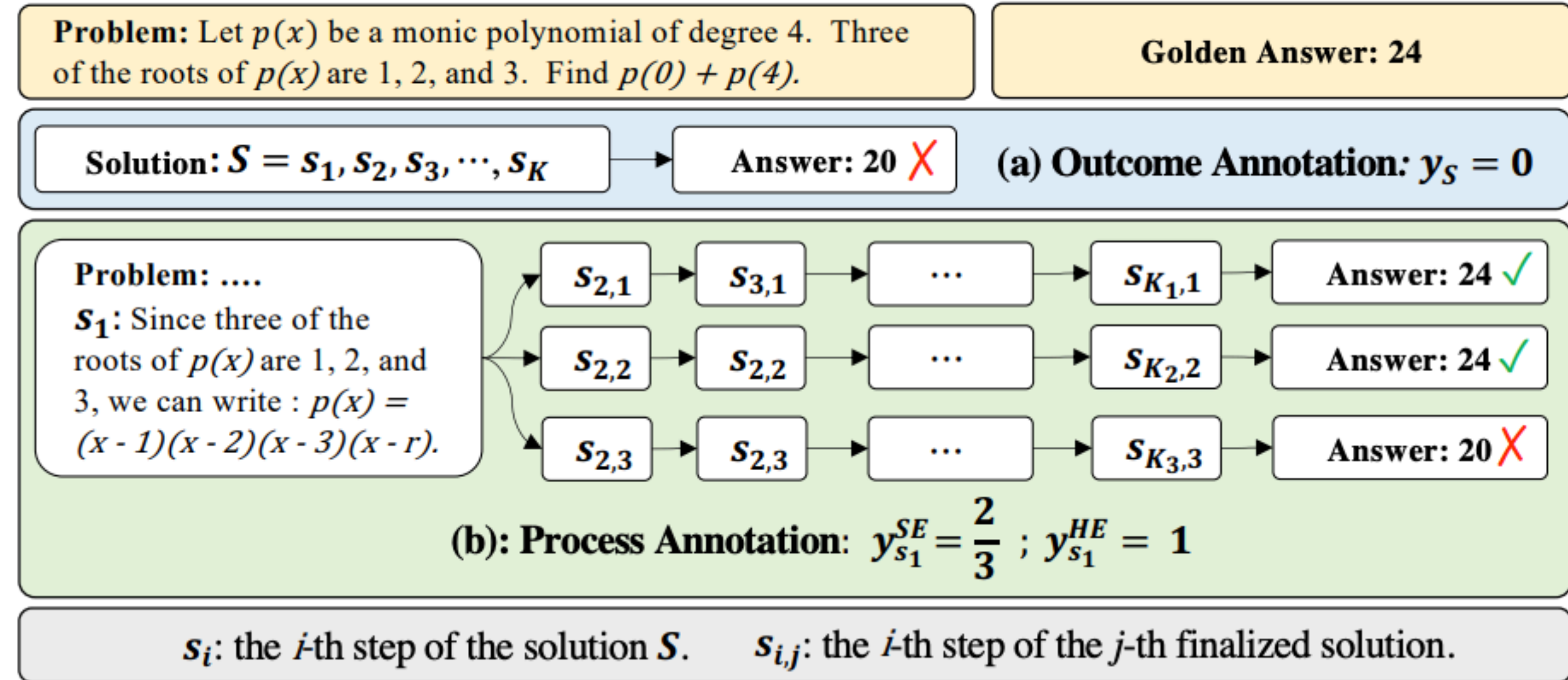
# Process supervision without human labels

## MATH-SHEPHERD: VERIFY AND REINFORCE LLMs STEP-BY-STEP WITHOUT HUMAN ANNOTATIONS

Peiyi Wang<sup>1†</sup> Lei Li<sup>3</sup> Zhihong Shao<sup>4</sup> R.X. Xu<sup>2</sup> Damai Dai<sup>1</sup> Yifei Li<sup>5</sup>  
 Deli Chen<sup>2</sup> Y. Wu<sup>2</sup> Zhifang Sui<sup>1</sup>  
<sup>1</sup>National Key Laboratory for Multimedia Information Processing, Peking University  
<sup>2</sup>DeepSeek-AI <sup>3</sup>The University of Hong Kong  
<sup>4</sup>Tsinghua University <sup>5</sup>The Ohio State University  
 {wangpeiyi9979, nlp.lilei}@gmail.com  
 li.14042@osu.edu szf@pku.edu.cn



Project Page: MATH-SHEPHERD



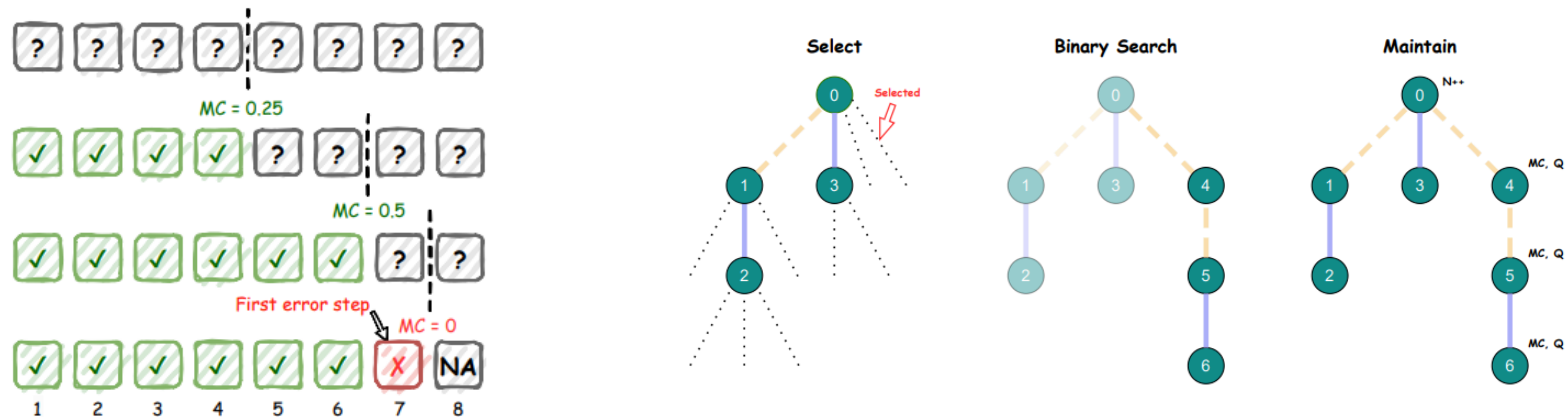
- **The quality of a reasoning step** = its potential to deduce the correct answer
- For each step, perform N rollouts, estimate how likely it will lead to the correct answer
- They did evaluations on a) best-of-n weighted; b) RL with PRM
- This is the method the Snell et al paper used!

# Process supervision without human labels

## Improve Mathematical Reasoning in Language Models by Automated Process Supervision

Liangchen Luo<sup>1\*</sup>, Yinxiao Liu<sup>1\*</sup>, Rosanne Liu<sup>1</sup>, Samrat Phatale<sup>1</sup>, Harsh Lara<sup>1</sup>, Yunxuan Li<sup>2</sup>, Lei Shu<sup>1</sup>, Yun Zhu<sup>1</sup>, Lei Meng<sup>2</sup>, Jiao Sun<sup>2</sup> and Abhinav Rastogi<sup>1</sup>

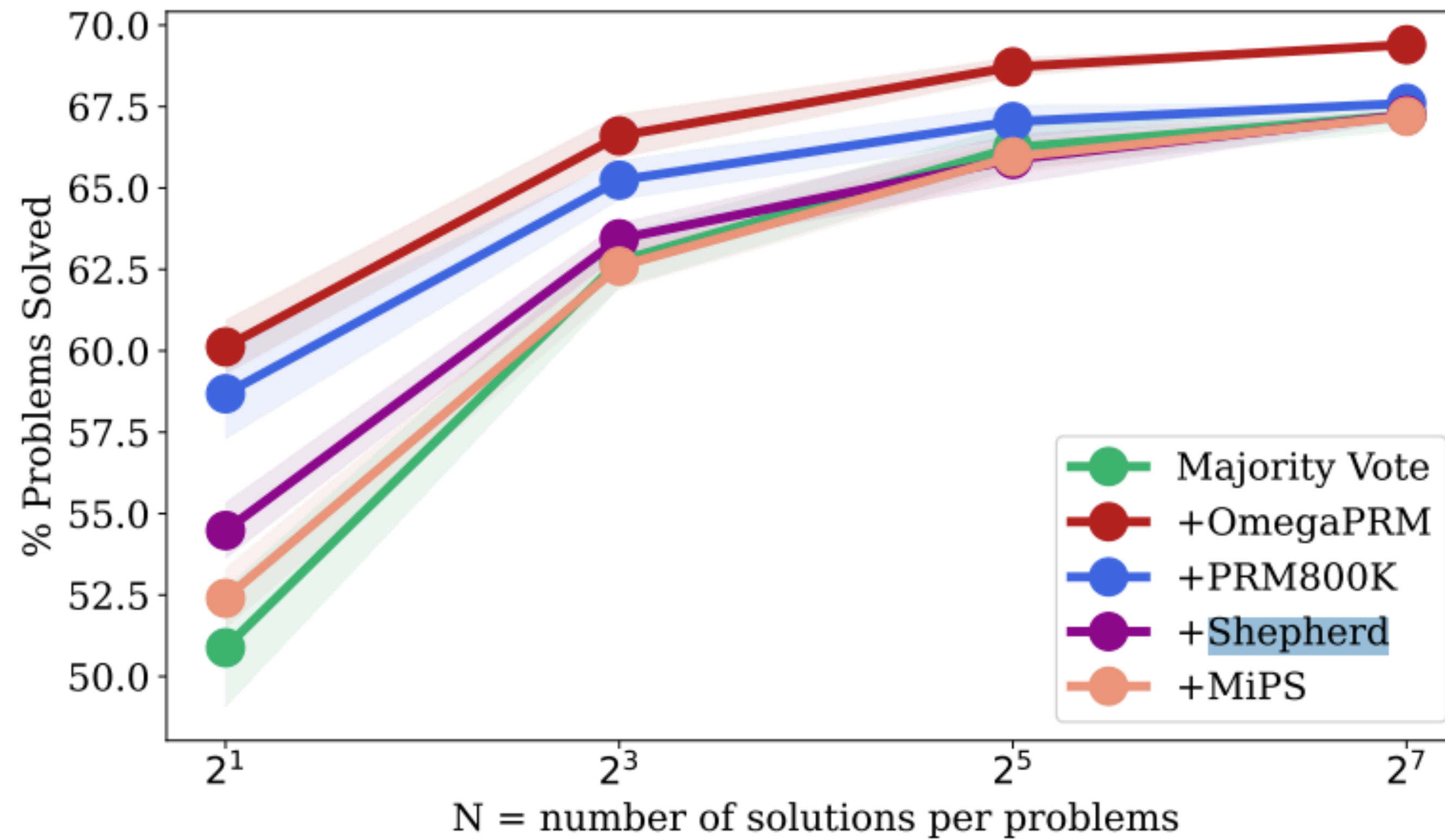
<sup>1</sup>Google DeepMind, <sup>2</sup>Google



- They claim using per-step Monte Carlo estimation as in Math-Shepherd is not efficient
- They use a complex MCTS process to decide how to do roll-outs and how to collect PRM data

# Process supervision without human labels

	Majority Vote	+OmegaPRM	+PRM800K	+Shepherd	+MiPS
% Solved (@128)	67.2	<b>69.4</b>	67.6	67.2	67.2



best-of-n sampling



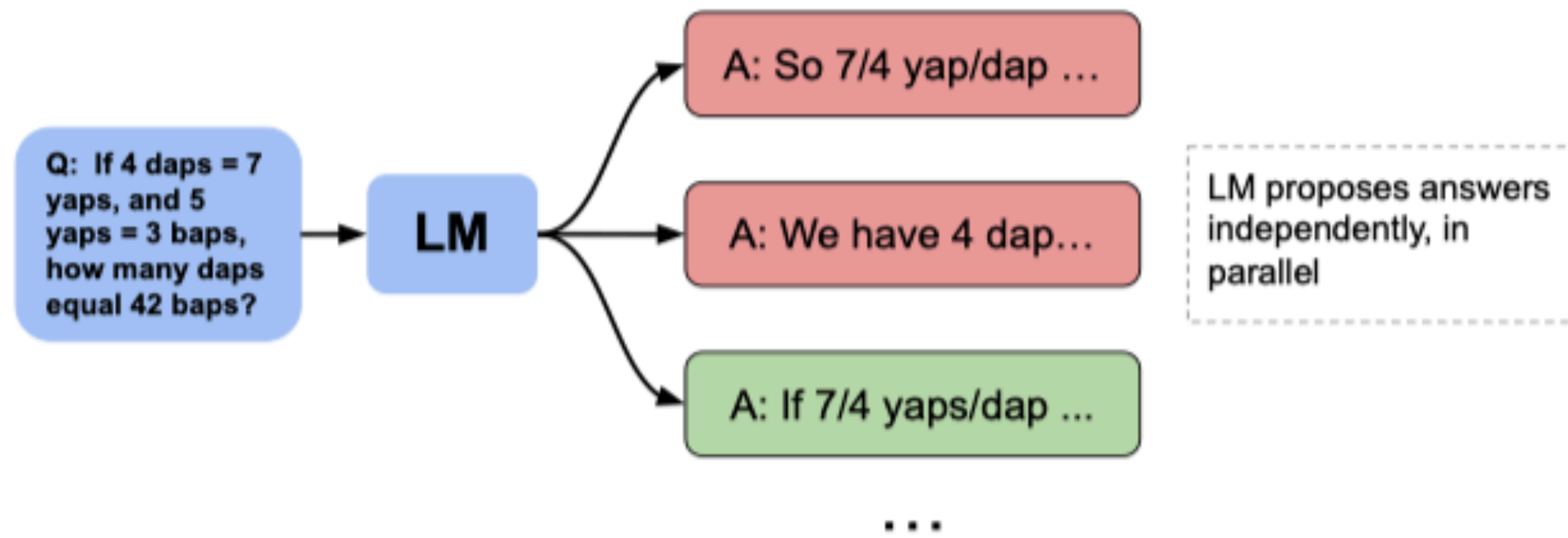
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# Refining the proposal distribution

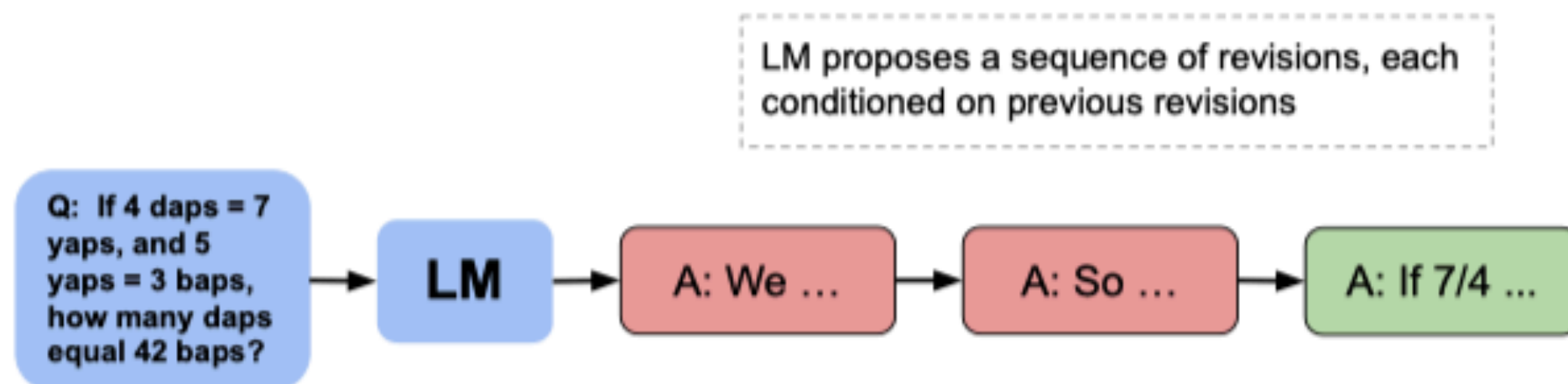


# Using a revision model

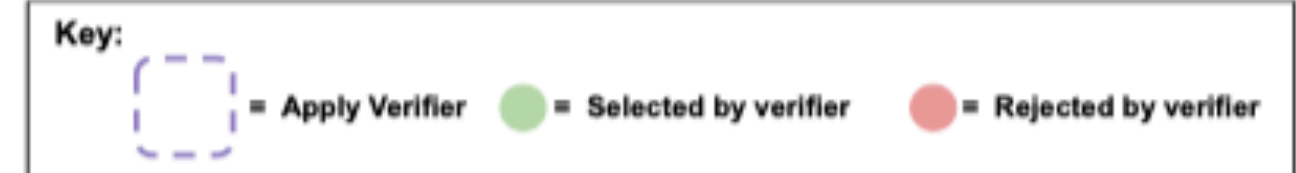
## Parallel Sampling



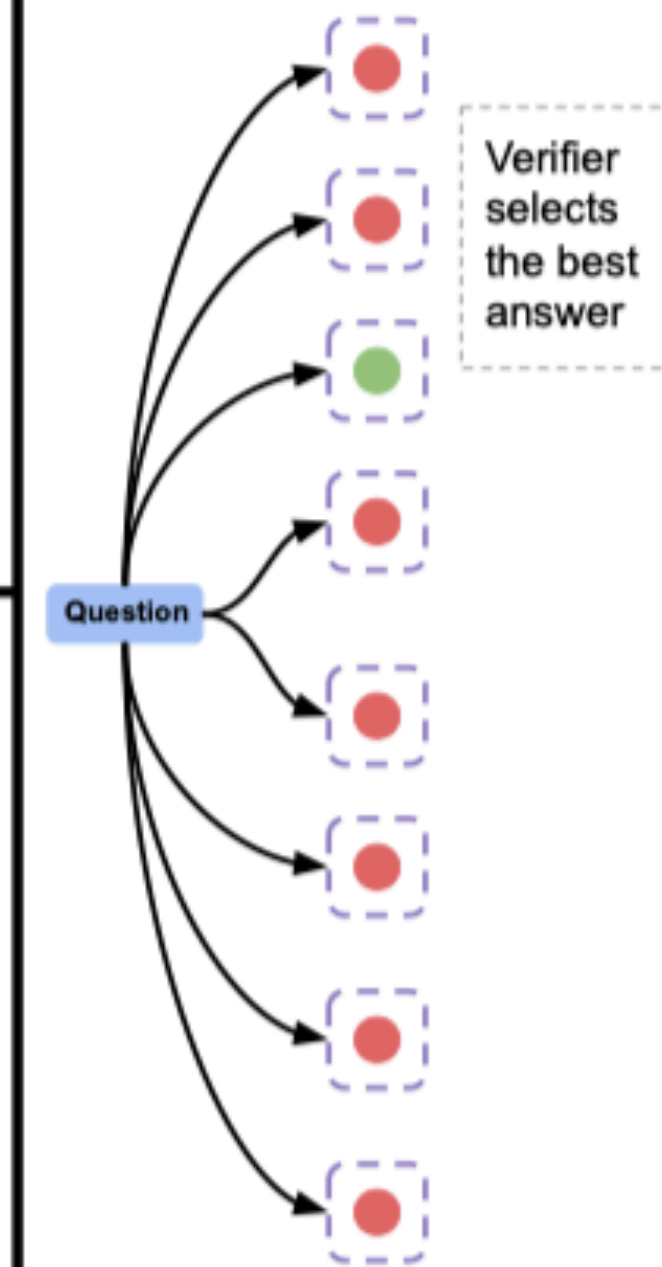
## Sequential Revisions



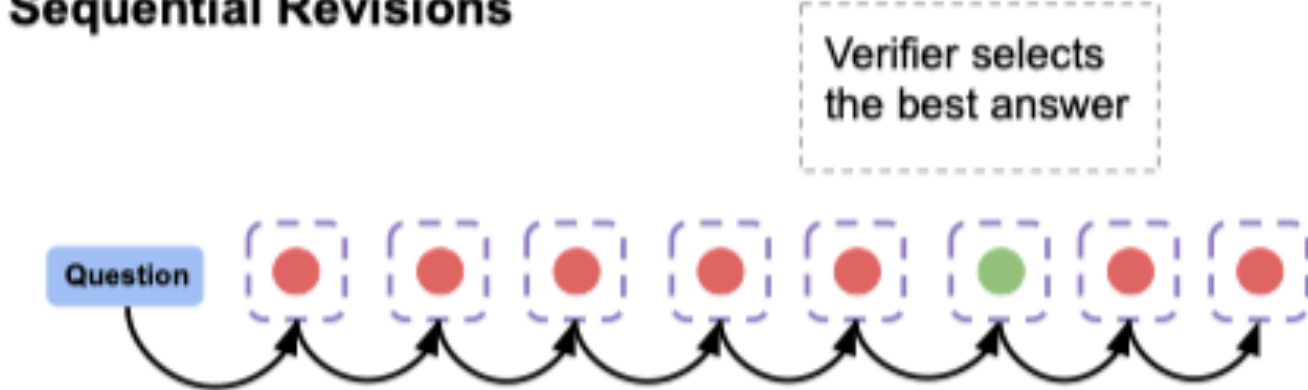
## Using Revision Model + Verifier at Inference Time



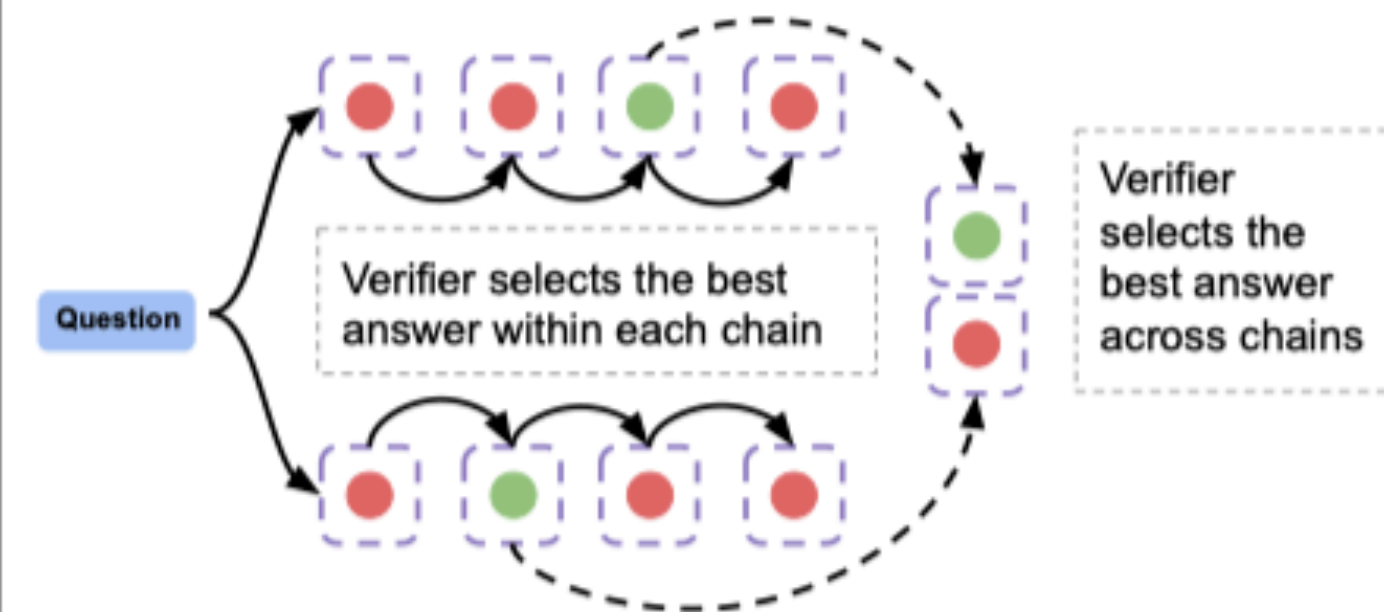
### Parallel Best-of-N



### Sequential Revisions



### Combining Sequential / Parallel



- The revision model takes the previous 4 responses and propose a new revision
- Pick the best output according to a verifier

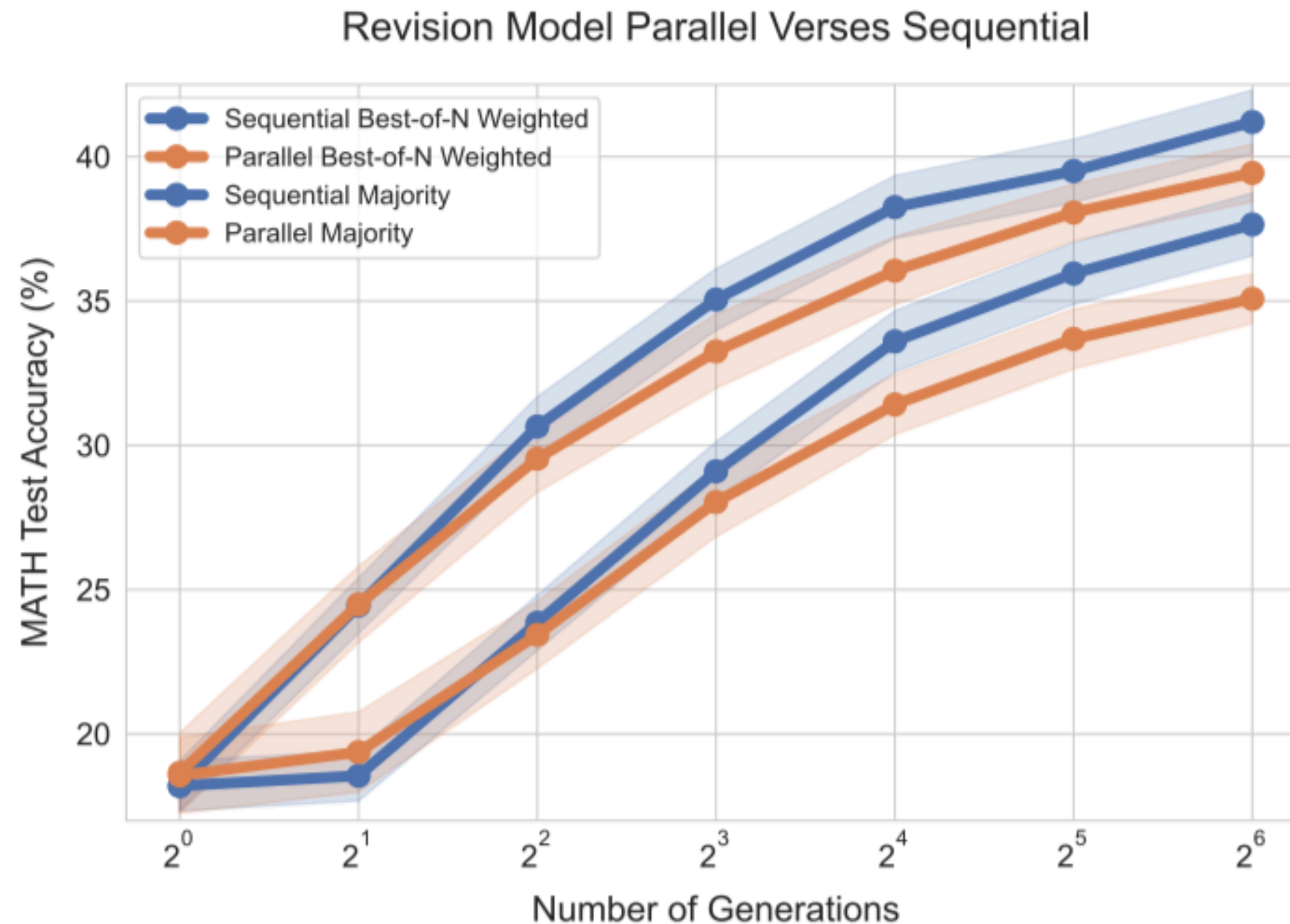
# How to train the revision model?

- **Data:** “Specifically, following the recipe of [1], we pair up each correct answer with a sequence of incorrect answers from this set as context to construct multi-turn finetuning data. We include up to four incorrect answers in context, where the specific number of solutions in context is sampled randomly from a uniform distribution over categories 0 to 4. We use a character edit distance metric to prioritize selecting incorrect answers which are correlated with the final correct answer.”

[1] Training revision models with synthetic data. Coming soon, 2024.

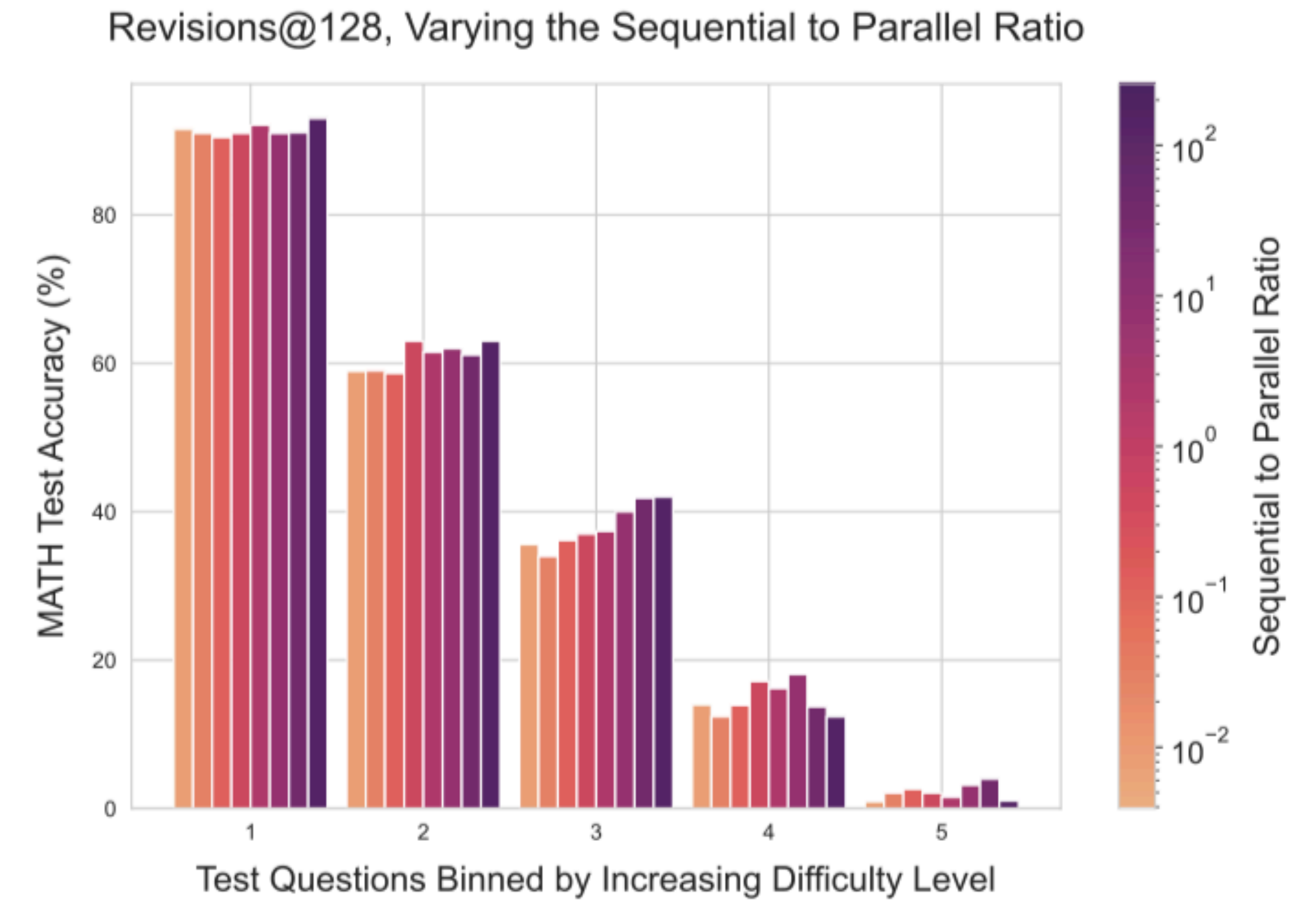
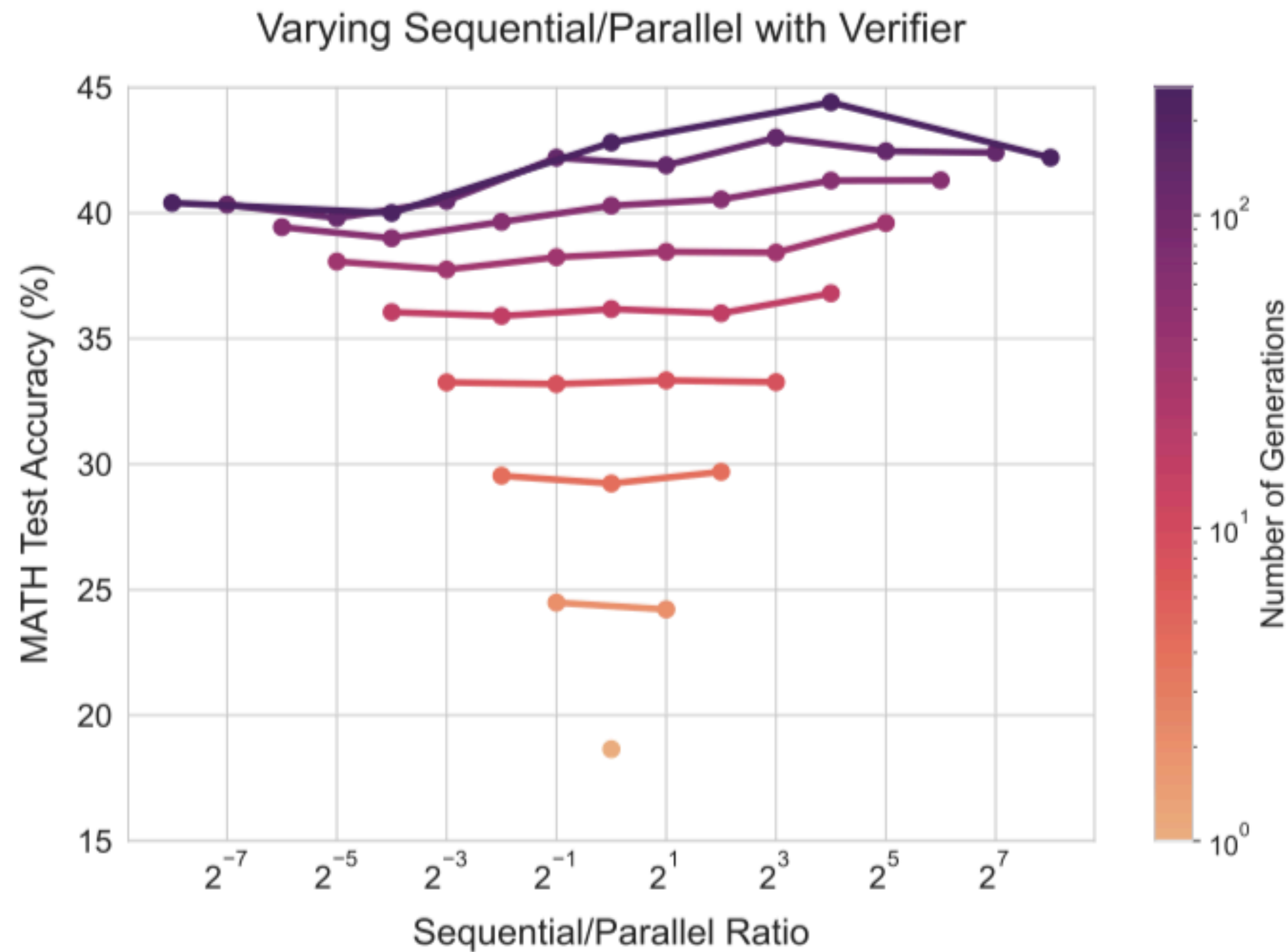
- Q: Do they have a separate revision model like the verifier model, or it is just the main model (= post-training)?

# Results: parallel vs sequential



- Using N sequential revisions is always better than N parallel samplings (when controlling # of generations)
- Q: What about FLOPs?

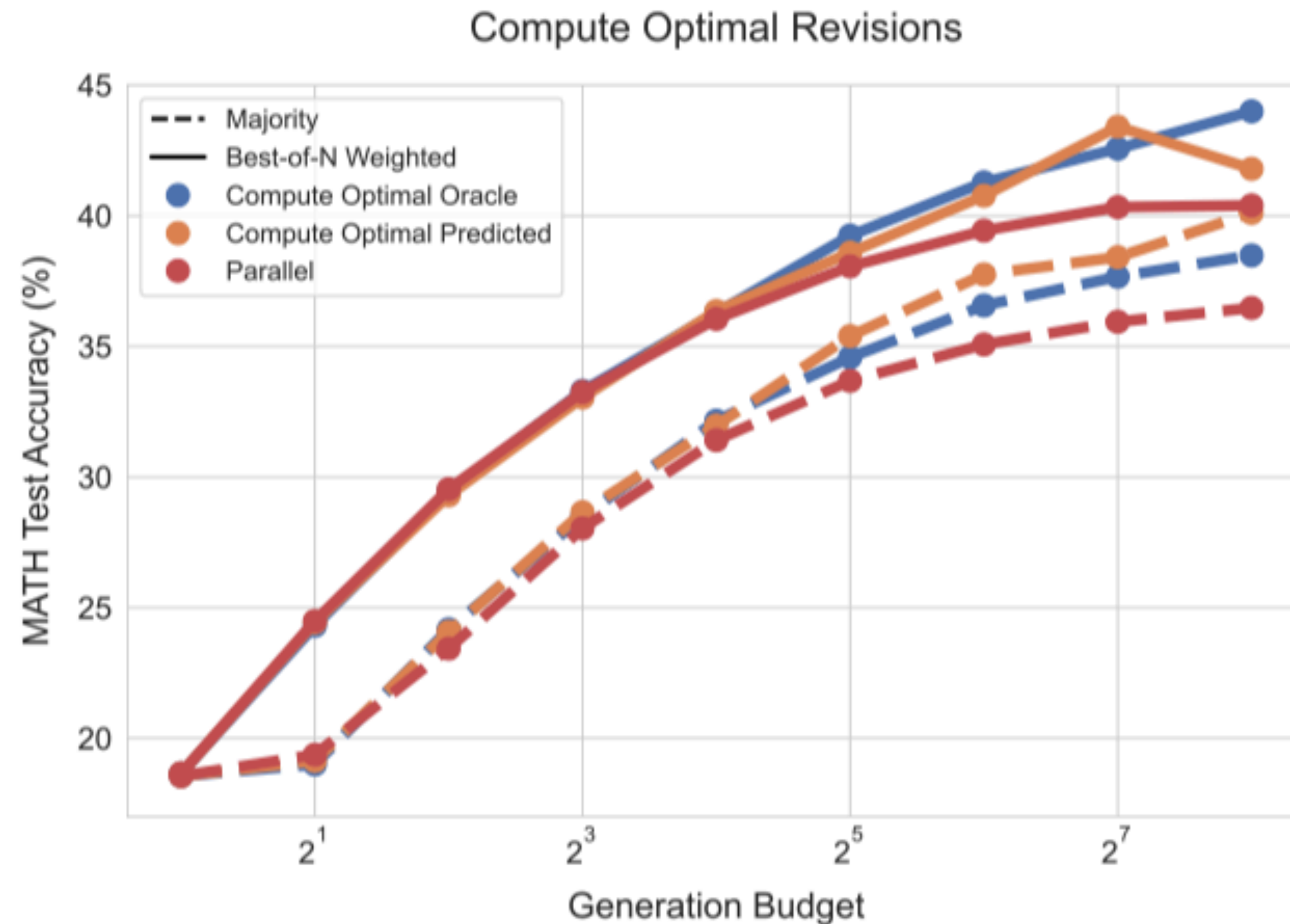
# Results: sequential-to-parallel ratio



- Difficult questions need more parallel computation



# Results: Adaptive compute-optimal strategy



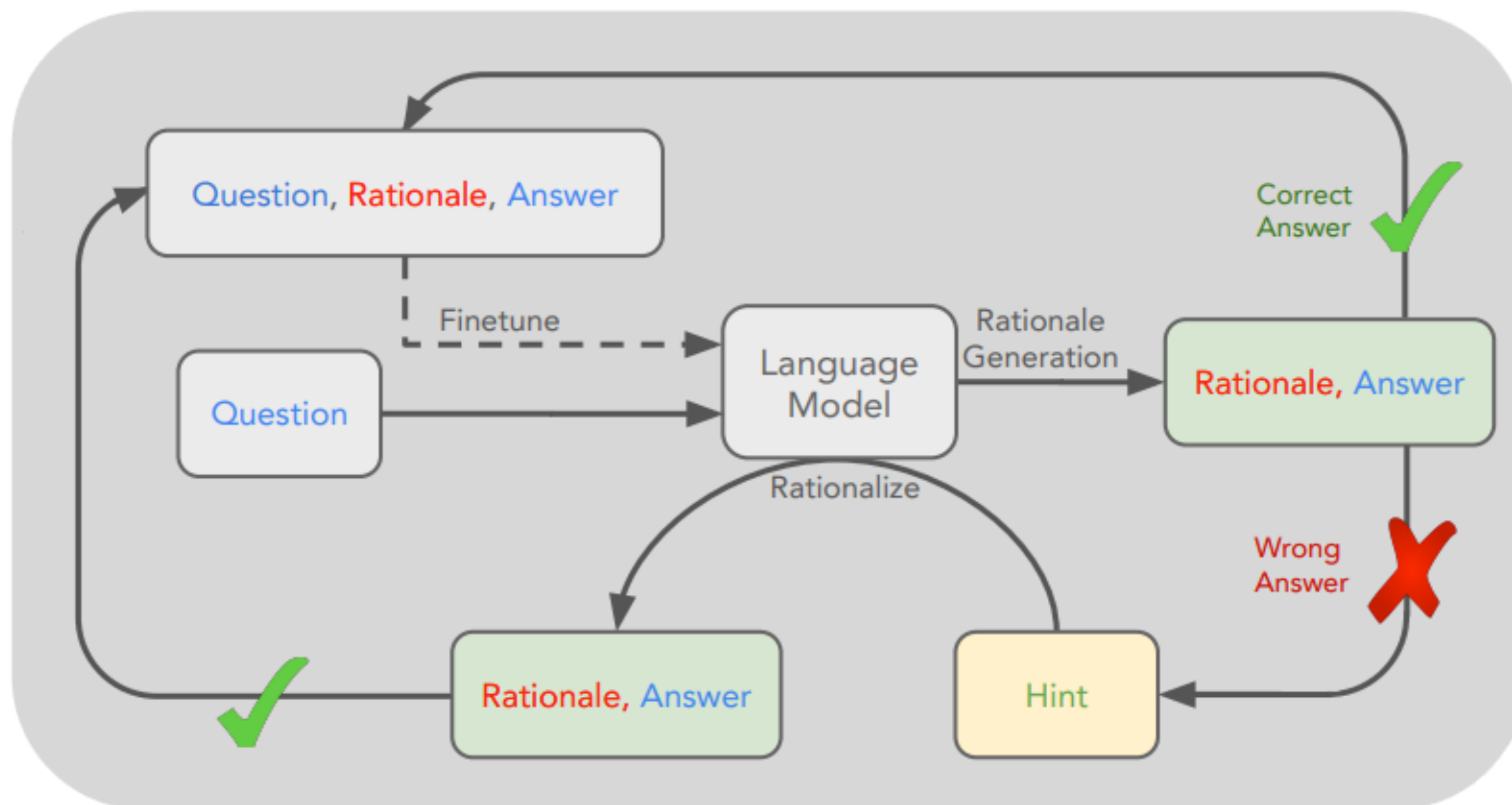
- The optimal test-time strategy should depend on question difficulty!
- Can outperform best-of-N up to 4x less test-time compute

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How to (post-)train LLMs for better reasoning?

# Self-Taught Reasoner (STaR)

## STaR: Self-Taught Reasoner Bootstrapping Reasoning With Reasoning



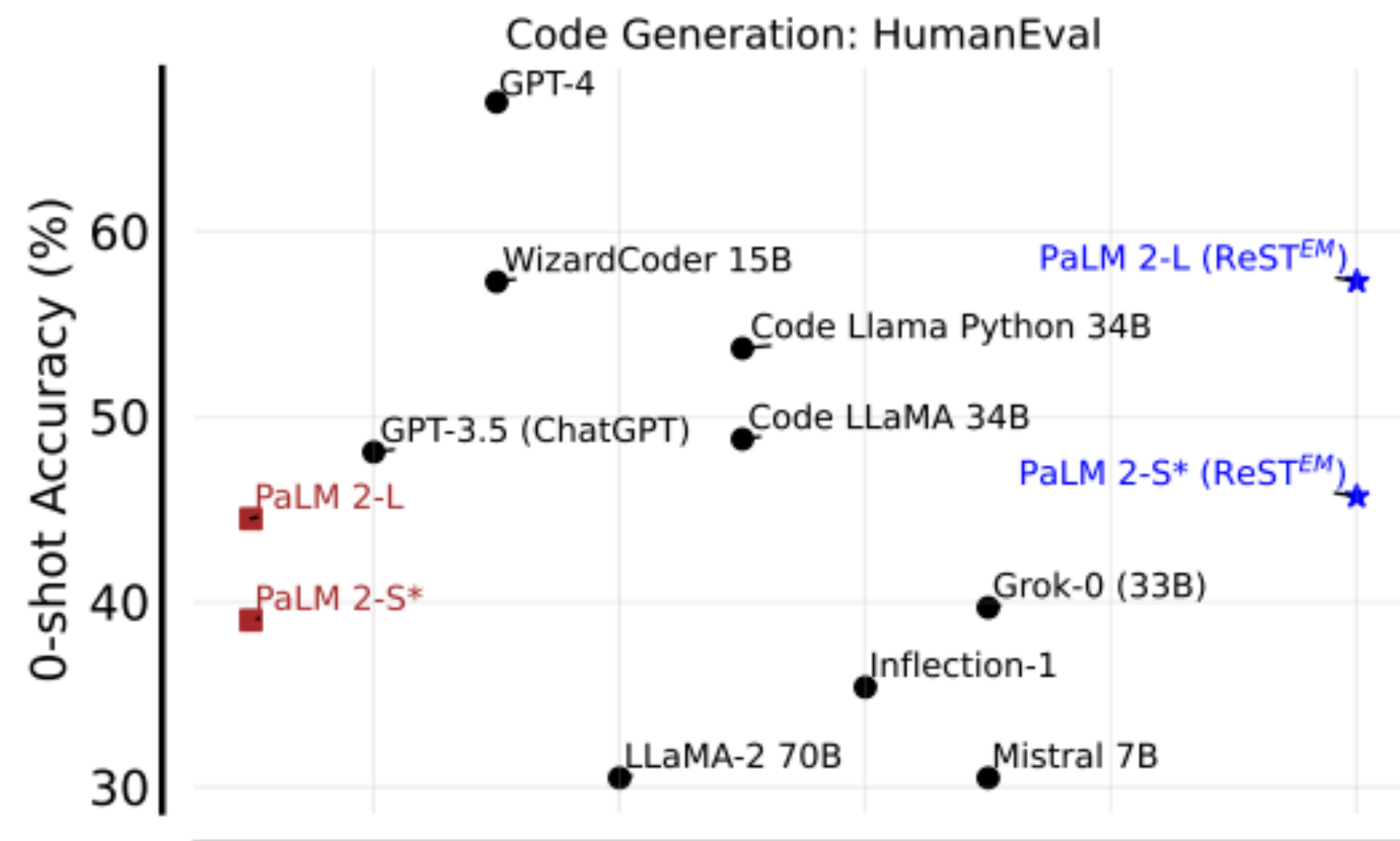
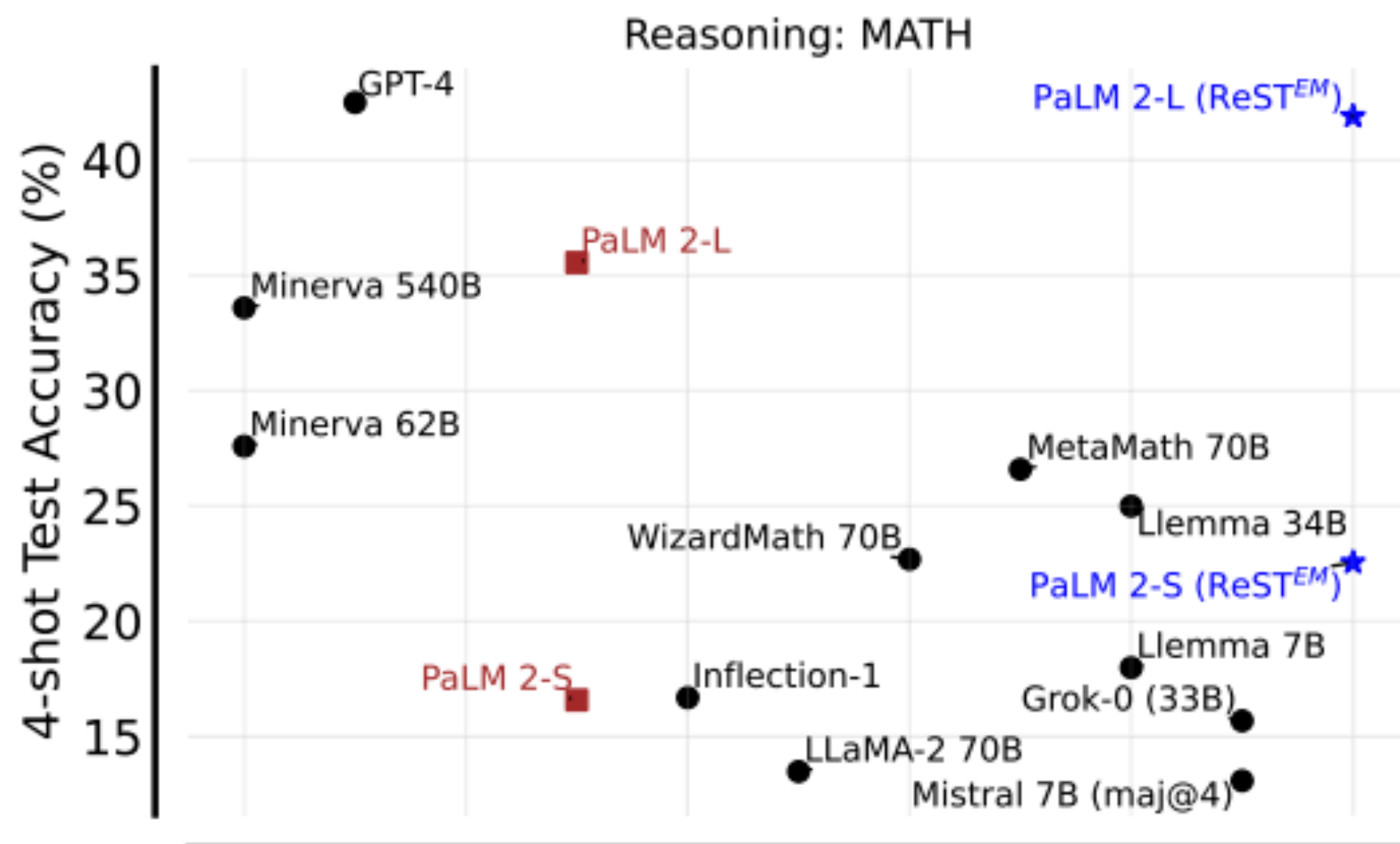
Q: What can be used  
to carry a small dog?  
Answer Choices:  
(a) swimming pool  
(b) basket  
(c) dog show  
(d) backyard  
(e) own home

A: The answer must be  
something that can be  
used to carry a small  
dog. Baskets are  
designed to hold things.  
Therefore, the answer  
is basket (b).

- Generate (rationale, answer)
- If answer is correct, add it back to the fine-tuning data

# Reinforced Self-training (ReST<sup>EM</sup>)

1. **Generate (E-step)**: The language model generates multiple output samples for each input context. Then, we filter these samples using a binary reward to collect the training dataset.
2. **Improve (M-step)**: The original language model is supervised fine-tuned on the training dataset from the previous **Generate** step. The fine-tuned model is then used in the next **Generate** step.





# Self-improvement and verification methods

Published as a conference paper at COLM 2024

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## V-STaR: Training Verifiers for Self-Taught Reasoners

METHOD	GENERATOR DATA	VERIFIER DATA	ITERATIVE
SFT	$\mathcal{D}_{\text{SFT}}$	$\times$	$\times$
VERIFICATION	$\mathcal{D}_{\text{SFT}}$	$\mathcal{D}_{\text{SFT}} \cup \text{GENERATED}$	$\times$
STAR	CORRECT GENERATED <sub><math>t-1</math></sub>	$\times$	$\checkmark$
RFT (STAR <sup>†</sup> [1 ITER])	$\mathcal{D}_{\text{SFT}} \cup \text{CORRECT GENERATED}$	$\times$	$\times$
STAR <sup>†</sup>	$\mathcal{D}_{\text{SFT}} \cup \text{CORRECT GENERATED}_{<t}$	$\times$	$\checkmark$
V-STAR [1 ITER]	$\mathcal{D}_{\text{SFT}} \cup \text{CORRECT GENERATED}$	$\mathcal{D}_{\text{SFT}} \cup \text{GENERATED}$	$\times$
<b>V-STAR</b>	<b><math>\mathcal{D}_{\text{SFT}} \cup \text{CORRECT GENERATED}_{&lt;t}</math></b>	<b><math>\mathcal{D}_{\text{SFT}} \cup \text{GENERATED}_{&lt;t}</math></b>	<b><math>\checkmark</math></b>

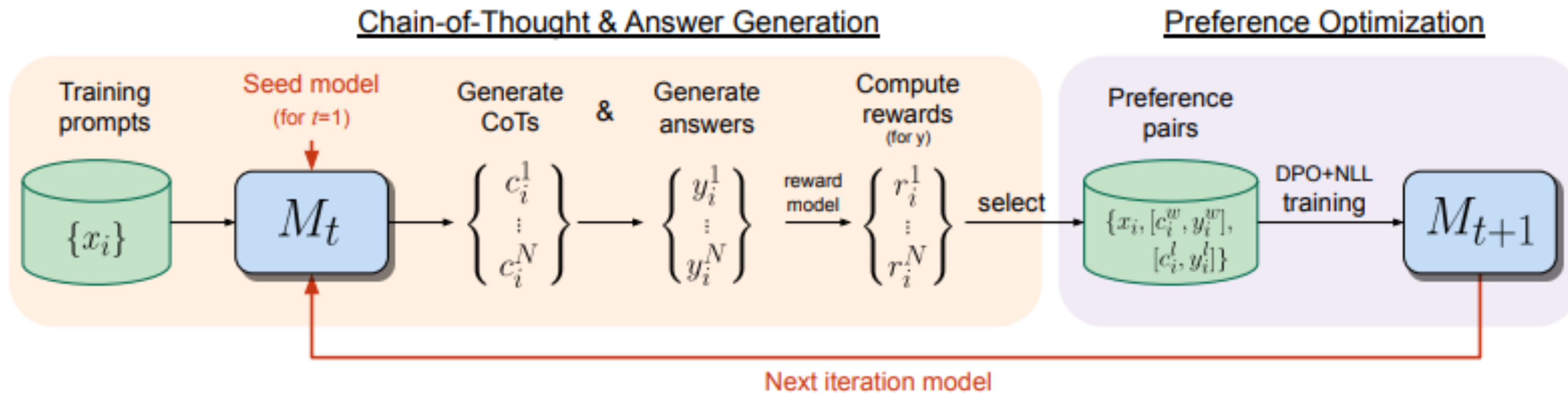
# Preference optimization for reasoning

## Iterative Reasoning Preference Optimization

Richard Yuanzhe Pang<sup>1,2</sup> Weizhe Yuan<sup>1,2</sup> Kyunghyun Cho<sup>2</sup>  
He He<sup>2</sup> Sainbayar Sukhbaatar<sup>1\*</sup> Jason Weston<sup>1,2\*</sup>

<sup>1</sup>FAIR at Meta

<sup>2</sup>New York University



# Final thoughts



Image: Jim Fan

- How do any of these findings generalize beyond a single task?
- Post-training: any generic solutions? What data to use?