Speculations on Test-Time Scaling

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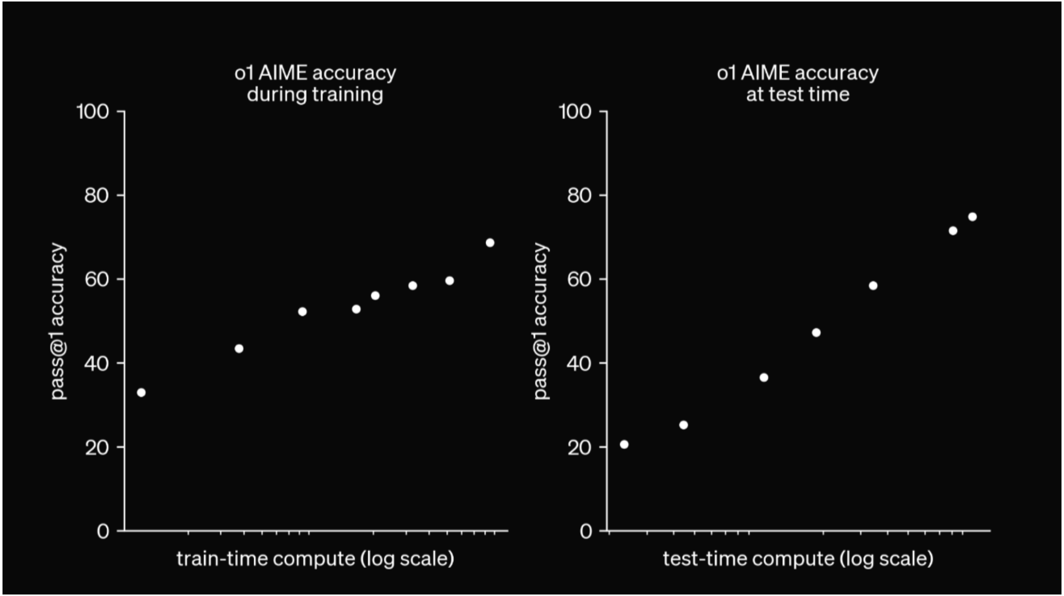
LLM (2018-2024) driven by training scaling

Speculation: Benefit of static data running out

o1 - Large-scale RL Training leading to search usage.



o1 AIME accuracy during training

o1 AIME accuracy at test time

Noam

This Talk

- Survey of the public literature
- Synthesis of discussions with expert
- Discussions (thx Lewis Tunstall, Edward Beeching, Aviral Kumar, Charlie Snell, Michael Hassid, Yoav Artzi, Risab Agarwal, Kanishk Gandhi, Wenting Zhao, Yuntian Deng, Nathan Lambert)

What we know

Our large-scale **reinforcement learning algorithm** teaches the model how to think productively using its **chain of thought** in a highly **data-efficient** training process.

What we know

- RL; Signal from verifiable problems

- CoT; “Thinking” occurs in token stream

- Data Efficient; Fixed set of good problems

From Gossip

- Single final model
- Not learned from expert examples

Chain of Thought

o1 learns to hone its chain of thought and refine the strategies it uses. It learns to recognize and **correct its mistakes**. It learns to **break down tricky steps** into simpler ones. It learns to try a **different approach** when the current one isn’t working.

Review: Chain of Thought

- In the process of answering a question, the model can generate a chain of intermediate steps.

- These steps provide a scratchpad for working on hard problems.

- OpenAI provided a limited number of examples.

o1 CoT: Outlining

Implementation Outline:

1. Capture input string as argument.
2. Remove any spaces (if any).
3. Parse the input string to extract numbers into arrays.

- Since the input is in the format ’[1,2],[3,4],[5,6]’, we can:
- Remove outer brackets if necessary.
- Split the string by ’],’ to get each row.
- For each row, remove ’[’ and ’]’, then split by ’,’ to get elements.

4. Build a 2D array in bash (arrays containing arrays).

o1 CoT: Planning

First, the cipher seems connected to the plaintext.
Given the time constraints, perhaps the easiest way is to try to see patterns.
Option 1: Try to find mapping from letters to letters.
Do any letters match?
First, let's write down the ciphertext and plaintext letters on top of each other.

o1 CoT: Backtracking

Similarly, m(x)⍰(−x2) = (−x2n + 2 + m2n−2x2n +lower terms)m(x)⍰(−x 2) = (−x 2n + 2 + m 2n−2x 2n +lower terms). Wait, actually, this may not help us directly without specific terms.An alternative is to consider the known polynomials. So m(x) = k …

o1 CoT: Self-Evaluation

Let's analyze each option.
Option A: "because appetite regulation is a field of staggering complexity."
Is that a good explanation? Hmm.
Option B: "because researchers seldom ask the right questions."
Does this make sense with the main clause?

Summary

- Solves problems by very long CoT
- CoT includes “thinking” (search / planning)
- Core novelty: Inducing this behavior

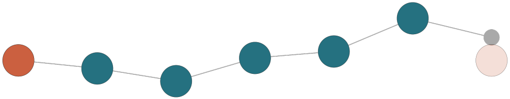
Notation: LLM Sampling (No learning yet!)

- x; problem specification
- $z_{1:T} \in \mathcal{S}^T$; chain of thought (CoT) stepsl
- $y \in \mathcal{Y}$; final answer

$$p(y|x) = \mathbb{E}_z p(y|x, z)$$

Warm-up: Ancestral Sampling

$$z_{1:T} \sim p(\cdot | x)$$
$$y \sim p(\cdot | x, z_{1:T})$$



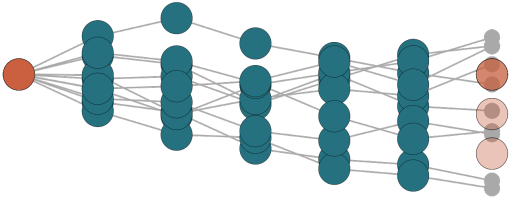
T is the amount of test-time compute

Warm-up: Monte-Carlo (Self-Consistency)

For N samples,

$$z_{1:T} \sim p(\cdot|x)$$
$$y^n \sim p(\cdot|x, z_{1:T})$$

Pick majority choice y^n



Assumption: Verifier

$$\text{Ver}_x : \mathcal{Y} \to \{0, 1\}$$

Examples:

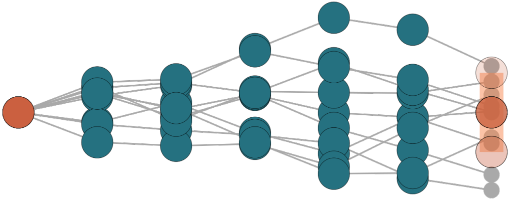
- Regular expression for math
- Unit test for code
- Test questions for science

Warm up: Rejection Sampling / Best-of-N

For $n = 1$ to N:

$$z^n \sim p(z|x)$$
$$y^n \sim p(y|x, z^n)$$

Verified set $\{y^n : \text{Ver}(y^n)\}$

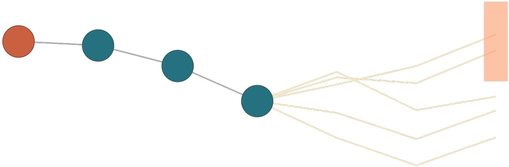


Warm up: Monte-Carlo Roll-Outs

Given partial CoT $z_{1:t}$, expected value,

$$\mathbb{E}_{y \sim p(y|z,x), z_{t:T}} \text{Ver}(y)$$

Rollout = Monte Carlo for this expectation.



Goal: Learning with Latent CoTs

Maximum likelihood;

$$\max_{\theta} \sum \log p(y|x;\theta) = $$
$$\sum \log \mathbb{E}_z p(y|x, z; \theta)$$

Classic combinatorial expectation

Outline

Introduction

The Clues

Warm-Up

The Suspects

What do we do now?

The Suspects

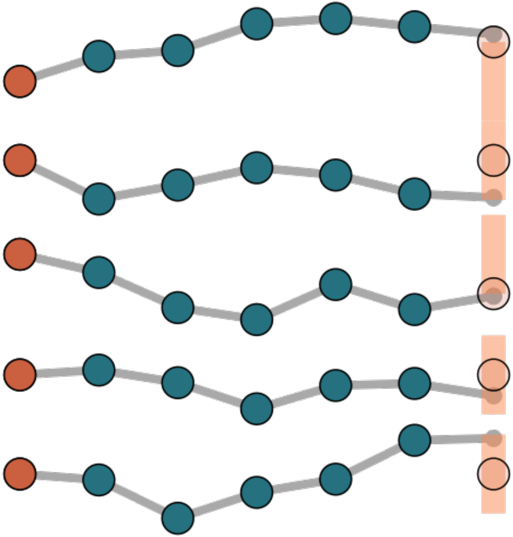
- Guess + Check
- Guided Search
- AlphaZero
- Learn to Search

Suspect 1: Guess + Check

- 1) Sample N CoTs

- 2) Check if successful

- 3) Train on good ones



G+C Formalization: Rejection Sampling EM

$$\max_{\theta} \sum \log E_{z \sim p(z|x;\theta)} p(y|x, z)$$

- E-Step: For $n = 1$ to N:

$$z^n \sim p(\cdot|x)$$
$$y^n \sim p(\cdot|x, z^n)$$

  Keep verified set $\mathcal{Z} = \{z^n : \text{Ver}(y^n)\}$

- M-Step: Fit $\theta' \leftarrow \arg\max_{\theta} \sum_{z \in \mathcal{Z}} \log p(z|x; \theta)$

G+C Variants

- STaR
- ReST
- ReST-EM
- Filtered Rejection Sampling
- Best-of-N Training

G+C Variants

- Batched -> Compute trajectories first, then train with behavioral cloning
- Online -> Use policy gradient-like steps to update after each example

G+C Empirical Results

[Singh et al., 2023]

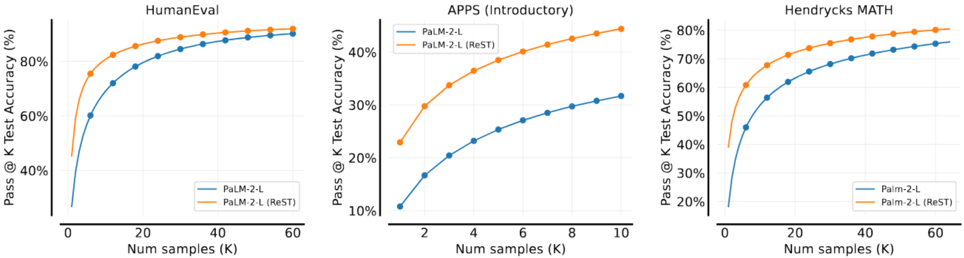


Figure 5 | **Pass@K results** for PaLM-2-L pretrained model as well as model fine-tuned with ReST^{EM}. For a fixed number of samples K, fine-tuning with ReST^{EM} substantially improves Pass@K performance. We set temperature to 1.0 and use nucleus sampling with $p = 0.95$.

G+C Why might this be right?

- Extremely simple and scalable

- Good baseline in past work

- No evidence this learns to correct, plan

- Well-explored in literature with marginal gains

More Structure?

- Rejection sampling may be really inefficient.

- Particularly on hard problems, may get no signal

Suspect 2: Guided Search

- During CoT sampling, use a heuristic to improve trajectories

- Check if final versions are successful

- Train on good ones

GS: Beam Search with Guide

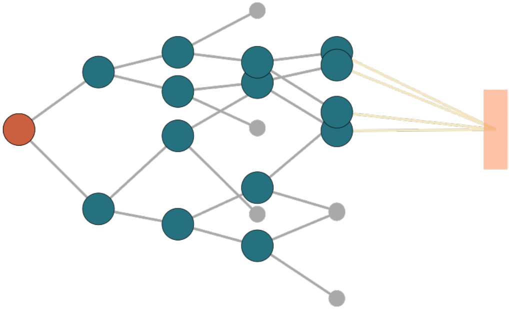
$r : \mathcal{S}^t \to \mathbb{R}$; Guide function

For each step t

1. Sample next step,

$$z_t \sim p(\cdot | x, z^i_{1:t-1})$$

2. Keep the top N samples, ordered by $r(z_t)$



What to use as Guide?

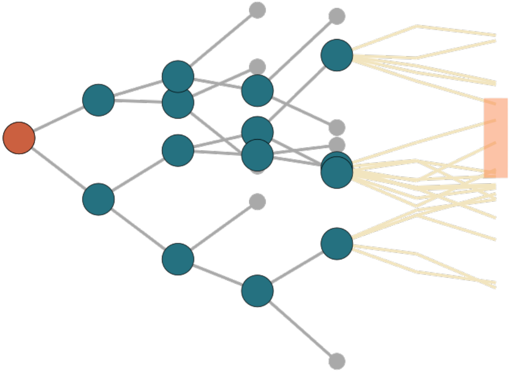
- Monte Carlo Roll-outs
- Learned Value Function
- Interleaved Value Function

Beam Search with Roll-Outs

For a z_t, sample answers

$$y^n \sim p(\cdot | x, z_{1:t-1})$$

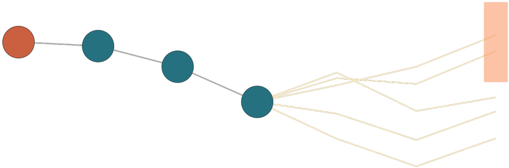
$$r_{MC}(z_t) = \frac{1}{N} \sum_{i=1}^{n} \text{Ver}(y^i)$$



Amortized Roll-Outs

[Wang et al., 2023]

- Rollouts are costly, so instead learn a model $r_\psi(z_t)$ to approximate rollouts
- Use r_{MC} to determine labels to train r_ψ



Interleaved

[Wang et al., 2023]

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What about test time?

- Learned rewards can improve test-time without verifier.
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Terminology

- Value
- PRM
- PAV
- Math Shepard.
- snell.

[Uesato et al., 2022, Setlur et al., 2024,
Wang et al., 2023, Lightman et al., 2023,
Snell et al., 2024]

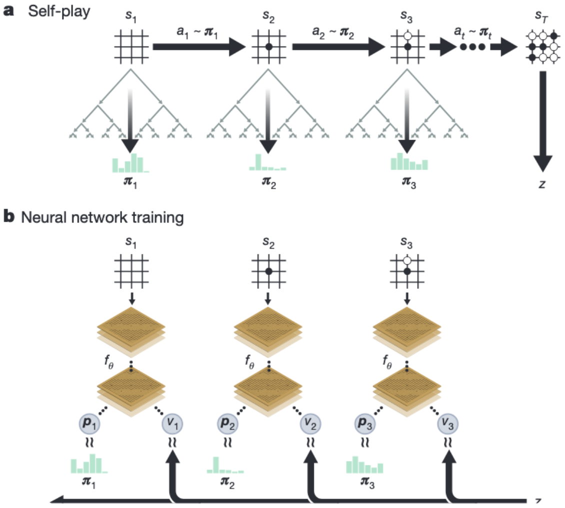
Why might this be right?

- OpenAI is exploring
- Makes RS more efficient.
- Learned rewards are effective
- Assumption: o1 is a single test-time model (although could train or distill-in)
- Not clear if it learns planning.

More Structure

- Improving search seems critical.

Reminder: AlphaZero



Suspect 3: AlphaZero

- Self-play using guided-search with exploration
- Label final outcomes of self-play games
- Train guide and generator

[Anthony et al., 2017]

Formalized: Expert Iteration

- Iterative algorithm combining learned model + expert search with a verifier.

- Generate samples using $p(y, z|x)$, reward model $r(z_t)$, and search algorithm (e.g. beam search)

- Label samples using $Ver(y)$

- Train $p(y, z|x)$, $r(z_t)$ on the labeled samples, and repeat

MCTS exploration

UCB for Language

- Selection: Walk down tree to leaf z_{t-1}
- Expand: Sample K next steps z_t^i, pick one at random
- Rollouts: Sample $z_{t+1} \ldots z_T$
- Backprop: Update nodes counts $z_{1:t}$ based on results

Compared with Search

- System builds in exploration
- Scales to more train-time search

- Costly to maintain open states
- More complex algorithmically

Empirical Results

[?]

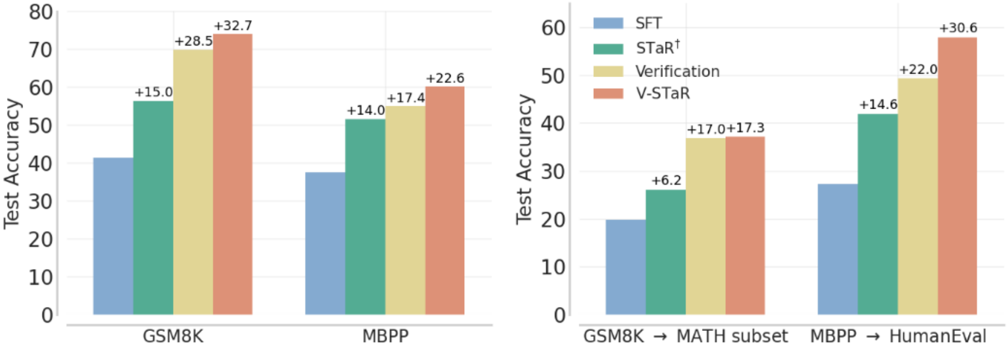


Figure 8: Test accuracy of 13B V-STaR compared to baselines. We report Best-of-64 for verification-based methods and Pass@1 for others. **(Left)** Test accuracy for training tasks. **(Right)** Transfer evaluation of GSM8K and MBPP trained models on MATH subset and HumanEval respectively.

Why might this be right?

- Major demonstrated RL result

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More Structure

- Can we force the model to search?

Suspect 4: Learning to Correct

- Sample N Successful CoTs
- Edit to inject incorrect expansions before correct ones.
- Train on correcting trajectories

Self-Correction

- Argument: Training on x, z_1^*, y is too easy.
- Train instead on x, z', z_1^*, y
- Model should learn to self-correct

Score

- Positive rewards

Challenge: Collapse

- Model may learn to just ignore negative
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[Gandhi et al., 2024]

Generalized: Stream of Search

- Find $z^*_{1:T}$ as optimal length CoT
- Find $z'_{1:T'}$ with $T' > T$ through backtracking tree search
- Train model on $z'_{1:T'}$

From Tree to Stream

Empirical Results

Score results

Why might this be right?

Less Structure?

- Maybe this is all too much…
- Could this be done without a verifier?

Outline

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What do we do now?

Replication

Does it need to be the same?

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