Speculations on Test-Time Scaling

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Cornell - Hugging Face

[\[Brown et al., 2020\]](#page-99-0)

[\[OpenAI, 2024\]](#page-105-0)

AIME

For any finite set X, let $|X|$ denote the number of elements in X. Define

$$
S_n = \sum |A \cap B|,
$$

where the sum is taken over all ordered pairs (A, B) such that A and B are subsets of $\{1, 2, 3, \dots, n\}$ with $|A| = |B|$. For example, $S_2 = 4$ because the sum is taken over the pairs of subsets

 $(A, B) \in \{(\emptyset, \emptyset), (\{1\}, \{1\}), (\{1\}, \{2\}), (\{2\}, \{1\}), (\{2\}, \{2\}), (\{1, 2\}, \{1, 2\})\}$ giving $S_2 = 0 + 1 + 0 + 0 + 1 + 2 = 4$. Let $\frac{S_2022}{S_2021} = \frac{p}{q}$ $\frac{p}{q}$, where p and q are relatively prime positive integers. Find the remainder when $p + q$ is divided by 1000.

[\[Sutton, 2019\]](#page-106-0)

The Bitter Lesson

The bitter lesson is based on the historical observations that 1) AI researchers have often tried to build knowledge into their agents, 2) this always helps in the short term, and is personally satisfying to the researcher, but 3) in the long run it plateaus and even inhibits further progress, and 4) breakthrough progress eventually arrives by an opposing approach based on scaling computation by **search and learning**.

Importance of Search

[\[Brown and Sandholm, 2017\]](#page-98-0),[https:](https://x.com/polynoamial/status/1840822629625688469) [//x.com/polynoamial/status/](https://x.com/polynoamial/status/1840822629625688469) [1840822629625688469](https://x.com/polynoamial/status/1840822629625688469)

The most important [lesson] is that I and other researchers simply didn't know how much of a difference scaling up search would make. If I had seen those scaling results at the start of my PhD, I would have shifted to researching search algorithms for poker much sooner and we probably would have gotten superhuman poker bots much sooner.

Scaling Laws for Board Games [\[Jones, 2021\]](#page-102-0)

Fig. 9. The trade-off between train-time compute and test-time compute. Each dotted line gives the minimum train-test compute required for a certain Elo on a 9×9 board

Search Against Learned Verifiers [\[Cobbe et al., 2021\]](#page-99-1)

$\circled{3}$ \bigcap $\left(2\right)$ Generate and label Train generator **Train Verifier** 100 solutions/problem Generator Generator Verifier Q_i questions S_i S_i S_i^j solutions Q_i S_i^1 Y_i^1 Q_i^j Y_i^j Y_i S^2_i Y_i^2 labels Q_i S_i^{100} $V100$

Figure 4: A diagram of the verification training pipeline.

Search Against Learned Verifiers [\[Cobbe et al., 2021\]](#page-99-1)

Sources

- Synthesis of discussions with expert
- Survey of the public literature
- Rumors from social media

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[\[OpenAI, 2024\]](#page-105-0)

o1 Description

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.

Implication

- RL; Signal from verifiable problems
- CoT; Test-time occurs in token stream
- Data-Efficient; Bounded set of problems

Current Assumptions

- Single final language model with coherent CoT
- Not following from expert examples
- Behaviors are learned

Review: Chain of Thought

[\[Wei et al., 2022,](#page-108-0) [Nye et al., 2021\]](#page-104-0)

- The model generates intermediate steps.
- These steps provide an scratchpad for technical problems.

Question: 4 baskets. 3 have 9 apples, 15 oranges, 14 bananas each. 4th has 2 less of each. Total fruits? Let's solve step-by-step: Fruits in one of first 3 baskets: $9 + 15 +$ $14 = 38$ Total in first 3 baskets: $38 * 3 = 114$ 4th basket: (9-2) + (15-2) + (14-2) = 32 Total fruits: 114 + 32 = 146

Answer: 146 fruits

[\[OpenAI, 2024\]](#page-105-0)

o1 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.

o1 CoT: Outlining

Implementation Outline:

- *1. Capture input string as argument.*
- *2. Remove any spaces (if any).*
- *3. Parse input string to extract numbers as arrays.*
- *Since the input is in the format '[1,2],[3,4]', 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) (−x 2) = (−x2n + 2 + m2n−2x2n + lower terms)m(x) * (−x 2) = (−x 2n + 2 + m 2n−2 x 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?

- CoT provides test-time scaling
- CoT looks like search / planning in a classical sense
- RL needed to induce this behavior

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[\[Cobbe et al., 2021\]](#page-99-1)

Technical Background

- Formalize sampling of latent reasoning
- No learning yet.

Question: 4 baskets. 3 have 9 apples, 15 oranges, 14 bananas each. 4th has 2 less of each. Total fruits?

- 1 Let's solve step-by-step:
- 2 Fruits in one of first 3 baskets: 9 + 15 $+ 14 = 38$
- 3 Total in first 3 baskets: 38 * 3 = 114
- 4 4th basket: $(9-2) + (15-2) + (14-2) =$ 32
- 5 Total fruits: 114 + 32 = 146

Answer: 146 fruits

[\[Welleck et al., 2024\]](#page-108-1)

Stepwise CoT Sampling

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

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

[\[Wei et al., 2022\]](#page-108-0)

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

[\[Wang et al., 2022\]](#page-107-0)

Self-Consistency / Majority Vote

For N samples,

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

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

Pick majority choice y^n

Assumption: Automatic Verifier at Training IUesato et al., 2022]

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

Common datasets:

- Regular expression for math [\[Cobbe et al., 2021\]](#page-99-1)
- Unit test for code [\[Hendrycks et al., 2021a\]](#page-101-1)
- Test questions for science [\[Hendrycks et al., 2021b\]](#page-101-2)

Automatic Verifier?

[\[Cobbe et al., 2021,](#page-99-1) [Lightman et al., 2023\]](#page-103-0)

- OpenAI primarily interested in learned verifiers (ORM)
- Spec: Large-scale annotation of on-policy outputs

6B verification test performance (a) when given varying numbers of completions per problem to rank.

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 $\{y^n : \mathsf{Ver}_x(y^n)\}$

[\[Nakano et al., 2021,](#page-104-1) [Lightman et al., 2023\]](#page-103-0)

[\[Wang et al., 2023\]](#page-107-2)

Monte-Carlo Roll-Outs

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

$$
\mathbb{E}_{y \sim p(\cdot|x)} \mathsf{Ver}(y)
$$

Monte Carlo for this expectation.

Goal: Learning with Latent CoTs

Maximum likelihood;

$$
\max_{\theta} \sum \log p(\text{Ver}(y)|x;\theta) =
$$

$$
\sum \log \mathbb{E}_{z} p(\text{Ver}(y)|x,z;\theta)
$$

Classic combinatorial expectation

Reinforcement Learning

Important practical choices:

- Batched? \rightarrow Compute trajectories first, then train
- On-policy? \rightarrow Sample from current model
- KL Constraints on learning.
- Specific algorithm choice (REINFORCE, PPO, etc)

When training a model for reasoning, one thing that immediately jumps to mind is to have humans write out their thought process and train on that. When we saw that if you train the model using RL to generate and hone its own chain of thoughts it can do even better than having humans write chains of thought for it. That was the "Aha!" moment that you could really scale this. [tEzs3VHyBDM](https://www.youtube.com/watch?v=tEzs3VHyBDM)

[https://www.youtube.com/watch?v=](https://www.youtube.com/watch?v=tEzs3VHyBDM)

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The Suspects

- \bullet Guess + Check
- Process Rewards
- Search / AlphaZero
- Learning to Correct

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Suspect 1: Guess + Check

- 1) Sample N CoTs
- 2) Check if successful
- 3) Train on good ones

[\[Neal and Hinton, 1998\]](#page-104-0)

Framework: Rejection Sampling EM

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

• E-Step: For $n = 1$ to N:

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

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

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

Variants

- Self-Training [\[Yarowsky, 1995\]](#page-109-0)
- Best-of-N Training [\[Cobbe et al., 2021\]](#page-99-0)
- STaR [\[Zelikman et al., 2022\]](#page-109-1)
- ReST [\[Gulcehre et al., 2023\]](#page-100-0)
- ReST-EM [\[Singh et al., 2023\]](#page-106-0)
- Filtered Rejection Sampling [\[Nakano et al., 2021\]](#page-104-1)

Empirical Results Empirical Results

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 $p = 0.95$.

Learned Verifier

- Ver available only at train
- Samples can be used to further train a learned verifier (amortization)
- Can be used for test-time rejection sampling.

Is this o1?

Pro

- \checkmark Extremely simple and scalable
- $\sqrt{ }$ Positive results in past work

Is this o1?

Pro

- $\sqrt{}$ Extremely simple and scalable
- $\sqrt{ }$ Positive results in past work
- \times No evidence this learns to correct, plan
- \times Computationally inefficient search

The Suspects

- Guess + Check
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Suspect 2: Process Rewards

- 1) During CoT sampling, use guidance to improve trajectories
- 2) Check if final versions are successful
- 3) Train on good ones

Process Rewards

[\[Uesato et al., 2022,](#page-107-0) [Lightman et al., 2023\]](#page-103-0)

• Early learned verification (PRM) improves over learned verification (ORM)

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

Learned Process Rewards

[\[Lightman et al., 2023,](#page-103-0) [Wang et al., 2023\]](#page-107-1)

- Rollouts are costly / require Ver
- Learn $r_{\psi}(z_t)$ to approximate
- Use Monte-Carlo for labels

Generative Verifiers

[\[Zhang et al., 2024,](#page-110-0) [Ankner et al., 2024\]](#page-98-0)

- Define $r_{\psi}(z_t)$ as an LLM
- Merges process reward with generation
- Note: allows for verification CoT

Open Process Rewards [\[Wang et al., 2023\]](#page-107-1)

Figure 3: Performance of LLaMA2-70B using different verification strategies across different numbers of solution candidates on GSM8K and MATH.

Incorporating at Test-Time

- Process Reward does not need Ver can be used at test-time.
- If generative, can be merge into a singel CoT stream

Let's analyze each option.

Option A: "because appetite regulation is a field of staggering complexity."

Is that a good explanation? Hmm.

Is this o1?

- $\sqrt{ }$ Intermediate guides are effective
- $\sqrt{\ }$ Removes challenges of full learned verifier

Is this o1?

- $\sqrt{ }$ Intermediate guides are effective
- $\sqrt{\ }$ Removes challenges of full learned verifier
- \times Not clear if this is enough for planning.
- \times Need to combine generator / guide into one $C₀$ T

The Suspects

- \bullet Guess + Check
- Process Rewards
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[\[Silver et al., 2017\]](#page-105-0)

Reminder: AlphaZero

- Canonical example of self-learning
- Scaling model without data

[\[Silver et al., 2017\]](#page-105-0)

AlphaProof

When presented with a problem, AlphaProof generates solution candidates and then proves or disproves them by searching over possible proof steps in Lean. Each proof that was found and verified is used to reinforce AlphaProof's language model, enhancing its ability to solve subsequent, more challenging problems.

Suspect 3: AlphaZero

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

Framework: Expert Iteration

- Iterative algorithm combining learned model + expert search with a verifier.
- Generate samples using $p(y, z|x)$, reward model $q(z_t)$, and search algorithm (e.g. beam search)
- Label samples using $\textsf{Ver}_x(y)$
- Train $p(y, z|x)$, $r(z_t)$ on the labeled samples, and repeat

Framework: Beam Search with Guide

$$
r: \mathcal{S}^t \rightarrow \mathbb{R}
$$

[\[Snell et al., 2024\]](#page-106-1)

Framework: Beam Search with Guide

$$
r: \mathcal{S}^t \rightarrow \mathbb{R}
$$

For each step t ,

1. Sample many next steps,

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

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

Beam Search with Roll-Outs

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

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

Beam Search with Roll-Outs

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y^n \sim p(\cdot | x, z_{1:t-1})
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r_{MC}(z_t) = \frac{1}{N} \sum_{n=1}^{N} \text{Ver}(y^n)
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$$

Empirical Results: Expert Iteration [\[Hosseini et al., 2024\]](#page-102-0)

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.

MCTS for Language

[\[Hubert et al., 2021,](#page-102-1) [Feng et al., 2023\]](#page-100-1)

- Selection: Walk down tree to leaf z_{t-1}
- $\bullet\,$ **Expand**: Sample ~ 5 next steps z_t , pick one at random
- **Rollouts:** Sample steps $z_{t+1} \ldots z_T$
- **Backprop:** Update nodes counts $N(z_{1:i})$ and wins $w(z_{1:i})$ for parents

Generalization: MCTS

Generalization: MCTS

Generalization: MCTS

Exploration

• MCTS-UCB explores states based on wins and amount of explorations

$$
\frac{w(z_{1:t})}{N(z_{1:t})} + \alpha \sqrt{\frac{\ln N(z_{1:t-1})}{N(z_{1:t})}}
$$

• Less strict search process

Learning from Search

[\[Xie et al., 2024,](#page-109-0) [Putta et al., 2024\]](#page-105-0)

- MCTS tree provides path preferences
- Can be used for preference learning (e.g. DPO)
- Alternative to learning on chains

Is this o1?

- $\sqrt{ }$ Major demonstrated RL result
- \checkmark Scales to more train-time search

Is this o1?

- $\sqrt{ }$ Major demonstrated RL result
- $\sqrt{\ }$ Scales to more train-time search
- \times Costly to maintain open states
- \times More complex algorithmically
- \times OpenAI comments / rumors

The Suspects

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What does exploration look like?

- Game Playing Explore alternative moves.
- Language Nearly infinite "moves"
- Exploration to learn strategies

Suspect 4: Learning to Correct

- 1) Start with failed CoT
- 2) Search to find successful corrections
- 3) Train on full CoT

[\[Welleck et al., 2022\]](#page-108-0)

Framework: Self-Correction

- Aim: Find similar CoT pairs z', z'' where z'' is better.
- Train the model to improve upon z'

Challenges: Learning Correction

- Collapse: Model may learn to just ignore negative
- Distribution Shift: Actual mistakes may deviate from examples

RL from Mistakes

[\[Gandhi et al., 2024\]](#page-100-0)

- Start with z'
- Learn to correct from verifier

Empirical Results

Figure 1 | Left: SCoRe achieves state-of-the-art self-correction performance on MATH; Right: SCoRe inference-time scaling: spending samples on *sequential* self-correction becomes more effective than only on *parallel* direct samples (Section 6.2).

[\[Gandhi et al., 2024\]](#page-100-0)

Generalization: Stream of Search

- Find z_1^* $_{1:T}^{\ast}$ as optimal length CoT
- Find $z'_{1:T'}$ with $T' > T$ through backtracking tree search
- Train model on z_1' $1:T'$

From Tree to Stream

- Tree search explores multiple paths
- Stream presents a linear sequence
- Allows model to mistakes in stream

Is this o1?

\checkmark Learns to correct and plan

 \checkmark Single test-time model

Is this o1?

- $\sqrt{}$ Learns to correct and plan
- \checkmark Single test-time model

 \times Complex training process

 \times Limited empirical evidence

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Replication

- Critical to have open-source versions
- Systems aspects are different
- Versions may not look the same

• Beyond Emergent Ablities

- Beyond Emergent Ablities
- Inference Time Systems

- Beyond Emergent Ablities
- Inference Time Systems
- From Prompting to Specification

- Beyond Emergent Ablities
- Inference Time Systems
- From Prompting to Specification
- Evaluations Need to Be Much Harder

- Beyond Emergent Ablities
- Inference Time Systems
- From Prompting to Specification
- Evaluations Need to Be Much Harder
- CoT Change Interpretability

Thank You

<https://github.com/srush/awesome-o1>

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