Tutorial: Test-Time Scaling for Mathematical Reasoning

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May 28, 2025

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Today's talk

Algorithms for generating outputs with a language model

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Algorithms for generating outputs with a language model

Why? Use **test-time compute** to improve performance

Language models

Al achieves silver-medal standard solving International Mathematical Olympiad problems
23 JULY 2004 AlphaProof and AlphaGasmentry teams

Solving olympiad problems

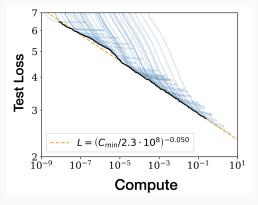


Writing code

Tasks framed as generating sequences: many other applications

Approach 1: scale pretraining compute

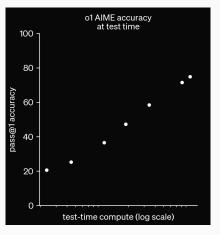
[2020-] Scale training-time compute: larger model, larger dataset



Scaling Laws for Neural Language Models [Kaplan et al., 2020]

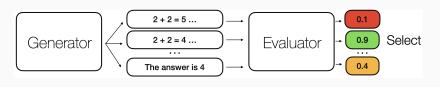
Approach 2: scale test-time compute

[Now] **Test-time scaling:** increase compute at generation time

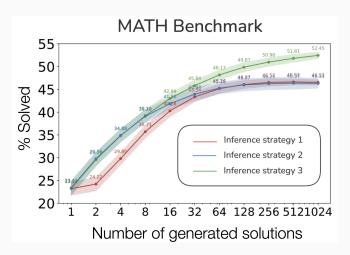


Test-time compute vs. accuracy ([OpenAI, 2024])

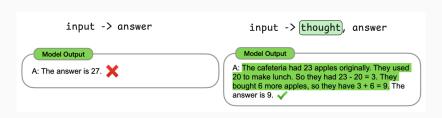
1. Generate multiple times



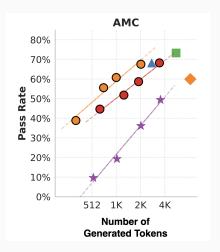
1. Generate multiple times

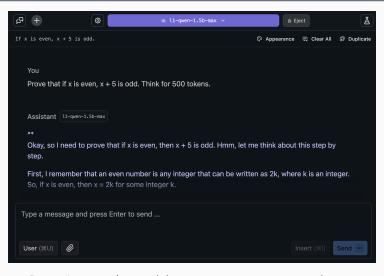


- 1. Generate multiple times
- 2. Generate longer outputs



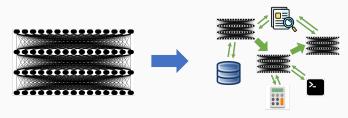
- 1. Generate multiple times
- 2. Generate longer outputs





Demo: L1 reasoning model [Aggarwal and Welleck, 2025] on a laptop

- 1. Generate multiple times
- 2. Generate longer outputs
- 3. Incorporate other models/tools



[Zaharia et al., 2024]

Verifiers, code interpreters, search engines, ...

Today's tutorial

- 1. Part 1: Generate multiple times
 - · Meta-generation: chain, parallel, refinement, tree search
- 2. Part 2: Generate longer outputs
 - Long chain-of-thought

Today's tutorial

- 1. Part 1: Generate multiple times
 - · Meta-generation: chain, parallel, refinement, tree search
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Recap: generation and decoding algorithms

Generator: Generates a sequence with a language model.

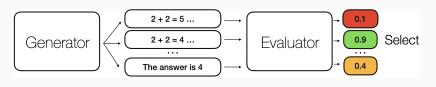


- · Example: calling an LLM API
- · Decoding algorithms
 - · Temperature sampling
 - ...

$$y \sim g(p_{\theta}, x; \phi)$$

Unified view: Meta-Generation

Meta-generator: Test-time strategies for calling a generator multiple times and incorporating external information¹

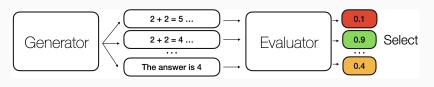


• Example: call API multiple times, select the best sequence with a separate model

¹From Decoding to Meta-Generation: Inference-time Algorithms for LLMs [Welleck et al., 2024]

Unified view: Meta-Generation

Meta-generator: Test-time strategies for calling a generator multiple times and incorporating external information¹



• Example: call API multiple times, select the best sequence with a separate model

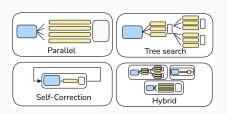
$$y \sim G(x, g; \Phi)$$

¹From Decoding to Meta-Generation: Inference-time Algorithms for LLMs [Welleck et al., 2024]

Meta-generators | outline

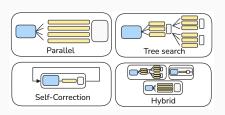
· Strategies

- · Parallel
- · Tree search
- · Refinement/self-correction
- · Chain (Part II)

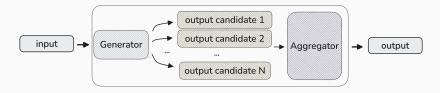


Meta-generators | outline

- Strategies
 - · Parallel
 - · Tree search
 - · Refinement/self-correction
 - · Chain (Part II)



Meta-generators | parallel



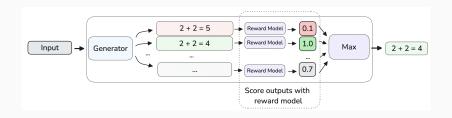
· Generate candidates:

$$\{y^{(1)}, \dots, y^{(N)}\} \sim G(\cdot | x)$$

· Aggregate:

$$y = h(y^{(1)}, \dots, y^{(N)})$$

Parallel | Best-of-N²



$$\underset{\{y^{(1)},...,y^{(N)}\}}{\operatorname{arg max}} \underbrace{v(y)}_{\text{reward model}}$$

²[Stiennon et al., 2020, Nakano et al., 2022]

Parallel | Best-of-N

Input: Let $f(r) = \sum_{j=2}^{2008} \frac{1}{j'} = \frac{1}{2^j} + \frac{1}{3^j} + \dots + \frac{1}{2008^l}$. Find $\sum_{k=2}^{\infty} f(k)$.

LLEMMA 34B solution:

We have

z:

$$\sum_{k=2}^{\infty} f(k) = \sum_{k=2}^{\infty} \sum_{j=2}^{2008} \frac{1}{j^k} = \sum_{j=2}^{2008} \sum_{k=2}^{\infty} \frac{1}{j^k} = \sum_{j=2}^{2008} \frac{1}{j^2} \sum_{k=0}^{\infty} \frac{1}{j^k} = \sum_{j=2}^{2008} \frac{1}{j^2} \frac{1}{1 - \frac{1}{j}}$$

$$= \sum_{j=2}^{2008} \frac{1}{j(j-1)} = \sum_{j=2}^{2008} \left(\frac{1}{j-1} - \frac{1}{j}\right)$$

$$= \left(\frac{1}{1} - \frac{1}{2}\right) + \left(\frac{1}{2} - \frac{1}{3}\right) + \dots + \left(\frac{1}{2007} - \frac{1}{2008}\right)$$

$$= 1 - \frac{1}{2008}$$

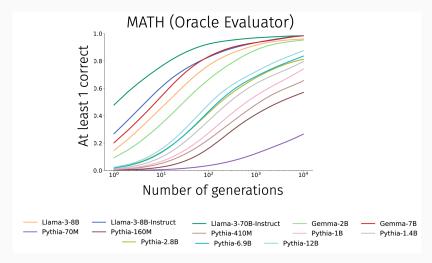
$$= \frac{2007}{2008}.$$

y:

Final Answer: The final answer is $\frac{2007}{2008}$.

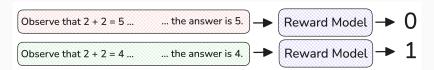
Example: solve a math problem

What if we had a perfect reward model $v^*(y)$?



[Brown et al., 2024]

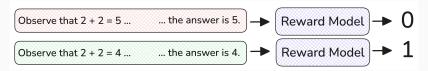
"Outcome reward model" $v(y) \rightarrow [0,1] \approx R(y)$:



Train reward model with correct and incorrect examples.³

³E.g., [Cobbe et al., 2021]

"Outcome reward model" $v(y) \rightarrow [0,1] \approx R(y)$:

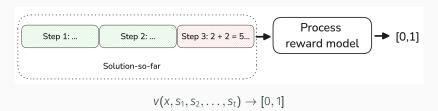


Train reward model with correct and incorrect examples.³

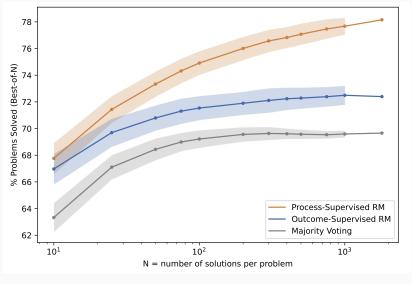
Terminology: Reward model pprox evaluator pprox critic pprox verifier pprox value pprox scoring model

³E.g., [Cobbe et al., 2021]

"Process reward model (PRM)"4



⁴[Uesato et al., 2022, Lightman et al., 2024, Wang et al., 2024a]



Lightman et al 2023

Note: Preference reward model



Train reward model with preference data.⁵

⁵E.g., [Stiennon et al., 2020]

Why Best-of-N?

· Approximates maximum (true) reward:

Best-of-
$$N = \underset{y \in \{y^{(1)}, \dots, y^{(N)}\}}{\text{arg max }} v(y)$$

$$\approx \underset{y}{\text{arg max }} v(y) \tag{1}$$

$$\approx \underset{y}{\text{arg max }} R(y) \tag{2}$$

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(1) gets better as number of generations N increases!

Why Best-of-N?

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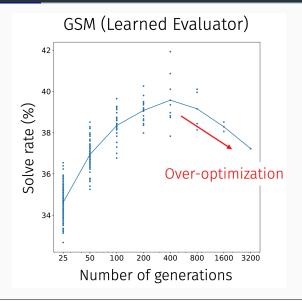
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$$\approx \underset{y}{\text{arg max }} v(y) \tag{1}$$

$$\approx \underset{y}{\text{arg max }} R(y) \tag{2}$$

- (1) gets better as number of generations N increases!
- (2) can suffer from imperfect reward model, aka "over-optimization"

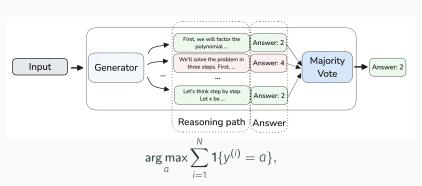
Parallel | Best-of-N⁶



⁶Plot adapted from *Training Verifiers to Solve Math Word Problems* [Cobbe et al., 2021]

Voting

Voting aggregation:7



⁷Also called *self-consistency* [Wang et al., 2023]

Weighted voting⁸

Weighted Voting:

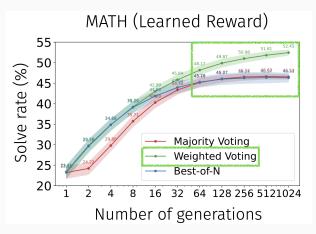


$$\arg\max_{a} \sum_{i=1}^{N} \underbrace{v(y^{(i)})}_{\text{reward model}} \cdot 1\{y^{(i)} = a\}$$

⁸[Li et al., 2023]

Voting

Can outperform Best-of-N, e.g.:9



⁹[Sun et al., 2024] Easy-to-Hard Generalization: Scalable Alignment Beyond Human Supervision.

Why (weighted) voting?

As the number of candidates $N \to \infty$, voting accuracy converges to...¹⁰

$$\frac{1}{M} \sum_{i=1}^{M} \mathbb{I} \left[a_i^* = \underset{a}{\operatorname{arg max}} \sum_{z} v(x, z, a) g(z, a | x) \right]$$
"Marginalize out paths z"

Notation:

- (x, z, a): (input, solution, answer)
- M: number of test examples

¹⁰Theorem 2, [Wu et al., 2024] *Inference Scaling Laws*. Y. Wu, Z. Sun, S. Li, S. Welleck, Y. Yang.

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Takeaway 1: Will accuracy keep improving with more samples?

No, it eventually converges to the accuracy shown above

¹⁰Theorem 2, [Wu et al., 2024] *Inference Scaling Laws*. Y. Wu, Z. Sun, S. Li, S. Welleck, Y. Yang.

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Takeaway 2: When is weighted voting better than voting?

• When $v \cdot g$ assigns more total mass to correct answers than g

¹⁰Theorem 2, [Wu et al., 2024] *Inference Scaling Laws*. Y. Wu, Z. Sun, S. Li, S. Welleck, Y. Yang.

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Takeaway 3: How do we improve performance further?

- \cdot Improve the reward model v
- Improve the generator *g* (better model and/or better algorithm)

¹⁰Theorem 2, [Wu et al., 2024] *Inference Scaling Laws*. Y. Wu, Z. Sun, S. Li, S. Welleck, Y. Yang.

Parallel

Improve the reward model:



Parallel generation in the reward model too¹¹

Active area of research! (More later in this tutorial!!)

¹¹[Zhang et al., 2024]

Meta-generation strategies | parallel

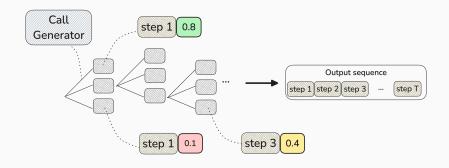
Parallel

- Explores output space by generating full sequences
- · Large performance gains in practice
- Bounded by the quality of the evaluator and generator
- · Next: Can we better leverage intermediate evaluation?

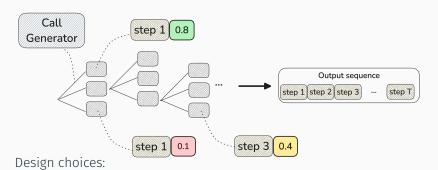
Strategies

- Strategies
 - Parallel
 - · Tree search
 - · Refinement

Tree search | basic idea



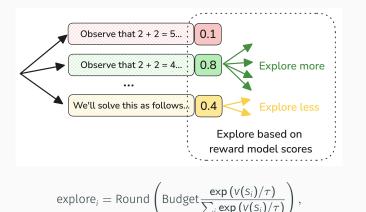
Tree search | basic idea



- States s
- Transitions $s \rightarrow s'$
- Scores v(s)
- · Strategy (breadth-first, depth-first, ...)

Tree search | example (REBASE)

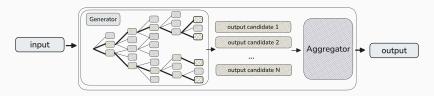
2. Reward Balanced Search (Rebase)¹²



(3)

¹²[Wu et al., 2024] Inference Scaling Laws: An Empirical Analysis of Compute-Optimal Inference.

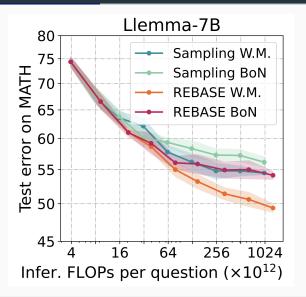
Tree search | example



Run tree search to get candidates for aggregation (e.g., voting).

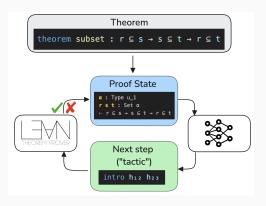
- · Key idea: Leverages scores on intermediate states
 - Backtracking
 - · Exploration

Tree search | examples¹³



¹³[Wu et al., 2024] Inference Scaling Laws: An Empirical Analysis of Compute-Optimal Inference.

Tree search | examples



Formal theorem proving [Polu and Sutskever, 2020]

Tree search | examples

```
type-checked candidates:

(-0.066) rintro rfl
(-0.307) rintro (rfl, rfl)
(-0.035) intro h
(-0.230) rintro (d, rfl)

(-0.453) cases c
```

Best-first search in formal theorem proving

Tree search | examples



Best-first search in web agents [Koh et al., 2024]

Meta-generation strategies | Tree search

Tree-search

- · Can backtrack and explore using intermediate scores
- Requires a suitable environment and value function
 - · Decomposition into states
 - · Good reward signal

Strategies

- Strategies
 - Parallel
 - · Tree search
 - · Refinement

Refinement / self-correction

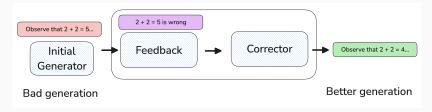


Improve a generation

Repeat:

•
$$y^{(i+1)} \sim g(x, y^{(i)})$$

Refinement / self-correction

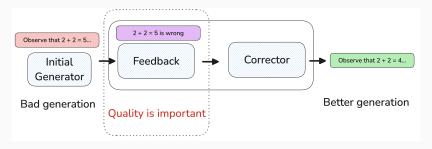


Improve a generation using feedback

Repeat:

•
$$y^{(i+1)} \sim g(x, y^{(i)}, F(y^{(i)}))$$

Refinement / self-correction



Improve a generation using feedback

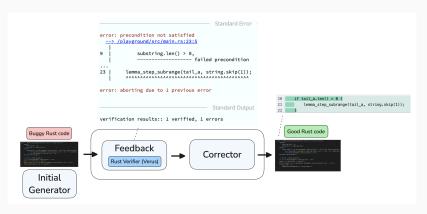
Meta-generators | refinement

In practice, the quality and source of feedback is crucial:

- Extrinsic: external information at inference time
- · Intrinsic: no external information at inference time

Meta-generators | refinement | extrinsic

1. Extrinsic: external feedback

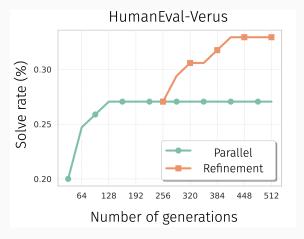


Feedback: external program verifier¹⁴

¹⁴ [Aggarwal et al., 2024], AlphaVerus. P. Aggarwal, B. Parno, S. Welleck.

Meta-generators | refinement | extrinsic

1. Extrinsic: external feedback



AlphaVerus. P. Aggarwal, B. Parno, S. Welleck.

Meta-generators | refinement | extrinsic

1. Extrinsic: external feedback

Several success cases:

- · Verifiers [Aggarwal et al., 2024]
- · Code interpreters [Chen et al., 2024]
- · Retrievers [Asai et al., 2024]
- · Tools + agent environment¹⁴

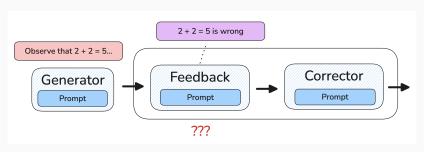
• ...

Intuition: adds new information, can detect and localize errors

¹⁴https://x.com/gneubig/status/1866172948991615177

Meta-generators | refinement | intrinsic

2. Intrinsic: Re-prompt the same model:



Re-prompt a single LLM, e.g. [Madaan et al., 2023]

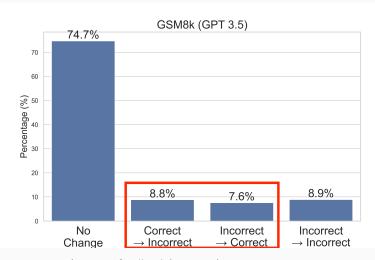
Meta-generators | refinement | intrinsic

Mixed results:

- Easy to evaluate tasks: positive [Wang et al., 2024b]
 - E.g., missing info [Asai et al., 2024]
- Mathematical reasoning: mixed¹⁵

¹⁵E.g., [Huang et al., 2024] Large Language Models Cannot Self-Correct Reasoning Yet

Meta-generators | refinement | intrinsic

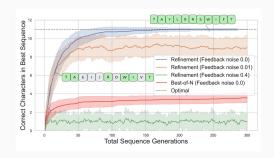


Takeaway: feedback is too noisy From [Huang et al., 2024]

Meta-generators | refinement

Generate "TAYLORSWIFT"

- · Generator:
 - p(character)
- · Feedback:
 - · Incorrect characters
- · Corrector:
 - · Regenerate incorrect



Meta-generators | refinement / self-correction

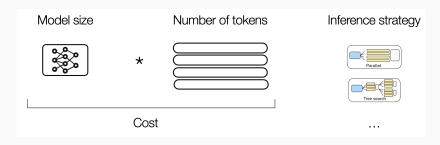
Refinement / self-correction

- Extrinsic
 - · Positive results for environments that detect or localize errors
- Intrinsic
 - · Mixed results, depends on difficulty of verification

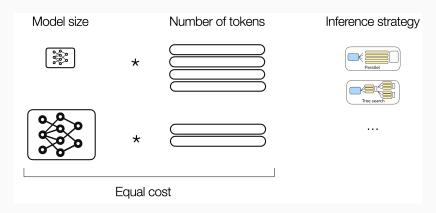
Meta-generators | outline

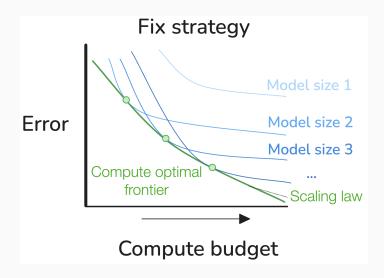
- Strategies
 - · Parallel
 - · Tree search
 - · Refinement
- · Inference scaling laws

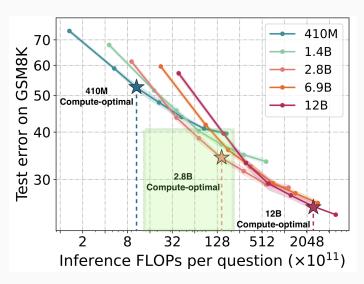
Compute is a function of model size and number of generated tokens



We can choose to increase model size or number of tokens







Using a smaller model and generating more is often best [Wu et al., 2024].

Inference scaling laws

Designing better strategies

- Example: design a better tree search [Wu et al., 2024]
- Example: select inference strategy based on problem difficulty [Snell et al., 2024]

• ...

Inference scaling laws | recap

- · When allocated optimally, performance improves with compute
- Best model size and strategy varies with the budget
 - · Sometimes smaller models are better!

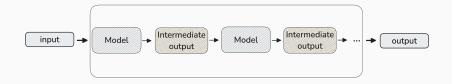
Meta-generation | recap

- Strategies for generating multiple sequences
- · Parallel, tree search, refinement
- · Choose methods based on task performance and cost

Today's lecture

- 1. Part 1: Generating multiple sequences
- 2. Part 2: Generating a single long sequence
 - · Long chain-of-thought

Meta-generators | chain



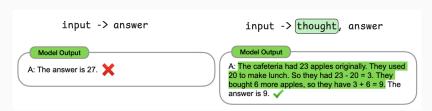
Compose generators:

$$y_1 \sim g_1(x)$$

 $y_2 \sim g_2(x, y_1)$
 $y_3 \sim g_3(x, y_2)$
:

Meta-generators | chain

Simple example: Chain-of-thought [Wei et al., 2022]:

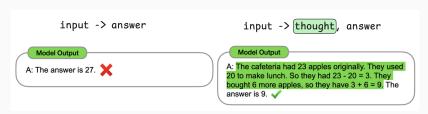


A simple decomposition:

- Generate a thought, $z \sim g(\cdot|x)$
- Generate an answer, $a \sim g(\cdot|x,z)$

Meta-generators | chain

Simple example: Chain-of-thought [Wei et al., 2022]:



Increases expressivity15

- · Variable output length, analogous to a writeable tape
- Idea: train a model that searches on its own in the thought!

¹⁵E.g., [Feng et al., 2023, Merrill and Sabharwal, 2024, Nowak et al., 2024]

Training a model to search: Basic idea

· Train a model to generate a "thought" prior to a final output

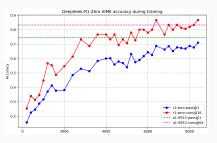
$$p_{\theta}(\underbrace{y}_{\text{"output"}}, \underbrace{z}_{\text{"thought"}}|x)$$

- · At inference time, just sample a thought+output
- In principle, the model can learn to try alternatives, perform refinement, backtrack within the thought

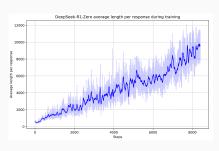
Training for long chain-of-thought [DeepSeek-AI et al., 2025]

- · Approach 1: reinforcement learning
 - Policy: given a math problem x, generate a thought + answer
 - · Reward: is the answer correct

Training for long chain-of-thought [DeepSeek-AI et al., 2025]



Accuracy improves during training



Response length increases to > 10,000

Training for long chain-of-thought [DeepSeek-AI et al., 2025]

Question: If a > 1, then the sum of the real solutions of $\sqrt{a - \sqrt{a + x}} = x$ is equal to

Response: <think>

To solve the equation $\sqrt{a-\sqrt{a+x}}=x$, let's start by squaring both \cdots

$$\left(\sqrt{a-\sqrt{a+x}}\right)^2 = x^2 \implies a - \sqrt{a+x} = x^2.$$

Rearrange to isolate the inner square root term:

$$(a-x^2)^2 = a+x \implies a^2 - 2ax^2 + (x^2)^2 = a+x \implies x^4 - 2ax^2 - x + (a^2 - a) = 0$$

. . .

Wait, wait. Wait. That's an aha moment I can flag here.

Let's reevaluate this step-by-step to identify if the correct sum can be \cdots

We started with the equation:

$$\sqrt{a-\sqrt{a+x}}=x$$

First, let's square both sides:

$$a - \sqrt{a + x} = x^2 \implies \sqrt{a + x} = a - x^2$$

Next, I could square both sides again, treating the equation: ...

. .

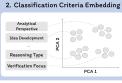
Example response

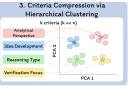
Long chain-of-thought patterns Credits: Weihua Du

- 1. Uncertainty
 - · Wait... / Hold on...
 - · Wait-actually, does this formula apply here?
- 2. Branching, backtracking, retrying
 - · Alternatively, generating functions could model this problem...
 - · Revisitina...
 - · Wait, I'm overthinking. Let's try again...
- 3. Verification
 - · Let's check if we made an error. We should verify...
 - This is a contradiction, so we must have made a mistake.
 - · Let's test this with...
- 4. Key Points
 - Key takeaway... | It's worth noting...
- 5. Clarification
 - · In other words... / To clarify...
- 6. Synthesis
 - · Ultimately... / Putting it all together...

CoT Encyclopedia [Lee et al., 2025]

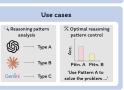










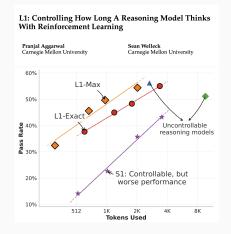


The COT ENCYCLOPEDIA: Analyzing, Predicting, and Controlling how a Reasoning Model will Think

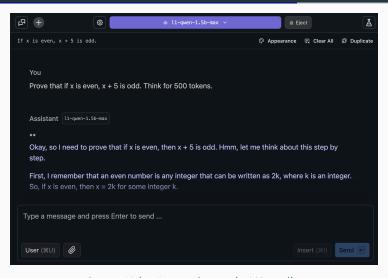
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Seongyun Lee<sup>1,21</sup> Seongone Kim<sup>21</sup> Minja Seo<sup>1</sup> Vongrae Ja<sup>2</sup>
Dongoung Ge<sup>1,2</sup> Hyeonbin Heung<sup>2</sup> Jihab Park<sup>1</sup>
Xing Yue<sup>2</sup> San Welfeck<sup>2</sup> Graham Noubig<sup>2</sup> Moontae Lee<sup>2</sup> Minjoon Seo<sup>1</sup>
KAST Al<sup>2</sup> Conegig Middu Biovensy<sup>2</sup>
LOA Hosensch<sup>2</sup> MVER South Un<sup>2</sup> Cornel University<sup>2</sup>
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```

Controlling the length: L1 [Aggarwal and Welleck, 2025]

- Train model with reinforcement learning to adhere to length constraints
- E.g. "use up to 1000 tokens" provided in the prompt
- Reward: correctness and length constraint penalty



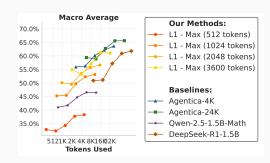
Controlling the length: L1 [Aggarwal and Welleck, 2025]



Demo: Using L1 on a laptop in LM studio

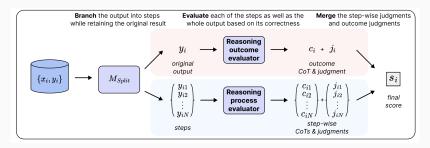
Long chain-of-thought | sequential vs. parallel

- Sequential: long chain-of-thought
- Parallel: majority voting (multiple long COTs)



[Aggarwal and Welleck, 2025]

Reasoning models as evaluators in Best-of-N [Kim et al., 2025]

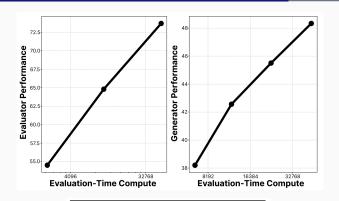


Scaling Evaluation-time Compute with Reasoning Models as Process Evaluators Seungene Kim¹- Inn Wu²- Jim Lee³- Xiang Yue¹ Seongun Lee² Mingreong Moor² Kiril Gastnewski²- Carolin Lawrence² Julia Hockenmider³ Graham Neubig³ Sean Welleck ¹CMU ² Juliacementa Researcher ² UUC ⁴ KAIST AI

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Reasoning models as evaluators in Best-of-N [Kim et al., 2025]



Scaling Evaluation-time Compute with Reasoning Models as Process Evaluators

Seungone Kim¹* Ian Wu²* Jinu Lee¹* Xiang Yue¹
Seongyun Lee¹* Mingyong Noon²* Kiril Gashtovssk¹C carolin Lawrence⁵
John Mindelson Gerhahn Noulg² Sean Welleck¹

LOMU ²Independent Researcher ²UIUC ⁴KAIST AI
⁶FEC Laboratories Europe ⁷58C yril and Meholius University of Skopje

Part 2 recap

- Train a model to generate a long sequence, then use a simple inference algorithm
- · Internally can perform backtracking, self-correction, etc.
- Emerging area of research!

Today's tutorial | recap

- 1. Test-time inference strategies take a trained model and improve performance by:
 - Generating tokens according to a strategy
 - Incorporate external information
 - · Reward models
 - · Environment feedback

Very active and evolving research area!

Today's tutorial | recap

- 1. Test-time inference strategies take a trained model and improve performance by:
 - · Generating tokens according to a strategy
 - Incorporate external information
 - · Reward models
 - · Environment feedback
- 2. Two complementary meta-generation strategies
 - · Call a generator to generate a thought prior to an answer
 - · Long chain-of-thought
 - · Call a generator multiple times in a structured way
 - · parallel, tree search, refinement

Very active and evolving research area!

Additional resources



TMLR Survey [Welleck et al., 2024]



NeurIPS 2024 LLM Inference Tutorial: https://cmu-l3.github.io/neurips2024-inference-tutorial/

Additional resources



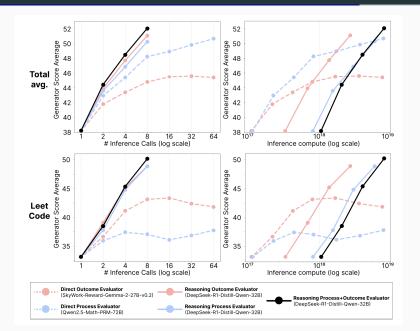
1st Workshop on Test-Time Scaling and Reasoning Models at COLM 2025 https://scalr-workshop.github.io/

Thank you!

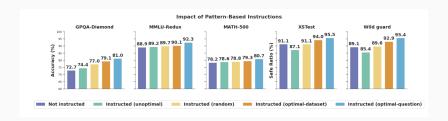
Sean Welleck
Carnegie Mellon University
Learning, Language, and Logic (L3) Lab
www.wellecks.com

Appendix

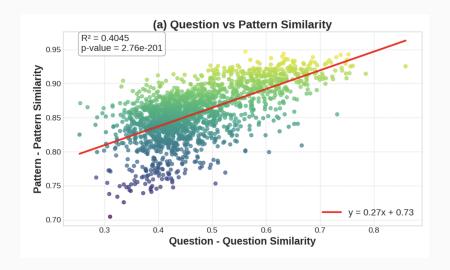
Additional results



Additional results



Additional results



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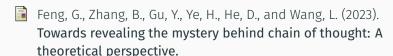
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