Beyond Decoding: Meta-Generation Algorithms for Large Language Models

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Meta-generators

Goal (system designer)

Design a system G that generates acceptable sequences:

$$\arg\max_G \mathbb{E}_{y \sim G(\cdot)} A(y) \tag{1}$$

Example acceptability: correctness, human preferences

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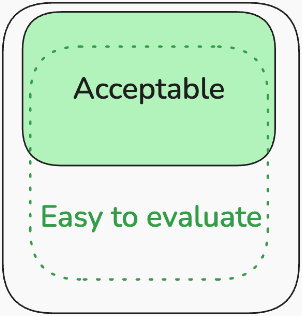
Example acceptability: correctness, human preferences

We know how to sample *probable* outputs, $y \sim p_\theta(y|x)$

- What if these outputs are not *acceptable*?

Meta-generation | Key ideas

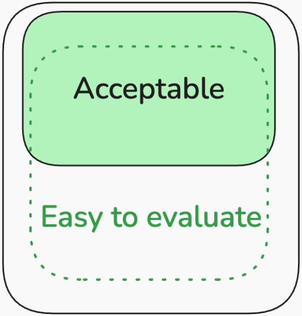
1. Take advantage of external information during generation



- Example: Learn an evaluator $v(y) \approx A(y)$ and use it in generation

Meta-generation | Key ideas

1. Take advantage of external information during generation

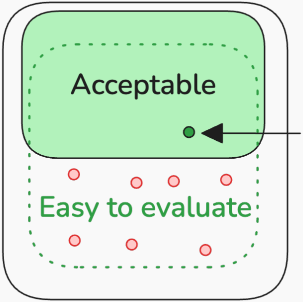


- Example: Learn an evaluator $v(y) \approx A(y)$ and use it in generation

Terminology: Evaluator ≈ critic ≈ verifier ≈ value ≈ reward model ≈ scoring model

Meta-generation | Key ideas

1. Take advantage of external information during generation
2. Call the generator more than once to search for good sequences



x:

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

LLEMMA 34B solution:
We have

z:

$$\sum_{k=2}^{\infty} f(k) = \sum_{k=2}^{\infty}\sum_{j=2}^{2008}\frac{1}{j^k} = \sum_{j=2}^{2008}\sum_{k=2}^{\infty}\frac{1}{j^k} = \sum_{j=2}^{2008}\frac{1}{j^2}\sum_{k=0}^{\infty}\frac{1}{j^k} = \sum_{j=2}^{2008}\frac{1}{j^2}\frac{1}{1-\frac{1}{j}}$$
$$= \sum_{j=2}^{2008}\frac{1}{j(j-1)} = \sum_{j=2}^{2008}\left(\frac{1}{j-1} - \frac{1}{j}\right)$$
$$= \left(\frac{1}{1} - \frac{1}{2}\right) + \left(\frac{1}{2} - \frac{1}{3}\right) + \cdots + \left(\frac{1}{2007} - \frac{1}{2008}\right)$$
$$= 1 - \frac{1}{2008}$$
$$= \boxed{\frac{2007}{2008}}.$$

y:

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

Example: solve a math problem

Meta-generation | Key ideas

What if we had an oracle verifier, $v(y)$?

Repeat:

- $z \sim p_\theta(z|x)$
- $y \sim p_\theta(y|x, z)$
- Stop if $v(y)$ says answer is correct

x:

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

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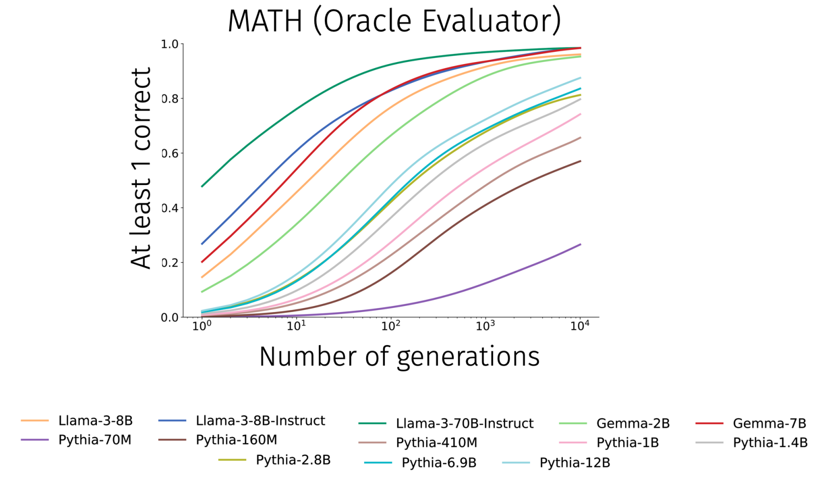
y:

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

Meta-generation | Key ideas[1]



[1] Adapted from [Brown et al., 2024]. See also [Li et al., 2022, Cobbe et al., 2021, Jiang et al., 2023]

Meta-generation

We formalize these kinds of strategies as *meta-generators* [2]

$$y \sim G(y|x; \underbrace{g_1, g_2, \ldots, g_G}_{\text{generators}}, \underbrace{\phi}_{\text{Other parameters}})$$

Key design choices:

- G: strategy for calling generators
- $g_1, g_2, \ldots, g_G$: choice of generators
- ϕ: other models, number of tokens to generate, ...

[2] [Welleck et al., 2024] *From Decoding to Meta-Generation: Inference-time Algorithms for LLMs.* S. Welleck, A. Bertsch*, M. Finlayson*, H. Schoelkopf*, A. Xie, G. Neubig, I. Kulikov, Z. Harchaoui.

Meta-generation

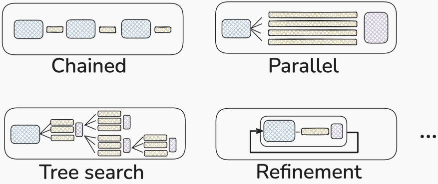
Token-level generators from part 1 are a special case of calling:

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

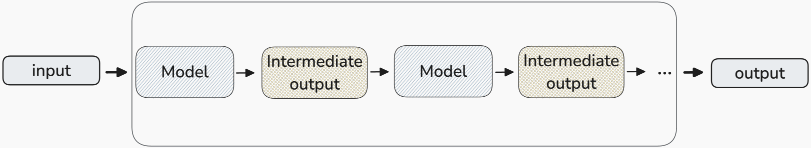
Design choices:

- g: sampling adapters, beam search, ...
- ϕ: temperature, beam width, ...

- Strategies
  - **Chain**
  - Parallel
  - Tree search
  - Refinement/Self-Correction
- Scaling meta-generators



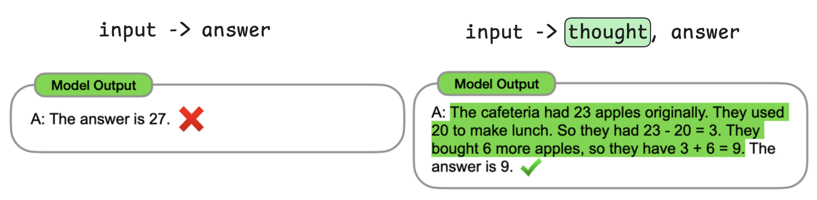
Meta-generators | chain



Compose generators:

$$
\begin{aligned}
y_1 &\sim g_1(x) \\
y_2 &\sim g_2(x, y_1) \\
y_3 &\sim g_3(x, y_2) \\
&\vdots
\end{aligned}
$$

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

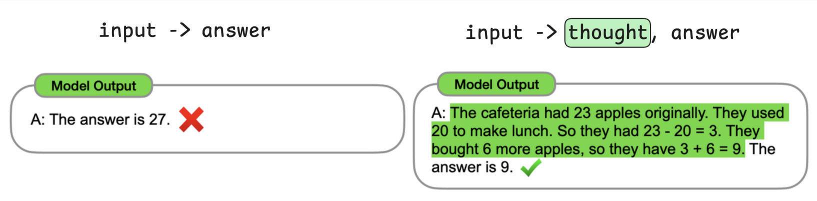


A simple decomposition:

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

Meta-generators | chain

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



Increases expressivity[3]

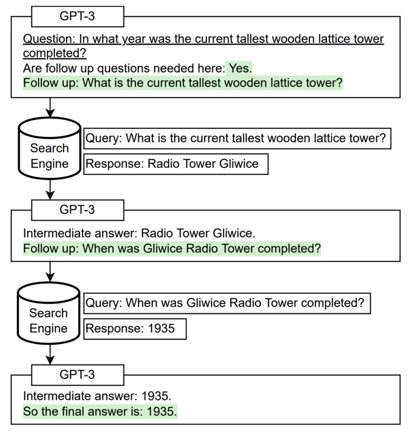
- Variable output length, analogous to a writeable tape

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

Meta-generators | chain

Extend to multiple steps:

- Each step:
    - Generate query
    - Call API
- Then generate an answer



Self-Ask [Press et al., 2023]

Meta-generators | chain[4]

View as programs:

- Outer function ≈ meta-generator
- Inner function ≈ generator

```
def search(x: Example) -> Example:
  x.hop1 = generate(hop_template)(x).pred
  x.psg1 = retrieve(x.hop1, k=1)[0]
  x.hop2 = generate(hop_template)(x).pred
  x.psg2 = retrieve(x.hop2, k=1)[0]
  return x

def predict(x: Example) -> Example:
  x.context = [x.psg1, x.psg2]
  x.pred = generate(qa_template)(x).pred
  return x
```

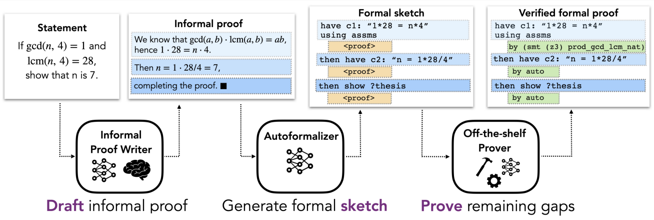
Demonstrate-Search-Predict (DSP)
[Khattab et al., 2022]

[4] [Khattab et al., 2022, Dohan et al., 2022, Schlag et al., 2023, Zheng et al., 2024]

Meta-generators | chain

Many other examples!

- Rewrite input before generating
  (*System-2 Attention* [Weston and Sukhbaatar, 2023])
- Sketch proof, fill gaps, check proof
  (*Draft-Sketch-Prove* [Jiang et al., 2023])
- ...



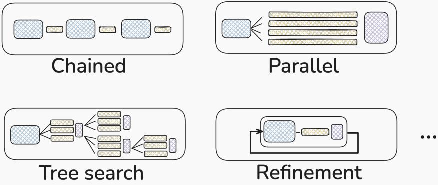
Meta-generators | chain

Chained meta-generation

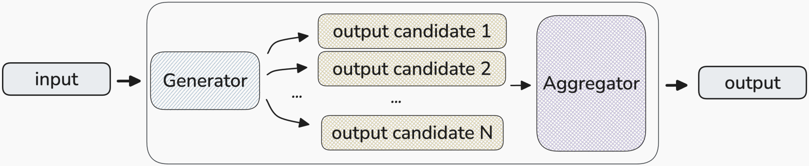
- **Key idea:** decompose generation and incorporate tools/models
- Chaining alone does not explore the output space

Meta-generators | outline

- Strategies
  - Chain
  - Parallel
  - Tree search
  - Refinement



Meta-generators | parallel



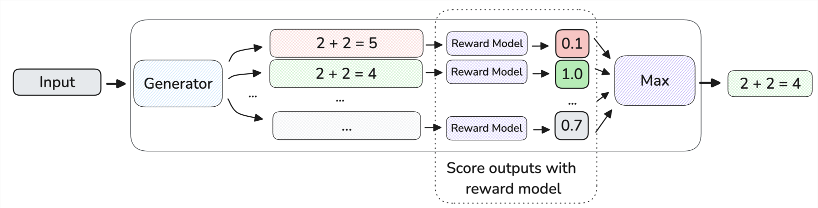
- Generate candidates:

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

- Aggregate:

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

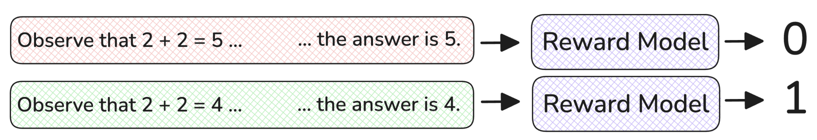
Meta-generators | parallel | Best-of-N/Rejection Sampling[5]



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

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

Reward model $v(y) \rightarrow [0, 1]$:

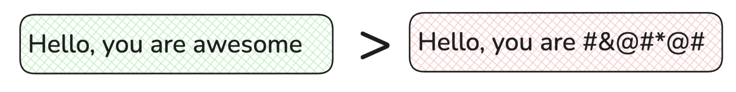


Train reward model with correct and incorrect examples.[6]

[6] E.g., [Cobbe et al., 2021]

Meta-generators | parallel | Best-of-N/Rejection Sampling

Reward model $v(y) \to [0, 1]$:



Train reward model with preference data.[6]

[6] E.g., [Stiennon et al., 2020]

Why Best-of-N?

- Approximates maximum acceptability:

$$
\begin{aligned}
\text{Best-of-}N &= \operatorname*{arg\,max}_{y \in \{y^{(1)},\ldots,y^{(N)}\}} v(y) \\
&\approx \operatorname*{arg\,max}_{y} v(y) && (2) \\
&\approx \operatorname*{arg\,max}_{y} A(y) && (3)
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(2) gets better as number of generations N increases!

Meta-generators | parallel | Best-of-N/Rejection Sampling

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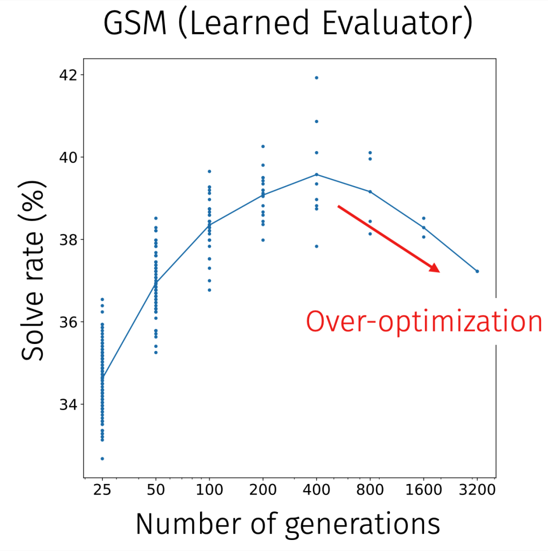
(2) gets better as number of generations N increases!

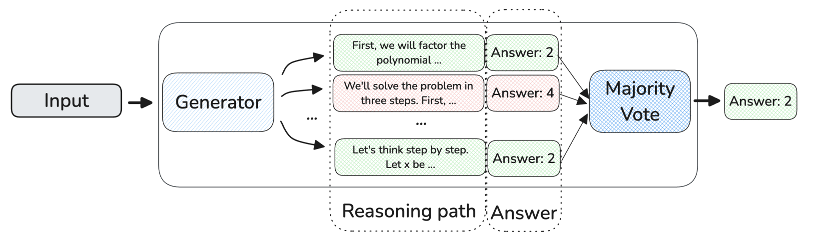
(3) Suffers from imperfect reward model, aka "over-optimization"

Meta-generators | parallel | Best-of-N / Rejection Sampling[7]



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

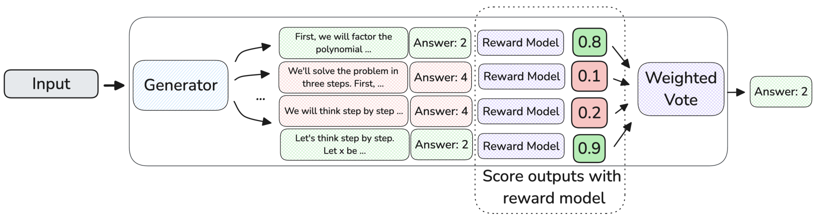
Voting aggregation:[8]



$$\arg\max_a \sum_{i=1}^{N} 1\{y^{(i)} = a\},$$

8[Wang et al., 2023]

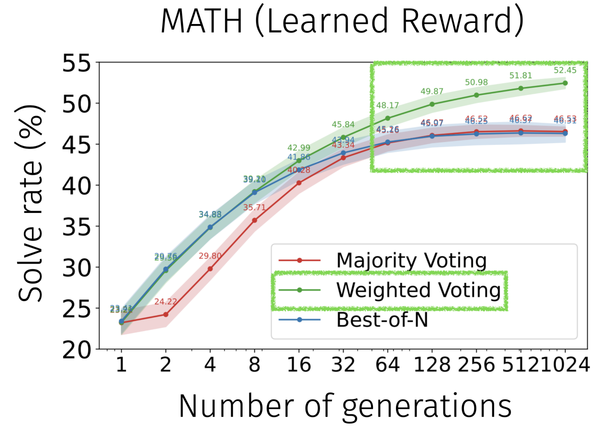
Weighted Voting:



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

[9] [Li et al., 2023b]

Can outperform Best-of-N, e.g.:[10]



[10][Sun et al., 2024] *Easy-to-Hard Generalization: Scalable Alignment Beyond Human Supervision.* Z. Sun, L. Yu, Y. Shen, W. Liu, Y. Yang, S. Welleck, C. Gan. NeurIPS 2024.

Meta-generators | parallel | why (weighted) voting?

As the number of candidates $N \to \infty$, voting accuracy converges to...[11]

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

Notation:

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

[11] Theorem 2, [Wu et al., 2024b] *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

[11] Theorem 2, [Wu et al., 2024b] *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

[11] Theorem 2, [Wu et al., 2024b] *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?

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

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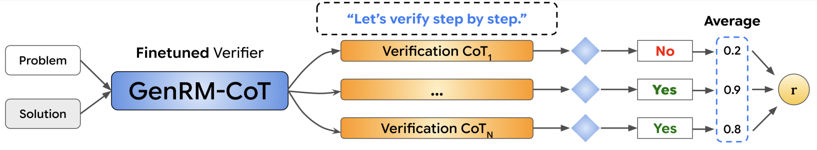
Improve the reward model:



Parallel generation *in the reward model too*[12]

Active area of research!

[12] [Zhang et al., 2024]

Meta-generators | parallel

Parallel meta-generators

- Explores output space by generating full sequences
- Large performance gains in practice
- Bounded by the quality of the evaluator and generator

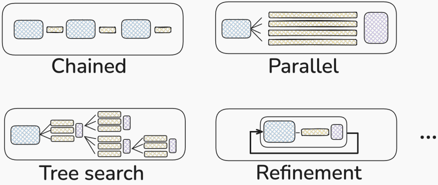
Parallel meta-generators

- Explores output space by generating full sequences
- Large performance gains in practice
- Bounded by the quality of the evaluator and generator

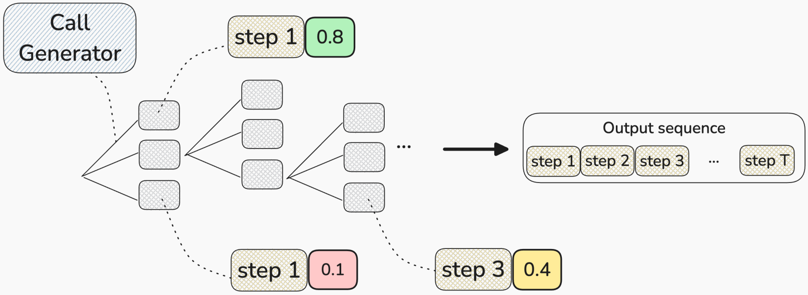
Insight: only uses the verifier at the end (on full sequences)

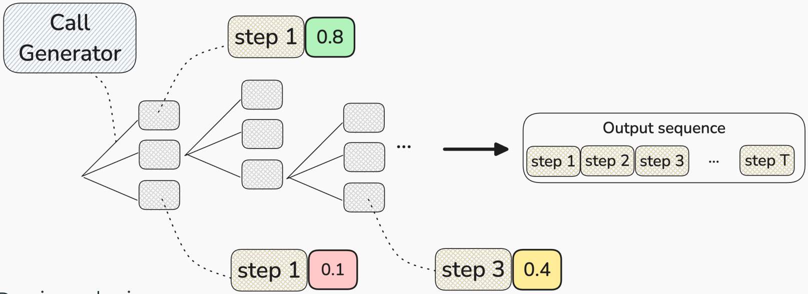
- *Next:* Can we better leverage *intermediate* evaluation?

- Strategies
    - Chain
    - Parallel
    - Tree search
    - Refinement



Meta-generators | tree search | basic idea

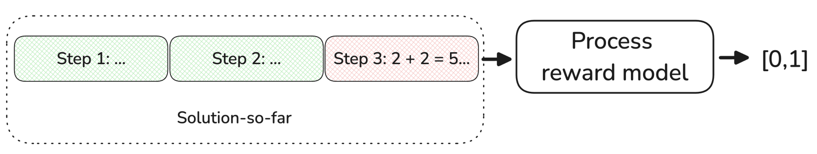




Design choices:

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

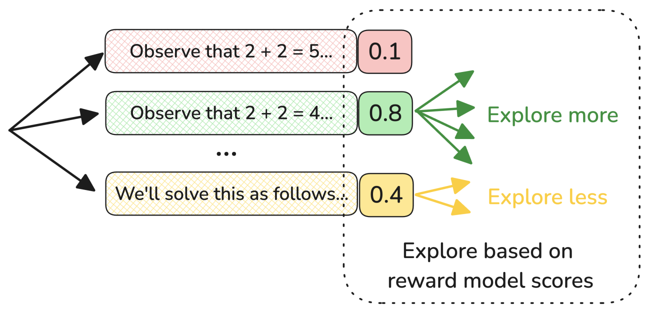
1. Scores: “process reward model (PRM)”[13]



$$v(x, s_1, s_2, \ldots, s_t) \rightarrow [0, 1]$$

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

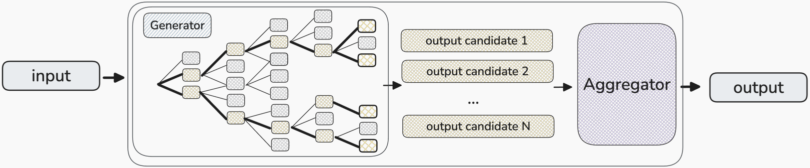
2. *Reward Balanced Search (Rebase)*[14]



$$\text{explore}_i = \text{Round}\left(\text{Budget}\frac{\exp\left(v(s_i)/\tau\right)}{\sum_j \exp\left(v(s_j)/\tau\right)}\right), \tag{4}$$

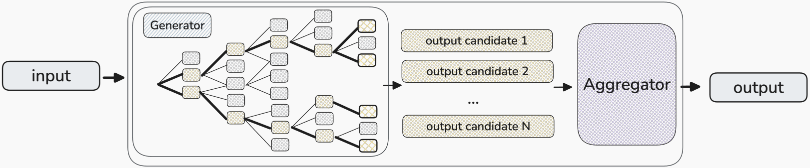
[14] [Wu et al., 2024b] *Inference Scaling Laws: An Empirical Analysis of Compute-Optimal Inference.*

Meta-generators | tree search | aggregation



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

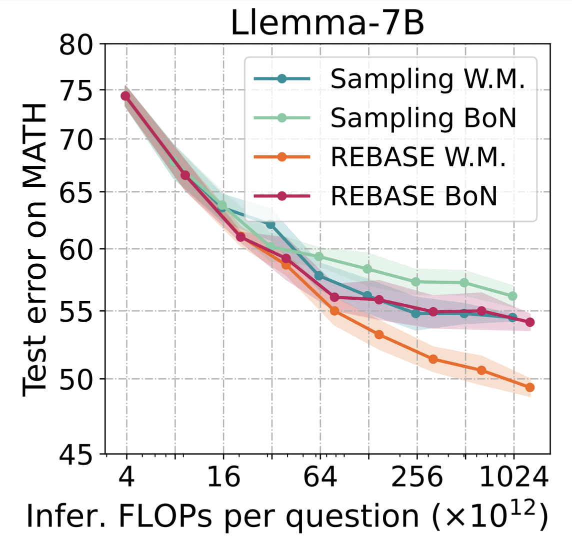
Meta-generators | tree search | aggregation



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

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

Meta-generators | tree search | example[15]



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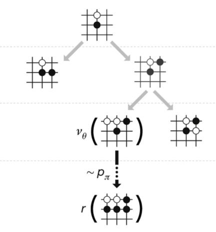
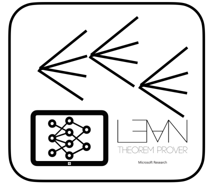
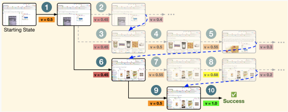
Meta-generators | tree search | example



Go [Silver et al., 2016]



Proofs [Polu and Sutskever, 2020]



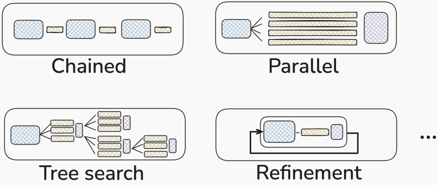
Agents [Koh et al., 2024]

Meta-generators | tree search

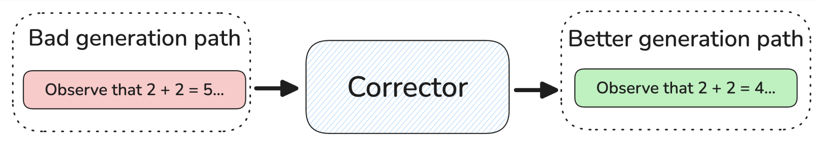
Tree-search meta-generators

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

- Strategies
  - Chain
  - Parallel
  - Tree search
  - Refinement/self-correction
- Scaling meta-generators

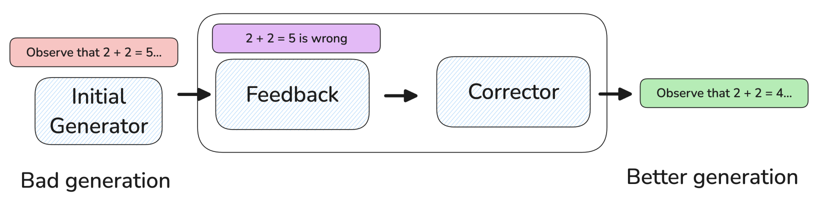


Meta-generators | refinement / self-correction



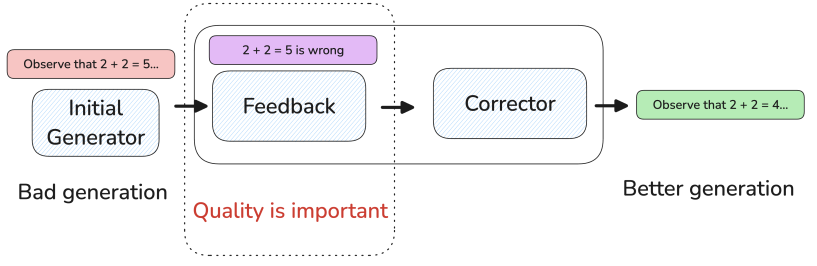
Improve a generation

Meta-generators | refinement / self-correction



Improve a generation using feedback

Meta-generators | refinement / self-correction

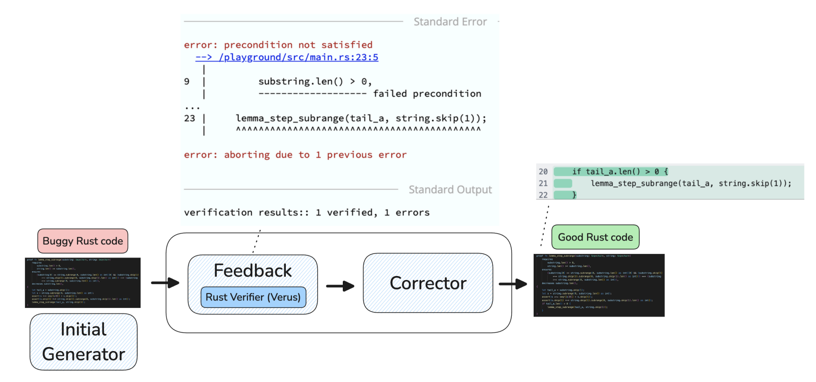


Improve a generation using feedback

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

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

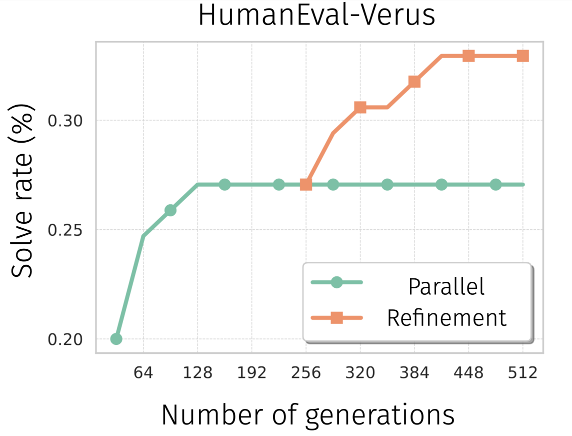
1. **Extrinsic**: external feedback



Feedback: external program verifier[16]

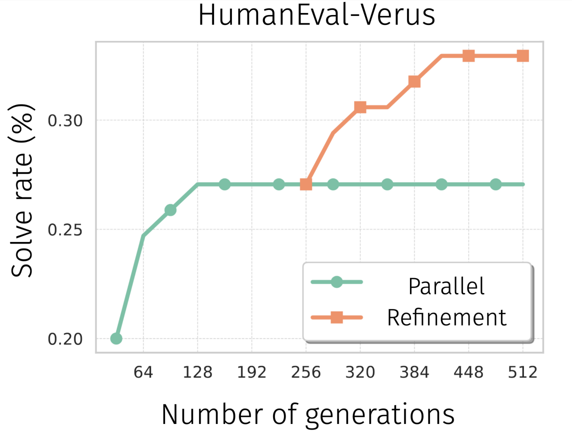
[16] [Aggarwal et al., 2024], *AlphaVerus*. P. Aggarwal, B. Parno, S. Welleck.

1. **Extrinsic**: external feedback



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

1. **Extrinsic**: external feedback



Tutorial code demo: github.com/cmu-l3/neurips2024-inference-tutorial-code

Meta-generators | refinement | extrinsic

1. **Extrinsic**: external feedback

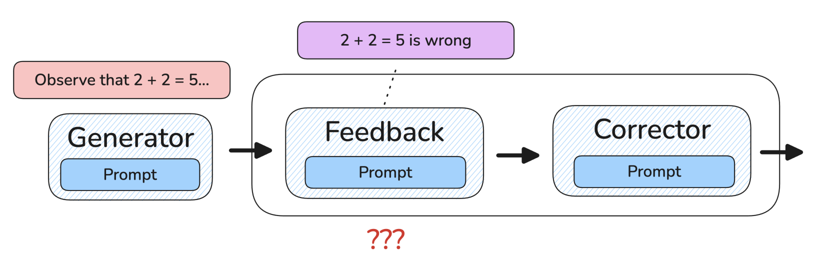
Several success cases:

- Verifiers [Aggarwal et al., 2024]
- Code interpreters [Chen et al., 2024b]
- Retrievers [Asai et al., 2024]
- Tools + agent environment[16]
- ...

Intuition: adds new information, can detect and localize errors

[16] https://x.com/gneubig/status/1866172948991615177

2. **Intrinsic**: Re-prompt the same model:



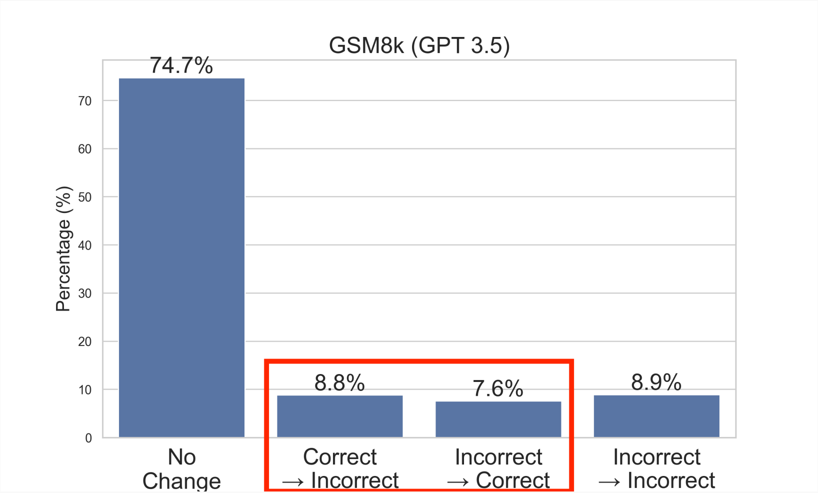
Re-prompt a single LLM, e.g. [Madaan et al., 2023]

Mixed results:

- Easy to evaluate tasks: positive [Wang et al., 2024b]
  - E.g., missing info [Asai et al., 2024]
- Mathematical reasoning: mixed[17]

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

Meta-generators | refinement | intrinsic

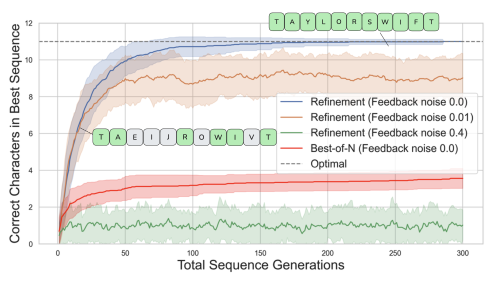


Takeaway: feedback is too noisy From [Huang et al., 2024]

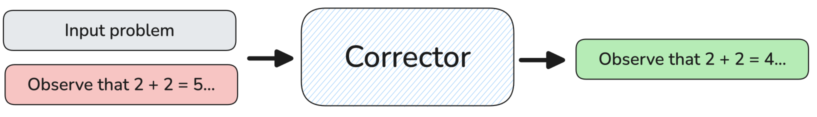
Meta-generators | refinement

Generate "TAYLORSWIFT"

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



3. **Intrinsic**: trained corrector



Directly *learn* to correct[17]

[17] [Welleck et al., 2023], *Generating Sequences by Learning to [Self-]Correct.*

Meta-generators | refinement | Case 3: fine-tuning

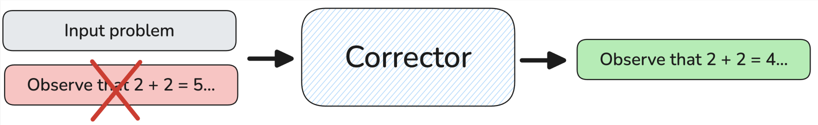
General pattern:[18]

- Collect (bad, better) pairs by generating and evaluating reward
- Update corrector $p_\theta(better|bad)$ using the collected data
- Repeat

[18] E.g., Self-corrective learning [Welleck et al., 2023], SCoRe [Kumar et al., 2024].

General pattern:[18]

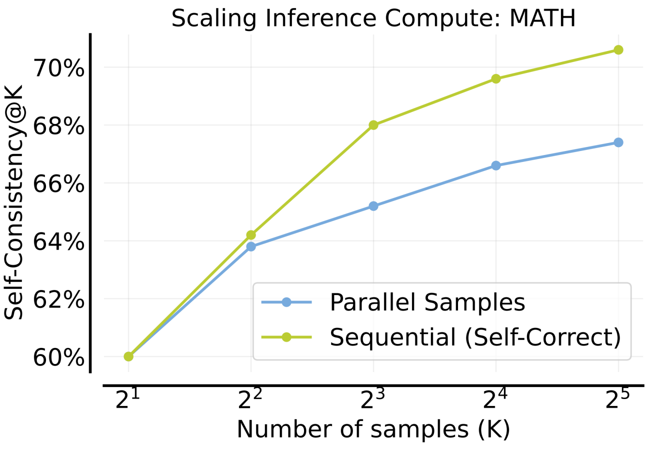
- Collect (bad, better) pairs by generating and evaluating reward
- Update corrector $p_\theta(better|bad)$ using the collected data
- Repeat



Prone to *behavior collapse*

- [Kumar et al., 2024]: overcome with regularization + RL

[18] E.g., Self-corrective learning [Welleck et al., 2023], SCoRe [Kumar et al., 2024].



From *SCoRe* [Kumar et al., 2024]

Meta-generators | refinement / self-correction

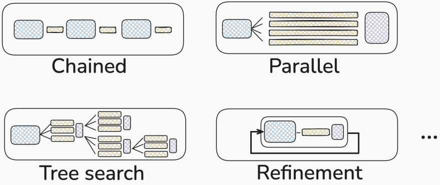
Refinement / self-correction

- Extrinsic
  - Positive results for environments that detect or localize errors
- Intrinsic, prompted
  - Mixed results, depends on difficulty of verification
- Intrinsic, trained
  - Possible improvements, requires specific training strategies

Meta-generators | outline

This talk:

- Strategies
  - Chain
  - Parallel
  - Tree search
  - Refinement
- Scaling meta-generators

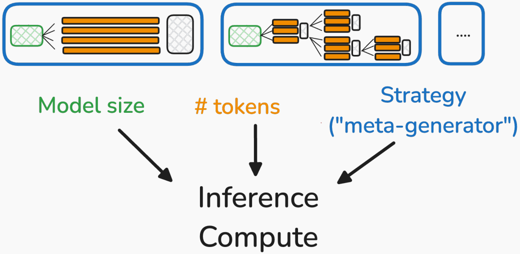


Meta-generation | how do we allocate test-time compute?

Choose strategies based on **task performance** and **compute cost**

Cost is a function of:

- Model size
- Number of generated tokens



Meta-generation | compute-optimal inference[19]

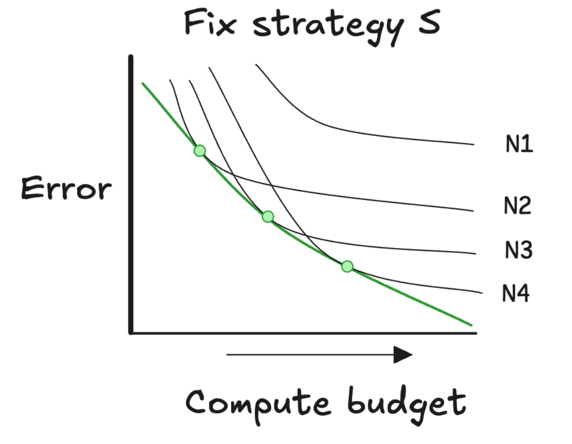
For a compute budget C:

$$\mathrm{argmin}_{N,T,S \text{ s.t. } cost(N,T,S)=C}\,\mathrm{error}(N,T,S)$$

- N: number of model parameters
- T: number of generated tokens
- S: inference strategy
- $cost(N,T,S)$: in floating-point operations

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

Meta-generation | compute-optimal inference[20]



Choose configurations on the *compute-optimal frontier* (green)

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

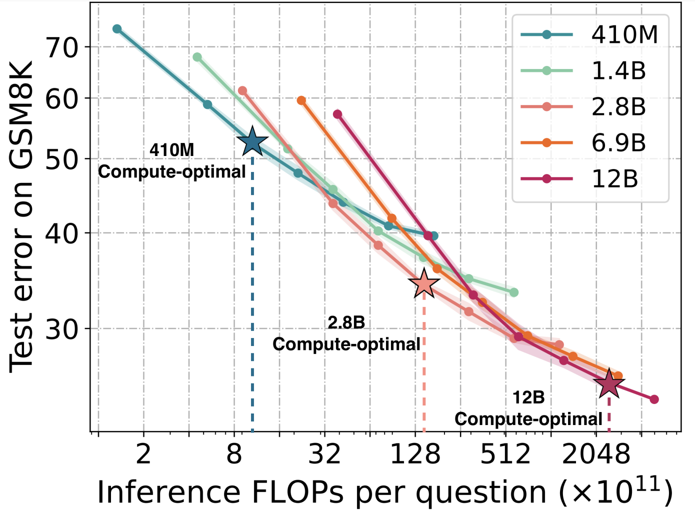
Meta-generation | how do we choose a meta-generator?

Question 1: is it better to use:

- A **small** model and more generations
- A **large** model and fewer generations

Experiment: Fix strategy, vary model size N and number of tokens T

Meta-generation | how do we choose a meta-generator?



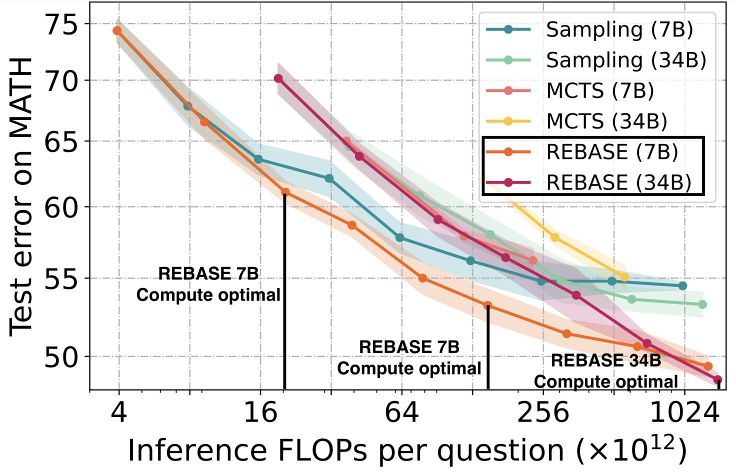
Smaller models can be compute optimal [Wu et al., 2024b].

Meta-generation | how do we choose a meta-generator?

Question 2: what is the compute-optimal meta-generation strategy?

Experiment: vary strategy (and model size and number of tokens)

Meta-generation | how do we choose a meta-generator?



Tree search (REBASE) can be compute-optimal [Wu et al., 2024b].

Meta-generation | recap

- Performance improves with increased compute…
  - … but it varies by the choice of model size and meta-generator
- The optimal model size and strategy varies with the compute budget
  - Sometimes smaller models are better!
  - Goal: design strategies that are universally optimal

Meta-generation | recap

- Meta-generators: strategies for calling generators and incorporating external information
- Several patterns: chain, parallel, tree search, refinement
- They can be combined and mixed together
- Choose and design methods based on task performance *and* cost

Meta-generation | speeding up

Next: The preceding meta-generators

- Generate many tokens
- In diverse ways (e.g., tree search)

How do we do this quickly and efficiently?

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