# CSE 493s/599s
# Lecture 8. Mixture-of-Experts and Test-time compute

Sewoong Oh

# Lecture notes

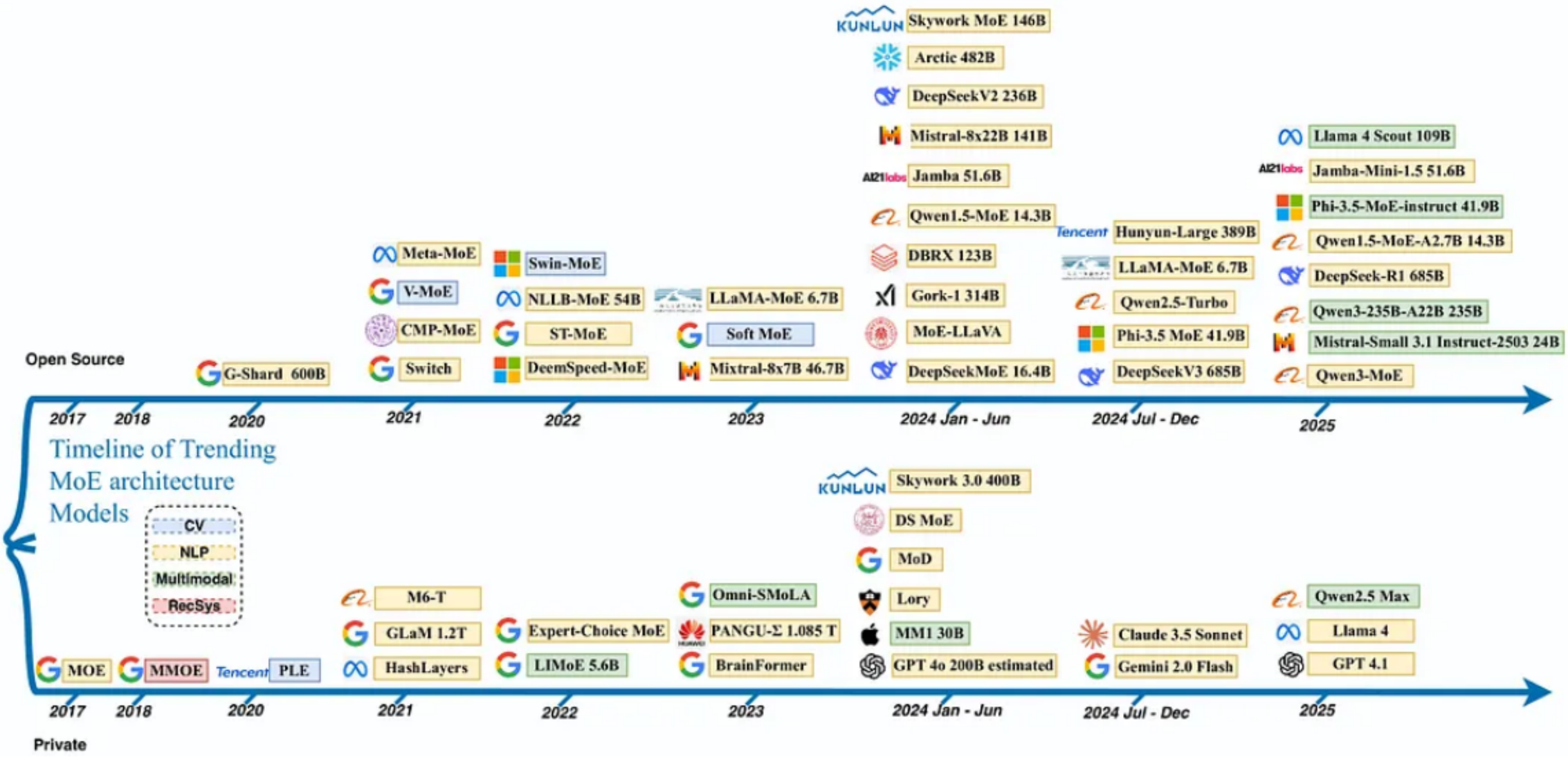
- These lecture notes are based on other courses in LLMs, including
  - CSE493S/599S at UW by Ludwig Schmidt: https://mlfoundations.github.io/advancedml-sp23/
  - EE-628 at EPFL by Volkan Cevher: https://www.epfl.ch/labs/lions/teaching/ee-628-training-large-language-models/ee-628-slides-2025/
  - ECE381V Generative Models at UT Austin by Sujay Sanghavi
  - and various papers and blogs cited at the end of the slide deck

# Outline

- Tokenizers
- Language models
- Architecture
    - Transformers
    - Mixture-of-experts
- Inference
    - Speculative decoding
    - In-context learning
    - Chain-of-thought prompting
    - Test-time compute
- Post-training
    - Parameter Efficient fine-tuning
    - Alignment

# Mixture-of-Experts (MoE)

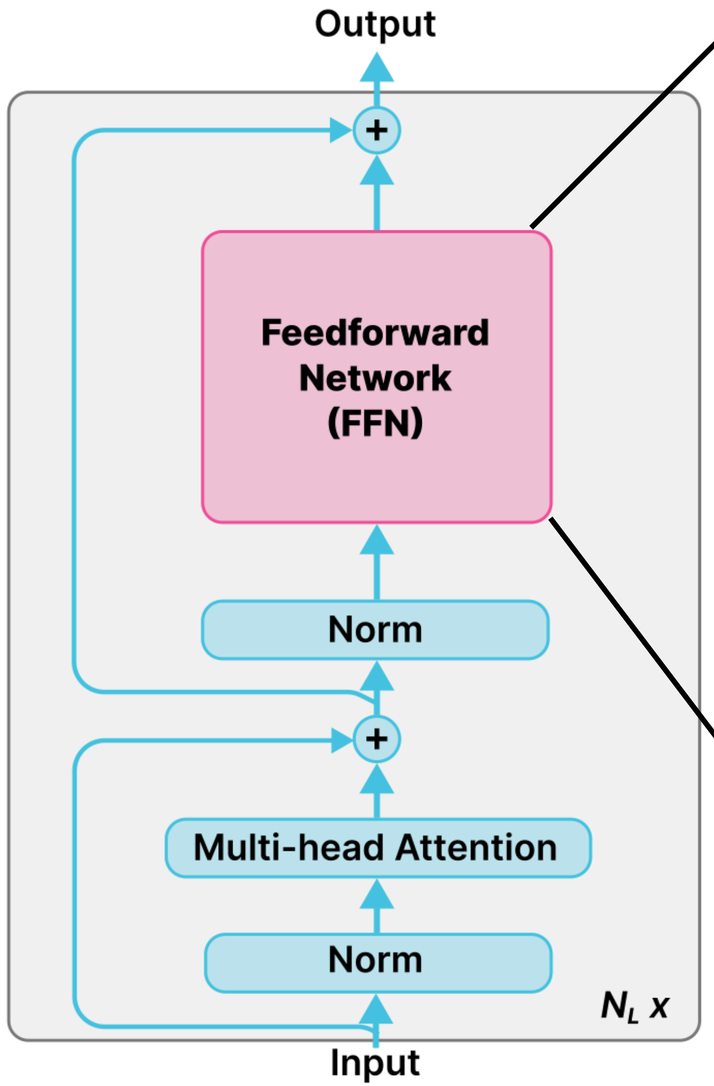
# Mixture-of-Expert (MoE) models are getting more popular




https://medium.com/data-and-beyond/the-ultimate-guide-to-mixture-of-experts-in-ai-286e5aa939be

- It is common for feed-forward layers to account for more than half of the parameters in a transformer.

| | GPT-3 |
|---|---|
| vocab | 50,257 |
| d_model | 12288 |
| n_heads | 96 |
| n_layers | 96 |
| d_ff | 49152 |
| LayerNorm (B) | 0.00 |
| Embedding (B) | 0.62 |
| Attention (B) | 57.99 |
| Feed-forward (B) | 115.97 |
| Total (B) | **174.57** |




output embedding of a token

$d_{\text{model}}$

$d_{\text{ff}} = 4 \times d_{\text{model}}$

$d_{\text{model}}$

input embedding of a token

FeedForward (FF) layer

$$\text{Feed-forward} = 2 \times d_{\text{model}} \times d_{\text{ff}}$$
$$= 1.2\,\text{B/layer}$$
$$= 116.0\,\text{B}$$

Figure from http://arxiv.org/abs/2409.02060 [Muennighoff et al. 2024]

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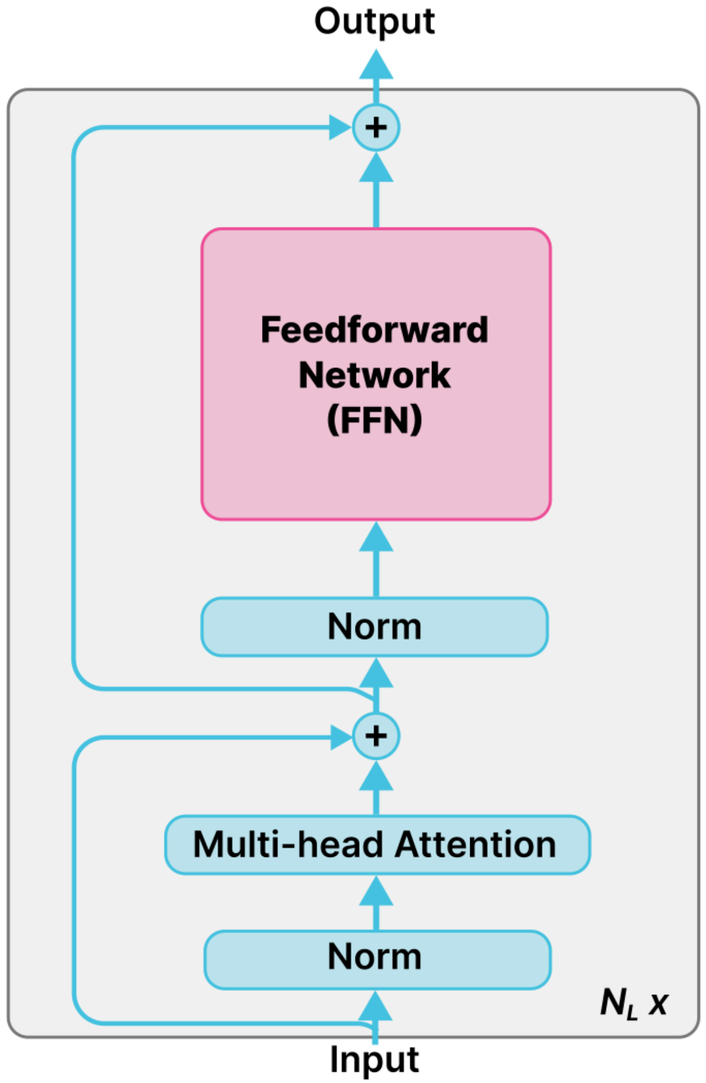


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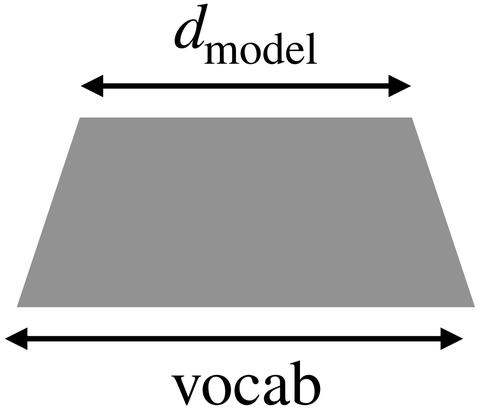
Embedding layer = vocab * d_model
= 50,257 * 12,288
= 0.614B

embedding of a token




input one-hot encoding of a token

Figure from http://arxiv.org/abs/2409.02060 [Muennighoff et al. 2024]

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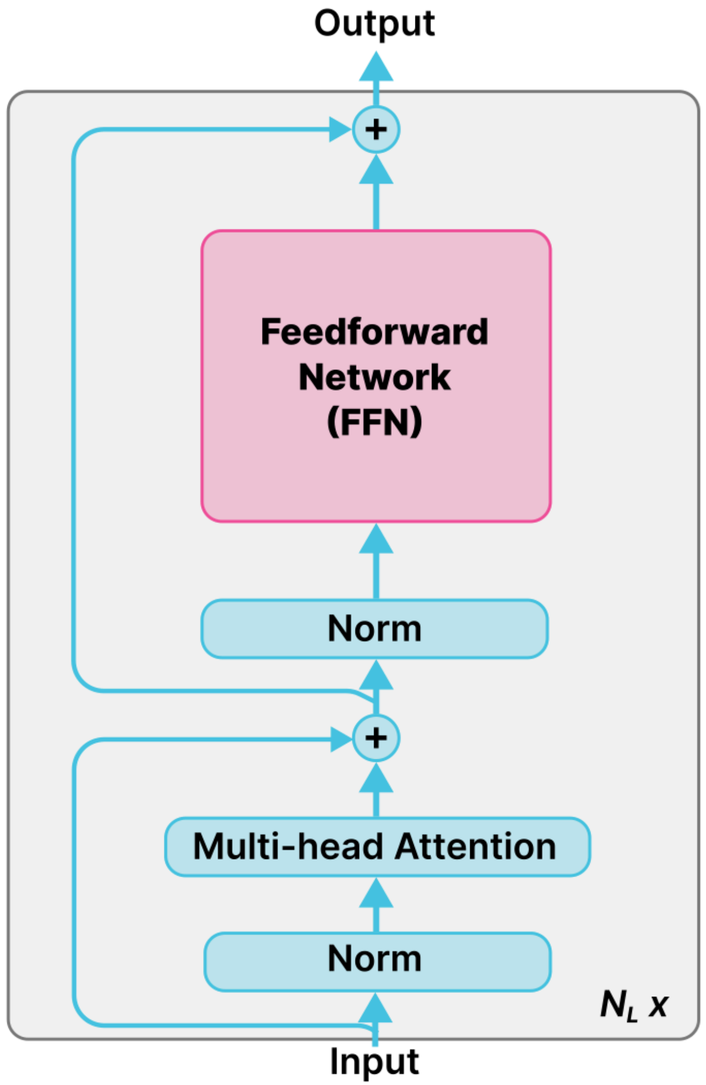


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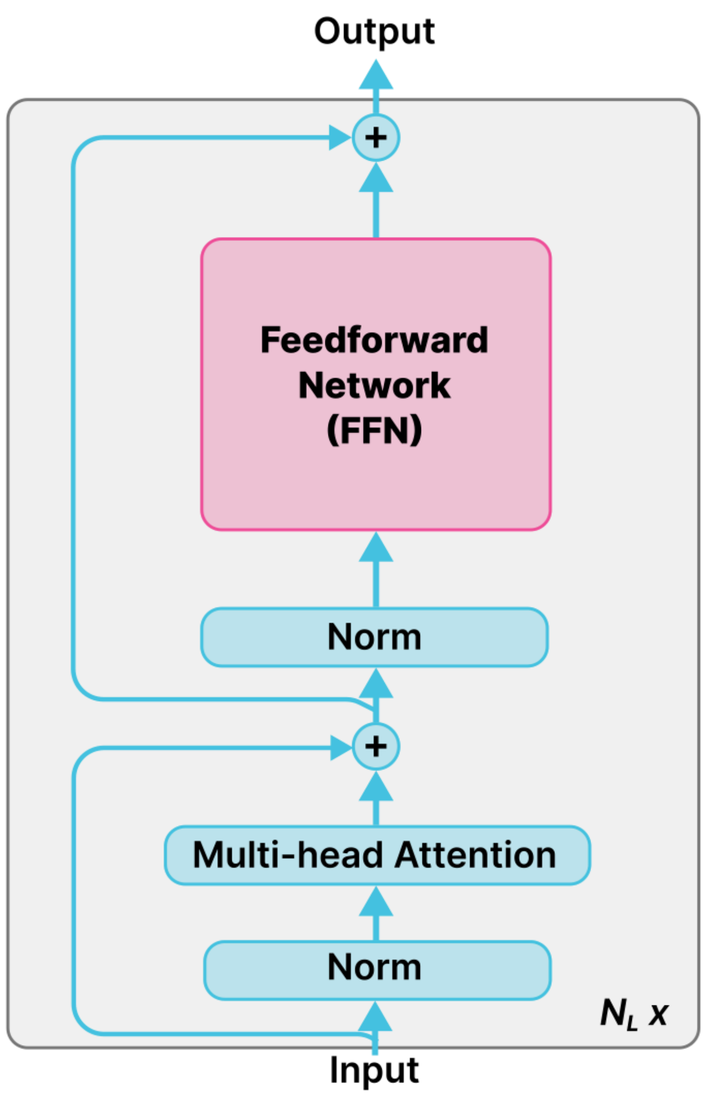
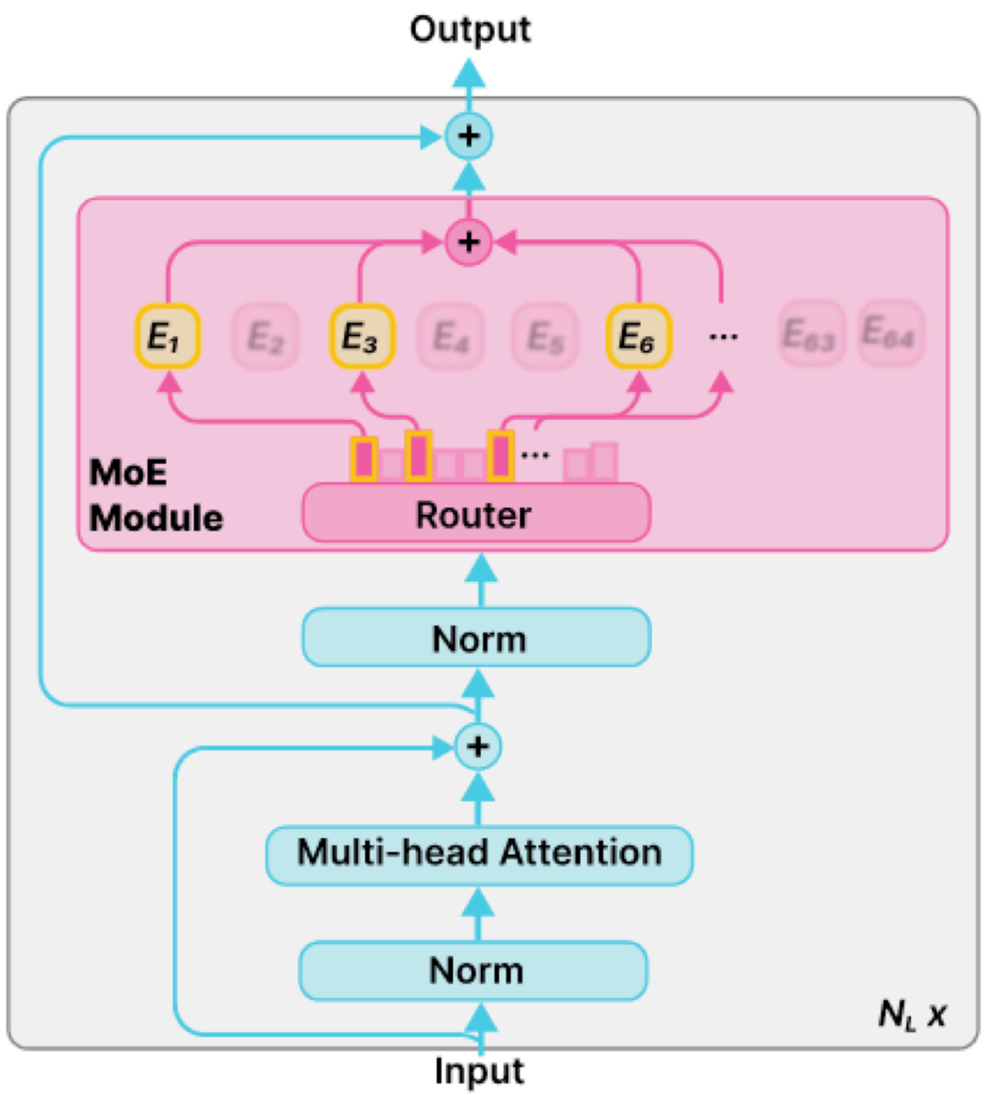
Self attention = $(W_Q, W_K, W_V, P)$
= 4*(d_model * d_model)
= $4 \times 12{,}288^2$
= $0.603\ \mathrm{B/layer}$
= 57.9 B

- Q: how do we increase model capacity (skills the model has) without increasing **inference time compute**?

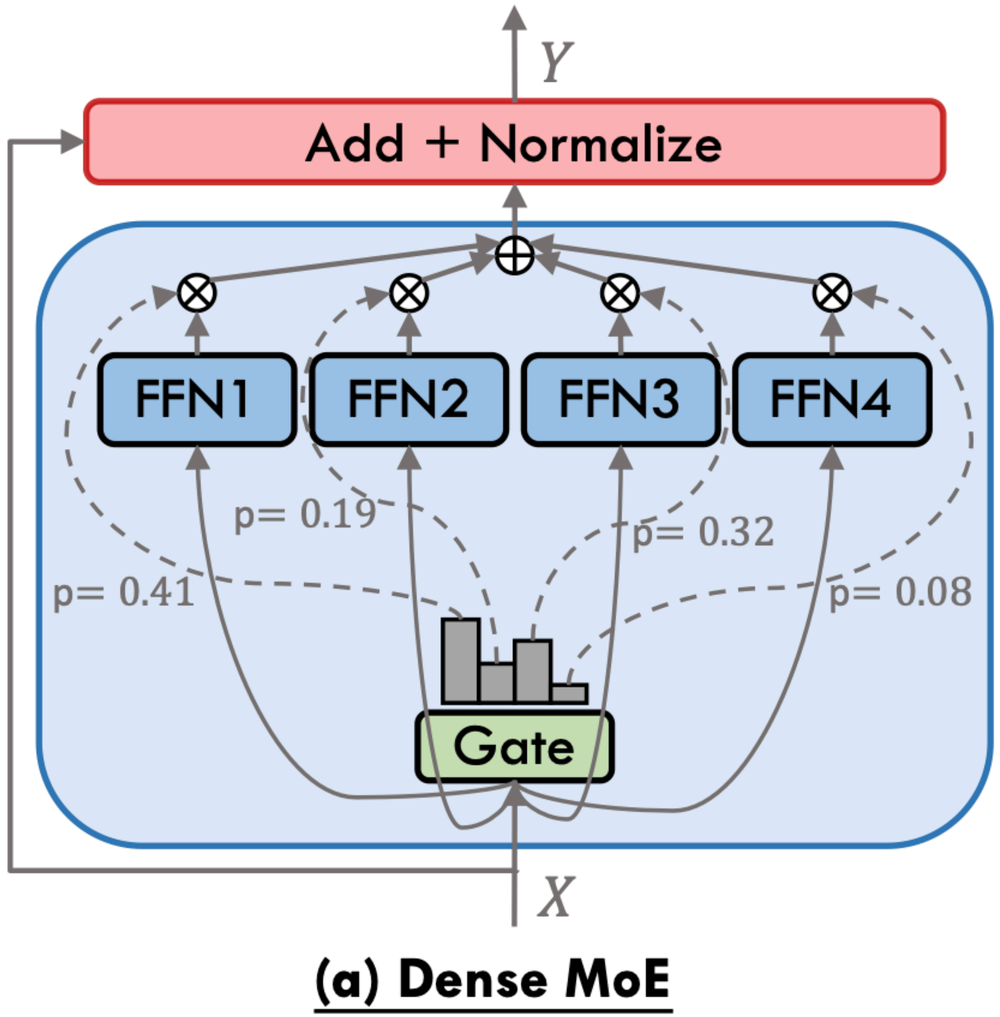
Figure from http://arxiv.org/abs/2409.02060 [Muennighoff et al. 2024]

- One can benefit from scaling up to larger models without increasing as much inference time and memory with **Mixture-of-Experts (MoE)**



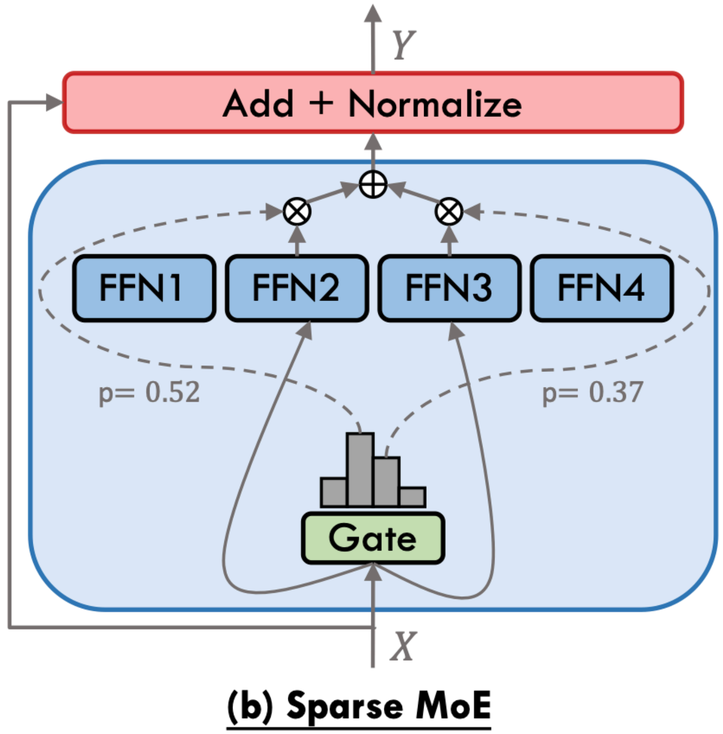



- **Dense MoE** gives every expert non-zero weights and computes weighted sum:
  - $$y = \sum_{i=1}^{N} \underbrace{G(x)_i}_{\text{MoE weight}} \times \underbrace{E_i(x)}_{\text{input emb.}}$$
  - Each expert is a small FFN:
    - $E_i(x) = W_2\,\sigma(W_1 x)$
  - Router is a **dense** softmax
    - $G(x) = \mathrm{Softmax}(W_G x)$




(a) Dense MoE

- **Sparse MoE** selects top-$k$ experts and is now popular
  - $$y = \sum_{i=1}^{N} \underbrace{G(x)_i}_{\text{sparse weights}} \times E_i(x)$$
  - Each expert is a small FFN:
    - $E_i(x) = W_2\,\sigma(W_1 x)$
  - Router is a **softmax over top-$k$ gating**
    - $G(x) = \text{Softmax}(\text{Top-}k(W_G x))$
  - $$\text{Top-}k(v) = \begin{cases} v_i, & v_i \text{ is in the Top } k \\ -\infty, & \text{otherwise} \end{cases}$$



(b) Sparse MoE

- **Sparse MoE** selects top-$k$ experts and is now popular
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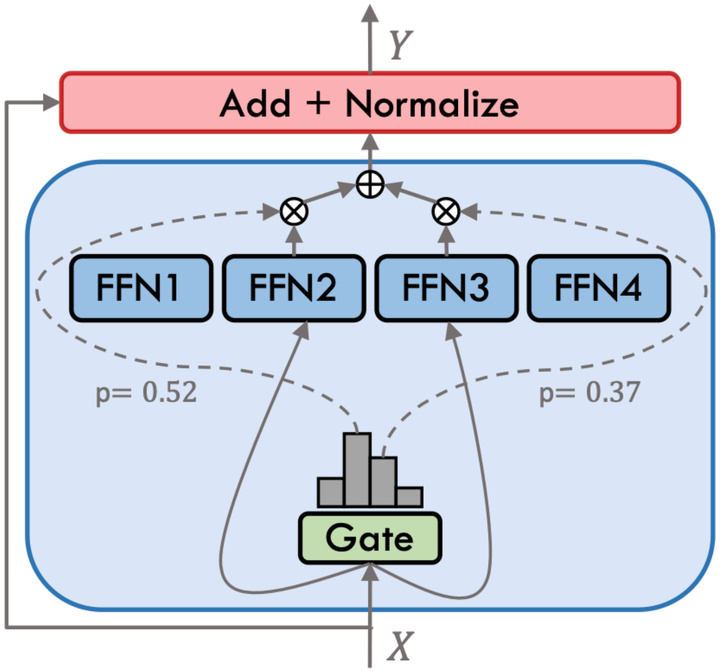
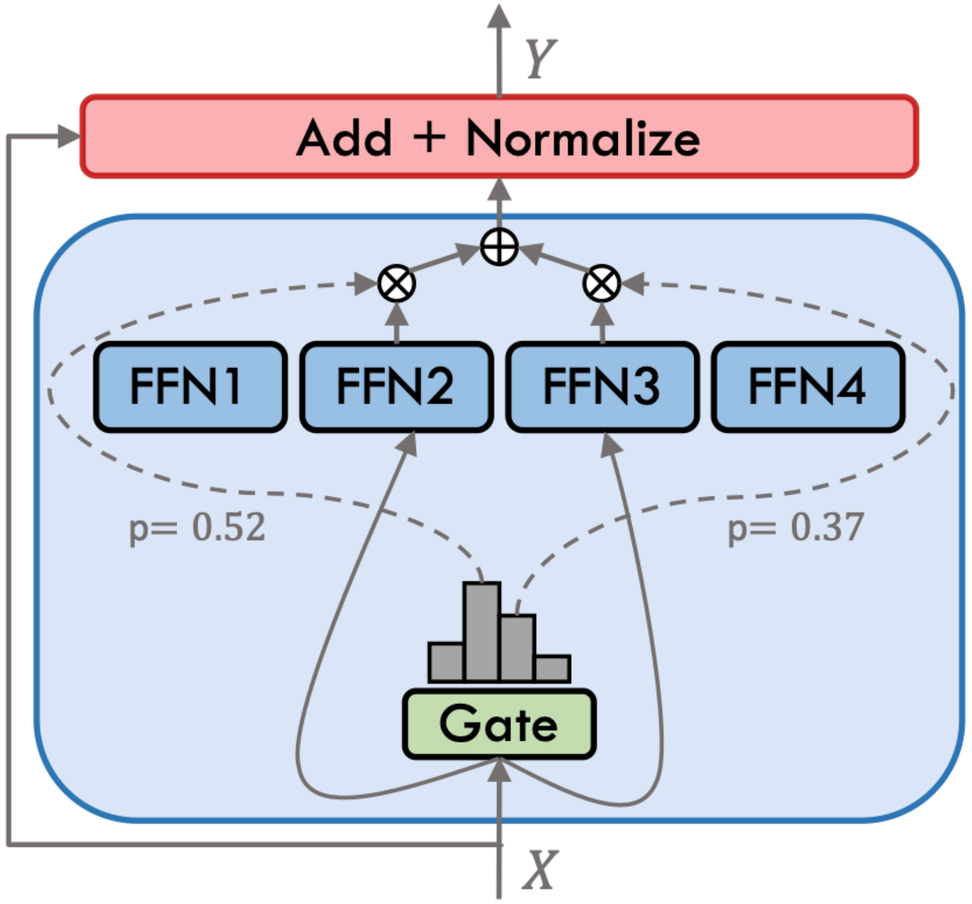


(b) Sparse MoE

- $v = [-7, 3, 8, -2]$
- **Top-$k$**$(v) = [-\infty, 3, 8, -\infty]$
- $\text{Softmax}(\textbf{Top-}k(v))$
$$= [0, \frac{e^3}{e^3 + e^8}, \frac{e^8}{e^3 + e^8}, 0]$$

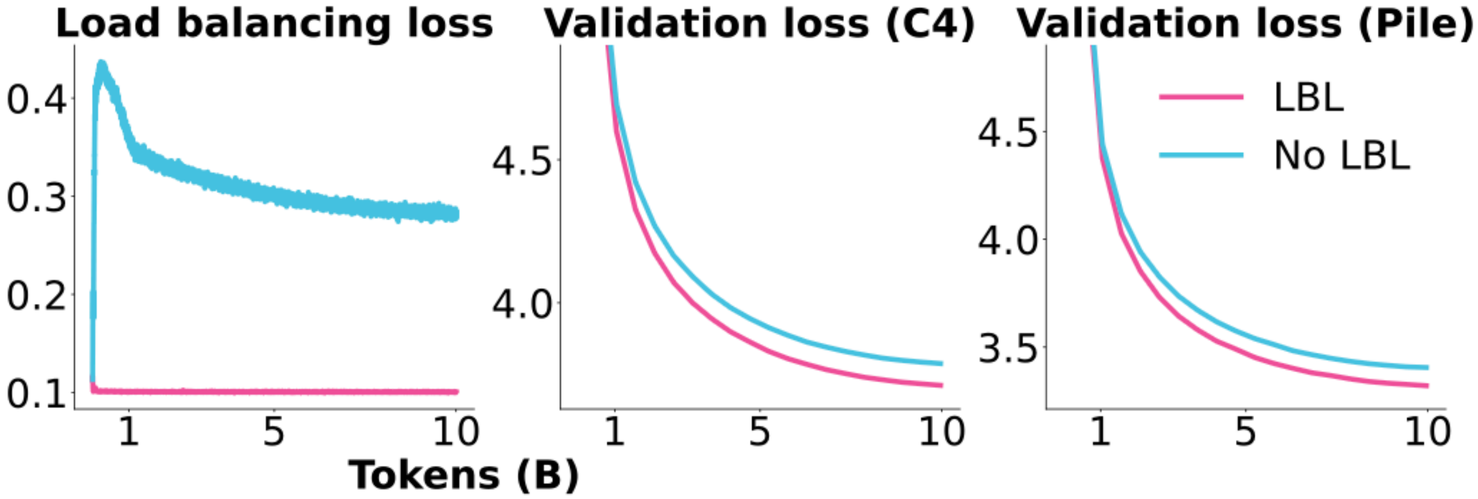
- Many variations of MoE architecture exist
- If left unchecked, the expert gate tends to concentrate on a small number of experts that are popular early in the training.




**(b) Sparse MoE**

- Many variations of MoE architecture exist
- If left unchecked, the expert gate tends to concentrate on a small number of experts that are popular early in the training.
- Proposed solution in OlMoE [Muennighoff et al. 2024]: **Load Balancing**

$$L = L_{\text{CE}} + \alpha L_{\text{LB}}$$




- **Load Balancing (LB)** regularizer: balances experts within a batch

$$L_{\text{LB}} = \sum_{i=1}^{N} f_i P_i$$

$f_i =$ fraction of tokens routed to expert $i$

$P_i =$ total routing probability allocated to $E_i$ in current batch

- Both $f = [f_1, \ldots, f_N]$ and $P = [P_1, \ldots, P_N]$ are non-negative and sum to one.
- Minimizing $f^T P$ encourages $P$ to be orthogonal from $f$, allocating more weight to infrequent modules

- The number of experts chosen, $k$, is typically small
  - Mixtral (MoE from mistral): $k = 1, N = 8$
  - OlMoE (MoE from AI2): $k = 8, N = 64$
- For MoEs the gain is in **inference-time computation**
  - GPU memory requirement ~= # of **total parameters**
  - FLOPS computation requirement ~= # of **active parameters**

  where **# of active parameters** is the count of parameters that are selected by the router

**DeepSeek V4 Parameter Counts at a Glance**

| Model | Total Parameters | Active Parameters | Download Size |
|---|---|---|---|
| DeepSeek-V4-Pro | 1.6 Trillion | 49 Billion | ~865 GB |
| DeepSeek-V4-Flash | 284 Billion | 13 Billion | ~160 GB |
| DeepSeek-V3.2 (predecessor) | 671 Billion | 37 Billion | ~380 GB |

$$k/N \simeq 3\,\%$$

- Naming convention:
    - **Mixtral 8x7B**: A popular, high-performance model with 8 experts of 7 billion parameters each.
    - **Qwen3.5-35B-A3B**: Indicates a Qwen model with 35 billion total parameters, and often implies the "A" refers to activated parameters during inference

- The difference in slopes show the better scaling of MoE w.r.t. active parameters

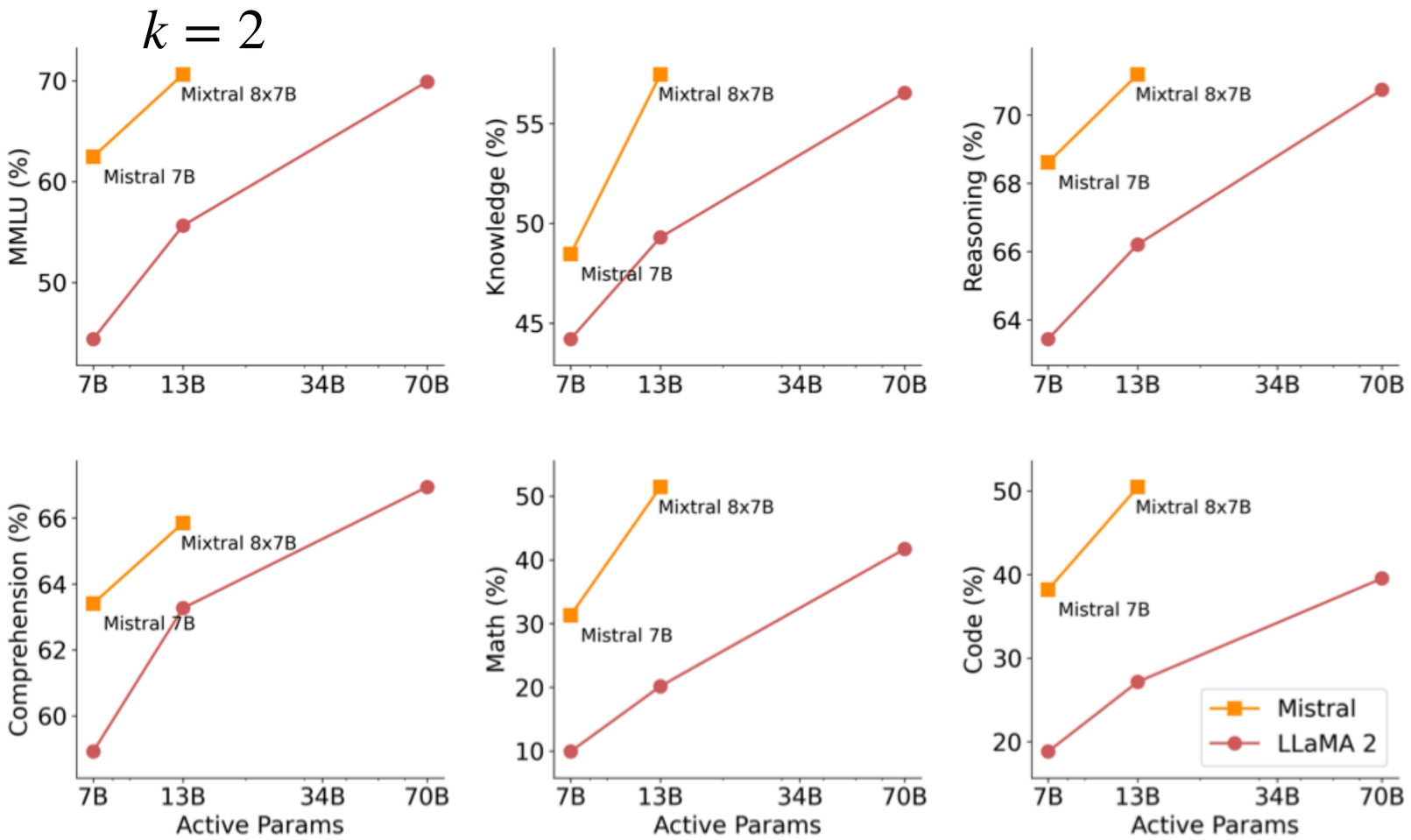
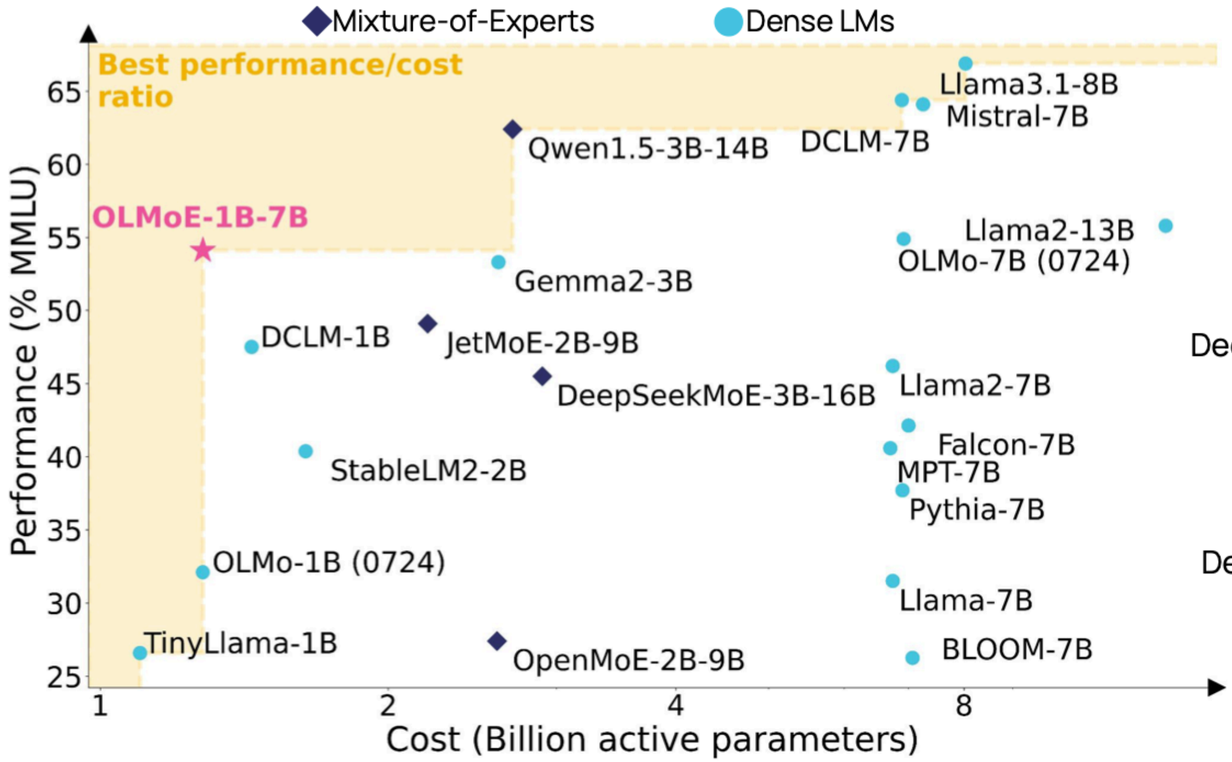



**Figure 3: Results on MMLU, commonsense reasoning, world knowledge and reading comprehension, math and code for Mistral (7B/8x7B) vs Llama 2 (7B/13B/70B).** Mixtral largely outperforms Llama 2 70B on all benchmarks, except on reading comprehension benchmarks while using 5x lower active parameters. It is also vastly superior to Llama 2 70B on code and math.

Figure from http://arxiv.org/abs/2401.04088

- MoEs achieve the frontier of **inference-cost** vs. performance trade-off for open-source models




**How open are open MoEs?**

| Name | Model | Data | Code | Logs | #ckpts |
|---|---|---|---|---|---|
| Grok-86B-314B | ✔ | ✘ | ✘ | ✘ | 1 |
| Mixtral-39B-141B | ✔ | ✘ | ✘ | ✘ | 1 |
| DBRX-36B-132B | !! | ✘ | ✘ | ✘ | 1 |
| Skywork-22B-146B | !! | ✘ | ✘ | ✘ | 1 |
| DeepSeekV2-21B-236B | !! | ✘ | ✘ | ✘ | 1 |
| Arctic-17B-480B | ✔ | !! | ✘ | ✘ | 1 |
| Qwen2-14B-57B | ✔ | ✘ | ✘ | ✘ | 1 |
| Mixtral-13B-47B | ✔ | ✘ | ✘ | ✘ | 1 |
| Jamba-12B-52B | ✔ | ✘ | ✘ | ✘ | 1 |
| DeepSeekMoE-3B-16B | !! | ✘ | ✘ | ✘ | 1 |
| Qwen1.5-3B-14B | !! | ✘ | ✘ | ✘ | 1 |
| OpenMoE-3B-9B | ✔ | ✔ | ✔ | ✘ | 6 |
| JetMoE-2B-9B | ✔ | !! | !! | ✘ | 1 |
| OLMoE-1B-7B | ✔ | ✔ | ✔ | ✔ | 244 |

Figure 1: **Performance, cost, and degree of openness of open MoE and dense LMs.** Model names contain rounded parameter counts: `model-active-total` for MoEs and `model-total` for dense LMs. `#ckpts` is the number of intermediate checkpoints available. We highlight MMLU as a summary of overall performance; see §3 for more results. **OLMoE-1B-7B** performs best among models with similar active parameter counts and is the most open MoE.

Figure from http://arxiv.org/abs/2409.02060

- MoEs achieve favorable **training-cost** vs. performance trade-off

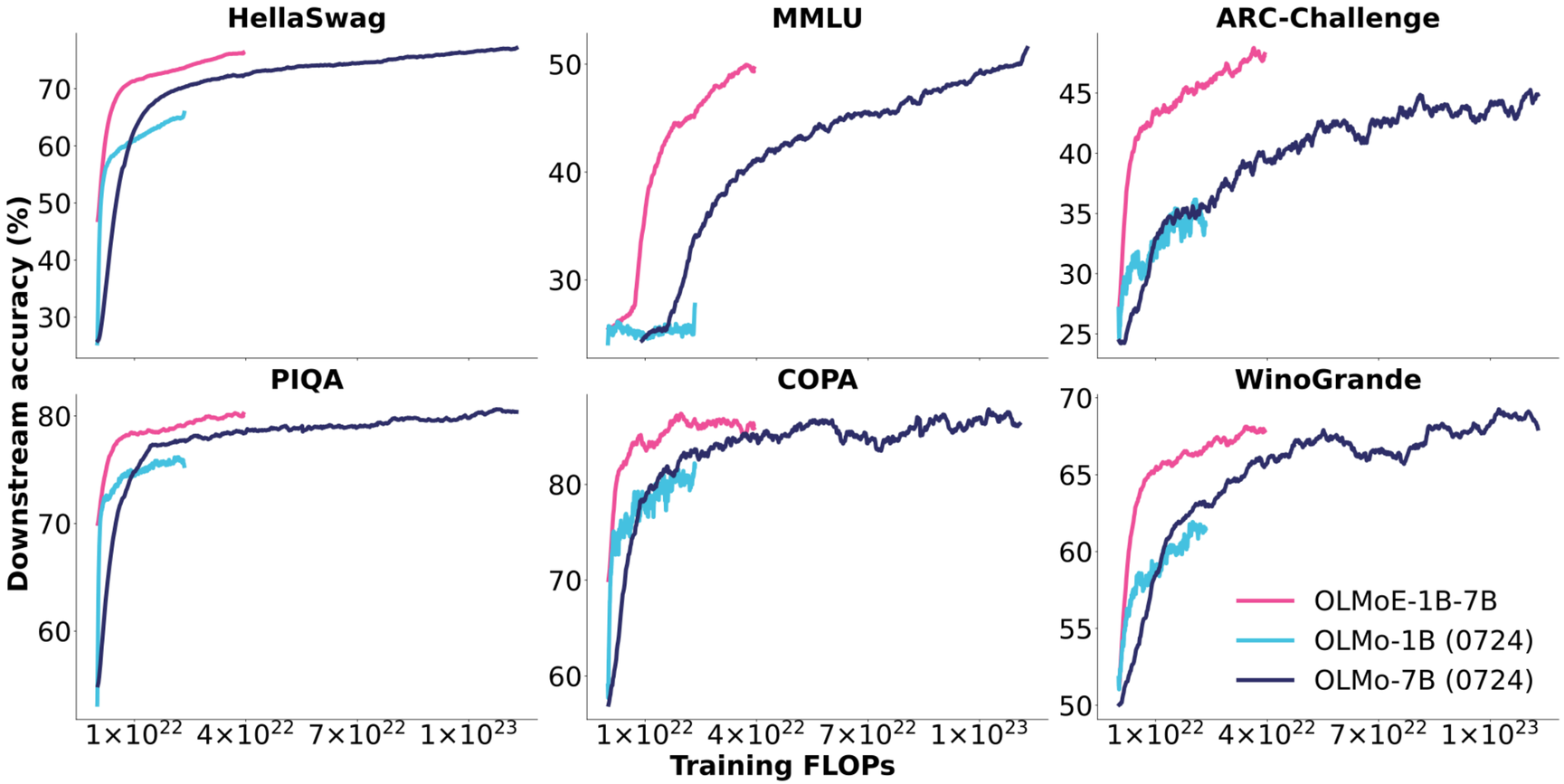
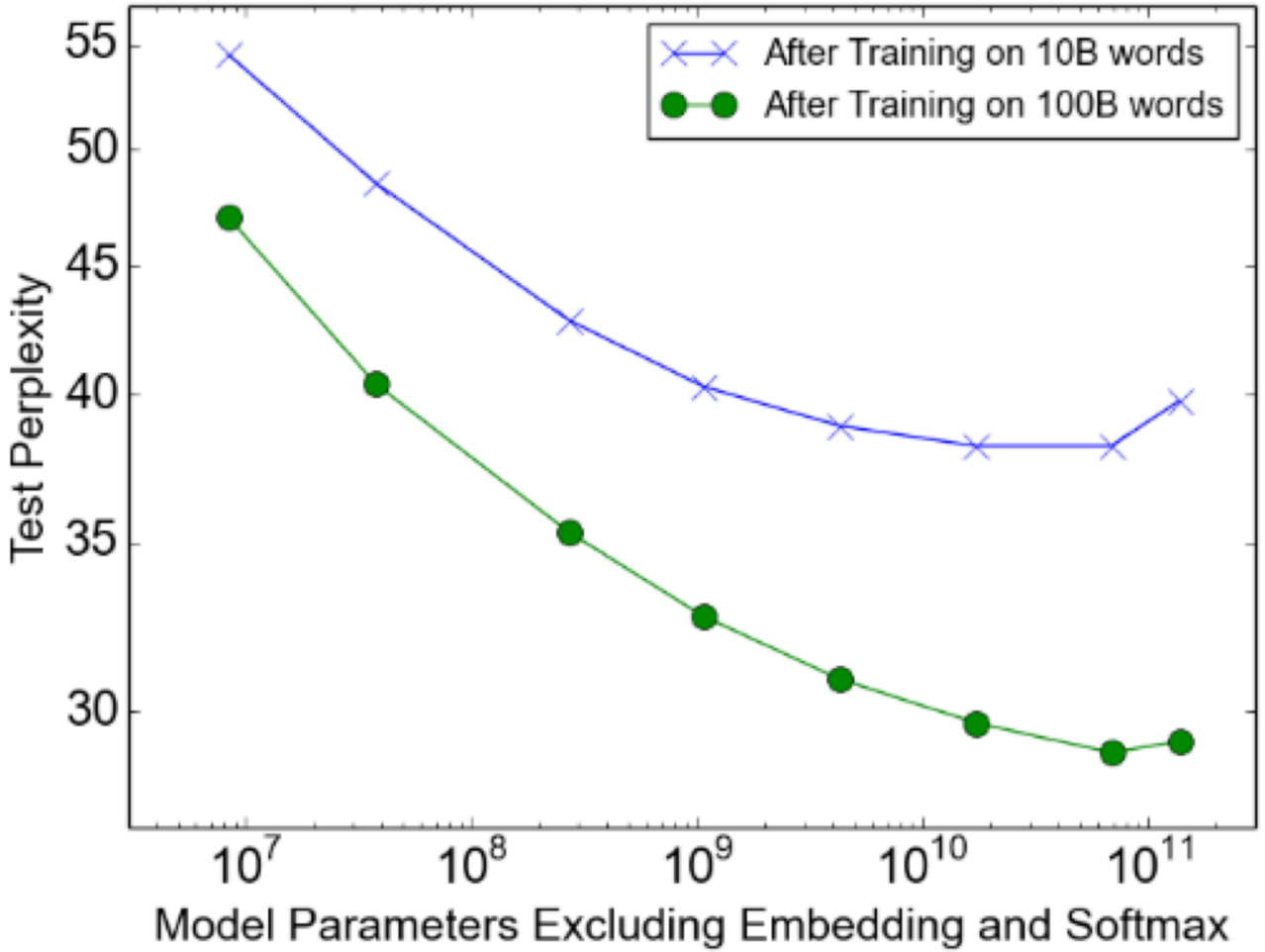



Figure 3: **Evaluation of OLMoE-1B-7B and the current best OLMo models during pretraining.** **OLMoE-1B-7B** differs from the OLMo models in its MoE architecture, several training hyperparameters, and its training dataset, see §2. A version of this plot with tokens as the x-axis and markers where annealing starts is in Appendix E. More results, logs, and configurations: https://wandb.ai/ai2-llm/olmoe/reports/Plot-OLMoE-1B-7B-vs-OLMo-7B-vs-OLMo-1B--Vmlldzo4OTcyMjEz

Figure from http://arxiv.org/abs/2409.02060

- Earlier works in **MoE designed for RNNs** favored very large number of experts, getting better with up to $N = 131{,}071$ experts




32, 256, 1024, 4096, 16384, 65536, and 131072 experts.

up to 137 billion parameters in the MoE layer.

- More recent **MoEs for transformers** require comparably smaller number of experts.

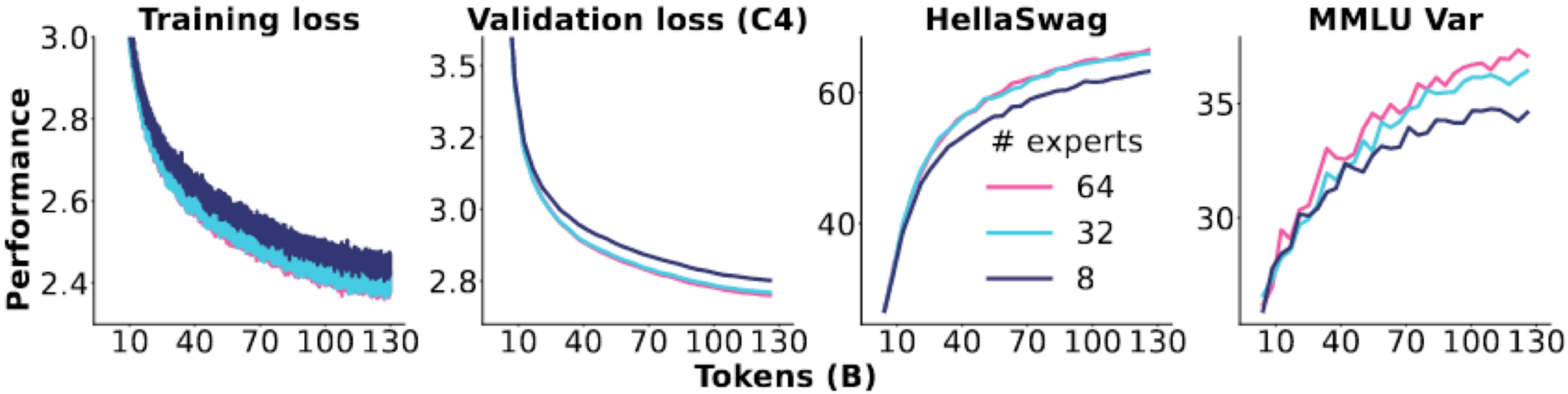



Figure 5: **Expert granularity.** We vary the number of experts in tandem with the FFN dimension to ensure that active and total parameters and thus compute cost remain the same. For example, for 64 experts, the FFN dimension is 1,024 and 8 experts are activated, while for 32 experts it is 2,048 with 4 activated experts. More results, logs, and configurations: https://wandb.ai/ai2-llm/olmoe/reports/Plot-Granularity--Vmlldzo4OTIxOTE4

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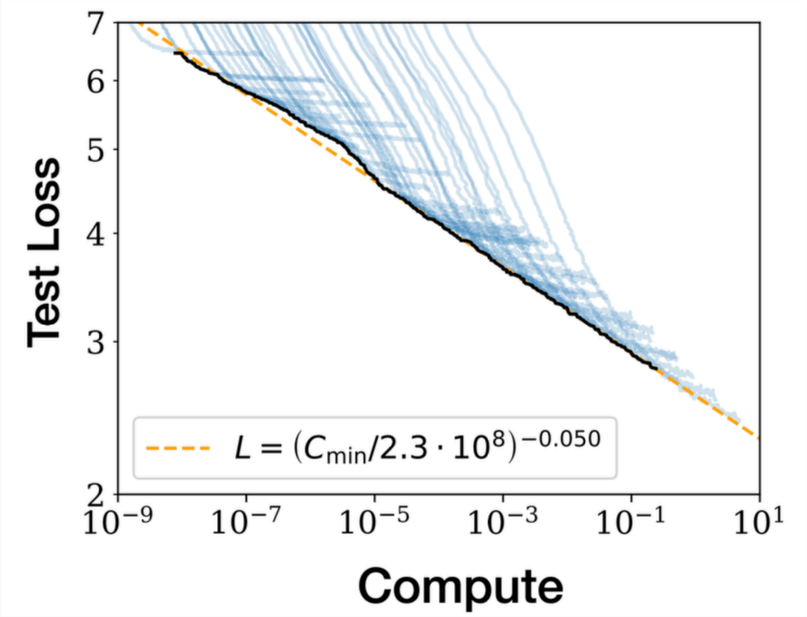
# Test-time scaling
# Test-time compute
# Test-time train

# How to improve performance of LMs?

- Scaling Pre-training

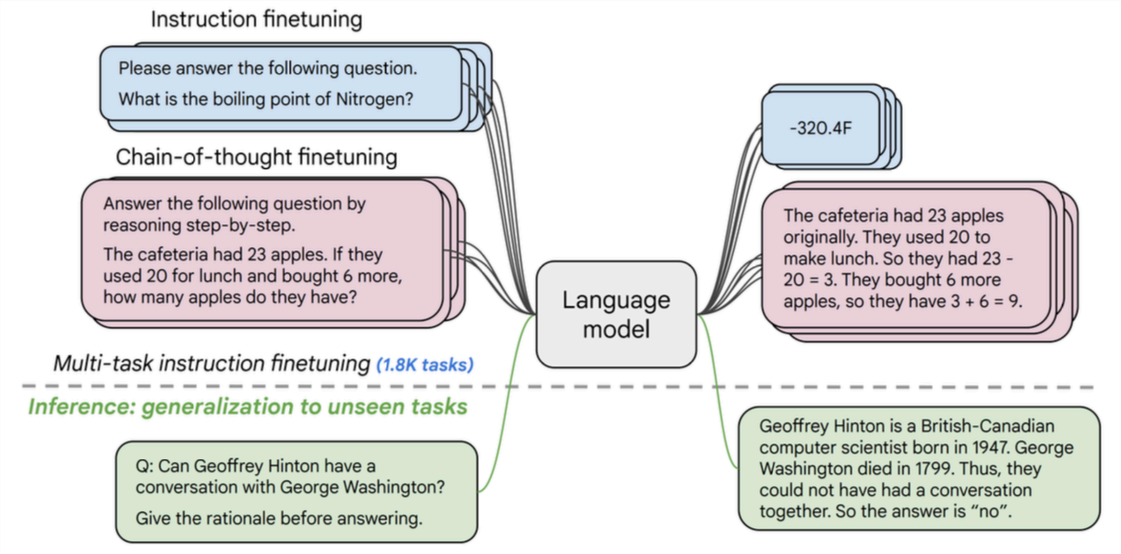
[2020-] **Scaling pretraining:** larger model, larger dataset




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

- Scaling Post-training

[2022-] **Scaling post-training:** e.g., fine-tune on (input, output) pairs




*Scaling Instruction-Finetuned Language Models* [Chung et al., 2022]

[Welleck et al. 2024]

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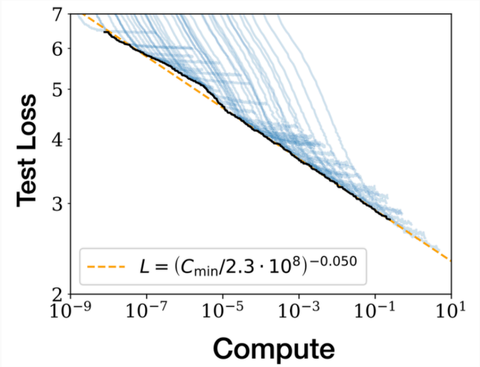


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- Scaling Post-training

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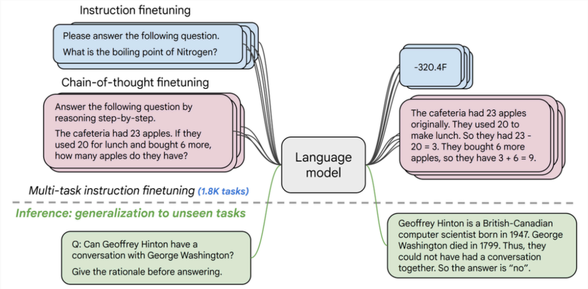


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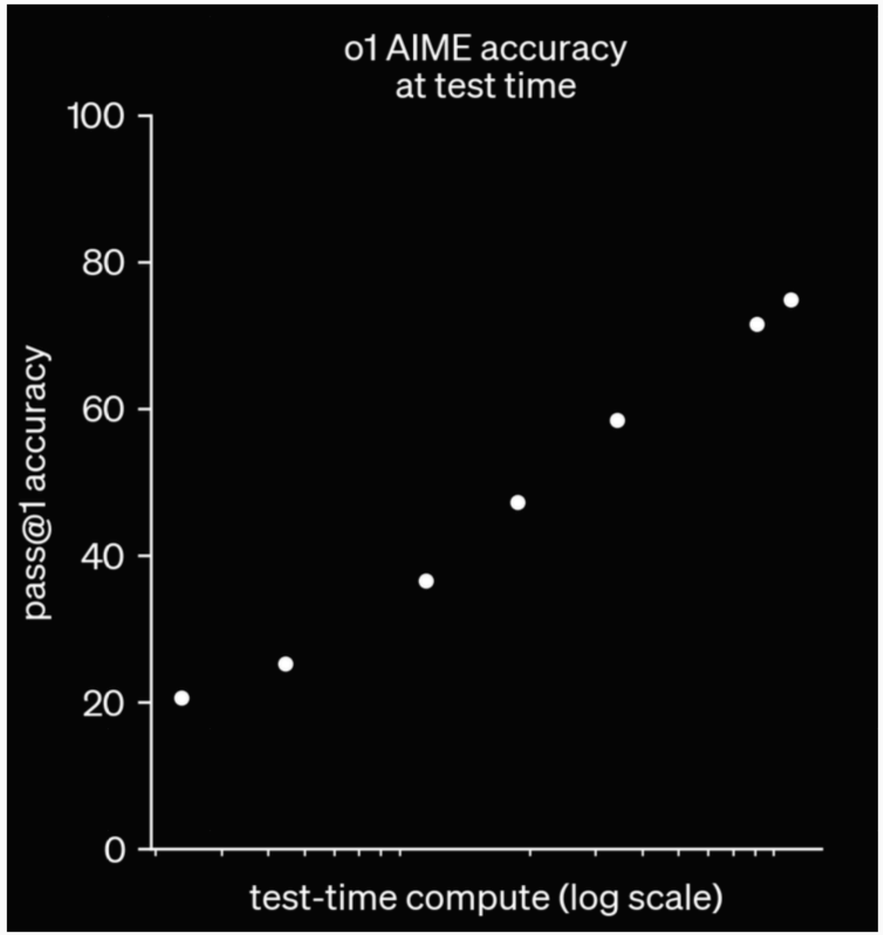
[Welleck et al. 2024]

- Test-time scaling

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



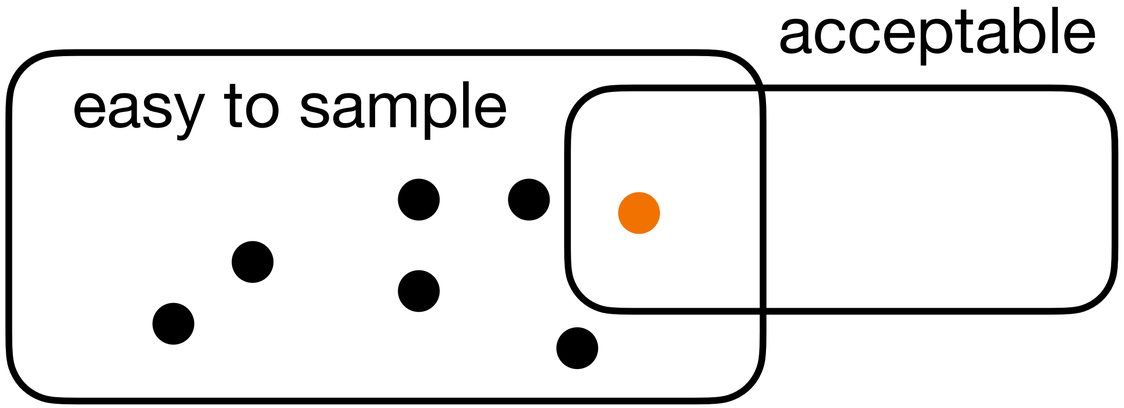

Test-time compute vs. accuracy ([OpenAI, 2024])

- Goal: design a system $G$ that generates acceptable sequences:

$$\arg\max_{G} \mathbb{E}_{y\sim G}\, A(y)$$

where acceptable, $A(\cdot)$, is measured by **correctness, human preference, etc**. (related to Reinforcement Learning with Verifiable Reward)

- We have a **pretrained model** that can sample from $y \sim P_\theta(y \mid x)$, which may produce unacceptable samples.



- If we have an oracle that can verify correctness of an output, one can repeat
  - $z \sim P_\theta(z \mid x)$
  - $y \sim P_\theta(y \mid x, z)$
- stop if oracle says it 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 $\sum_{k=2}^{\infty} f(k)$.

z:

**LLEMMA 34B solution:**
We have

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

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

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

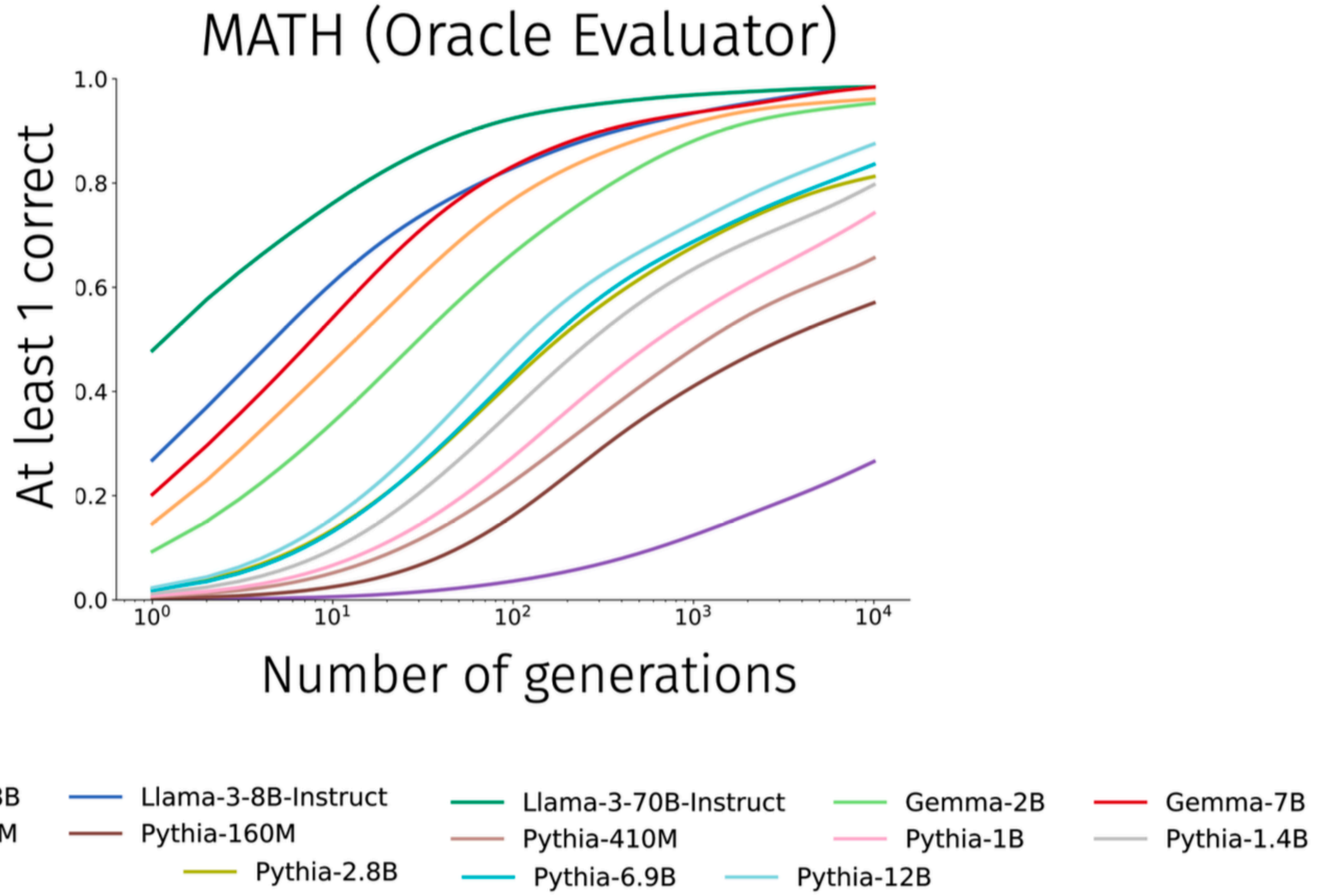
$$= 1 - \frac{1}{2008}$$

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

y:

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

- When oracle is correct, this strategy increases accuracy.



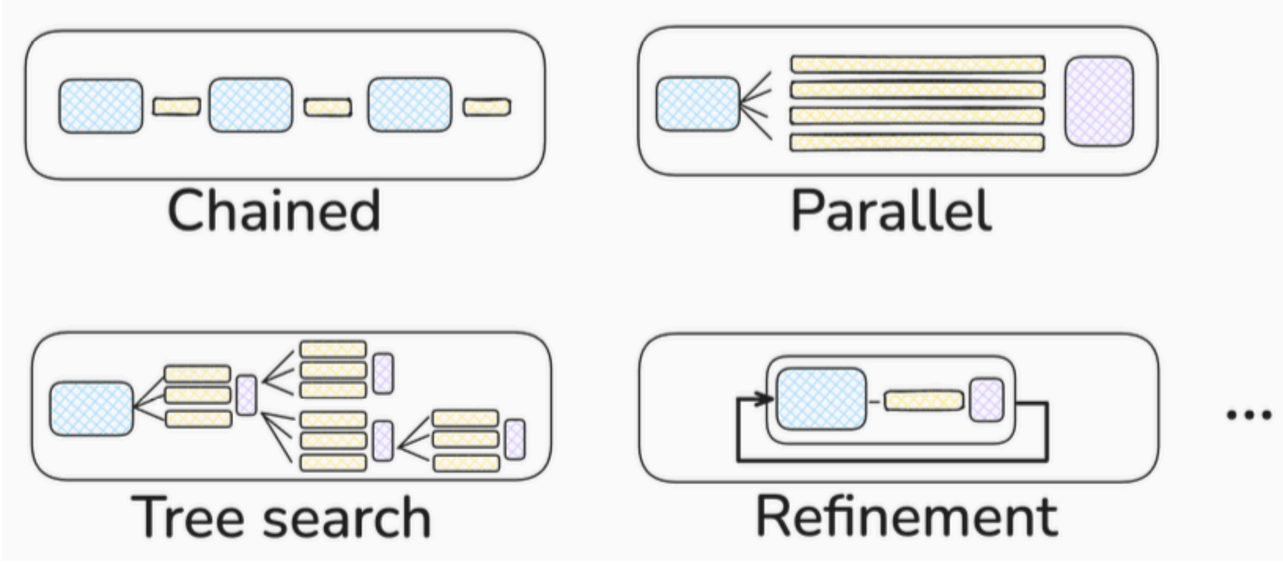

[1]Adapted from [Brown et al., 2024]. See also [Li et al., 2022, Cobbe et al., 2021, Jiang et al., 2023]

- In general, a **meta-generator** $G$ uses multiple generative model calls and other tools, hyper-parameters, prompts:

$$y \sim G(y \mid x; g_1, \ldots, g_G, \phi)$$

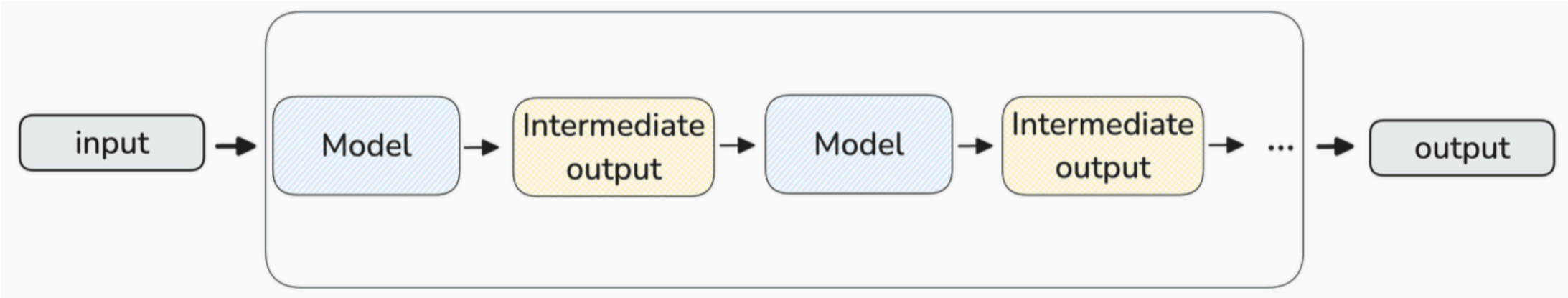
- Design choices:
  - $G$ : strategy for calling generators
  - $g_1, \ldots, g_G$ : choices of generators
  - $\phi$ :other models, number of tokens, etc.

- **Meta-generation strategies** include:
  - Chain
  - Parallel
  - Tree search
  - Refinement/self-correction

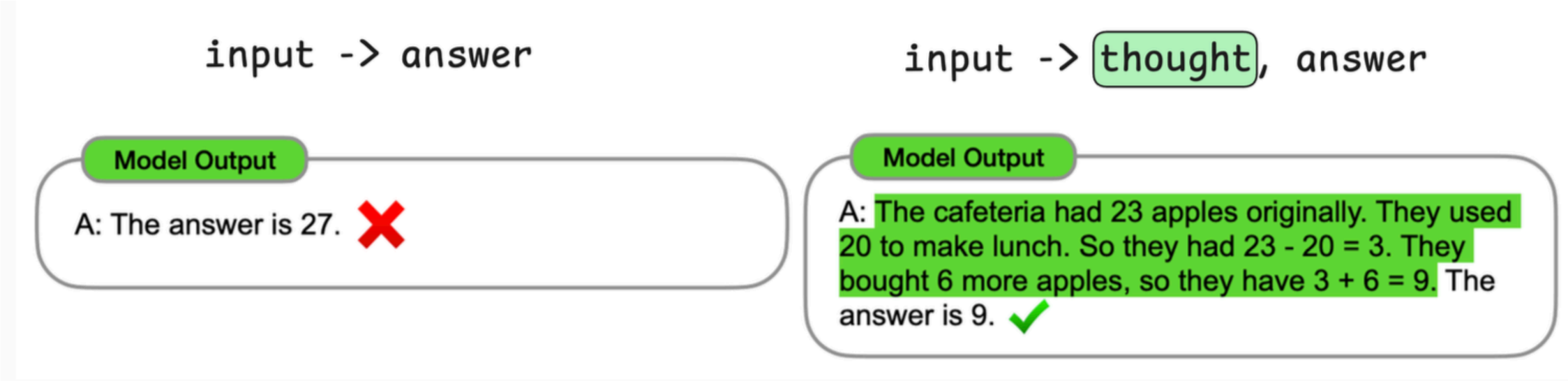


1. **Chained meta-generators** call the LM repeatedly, with augmented prompts.

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



- **Chain-of-Thought** is an example:

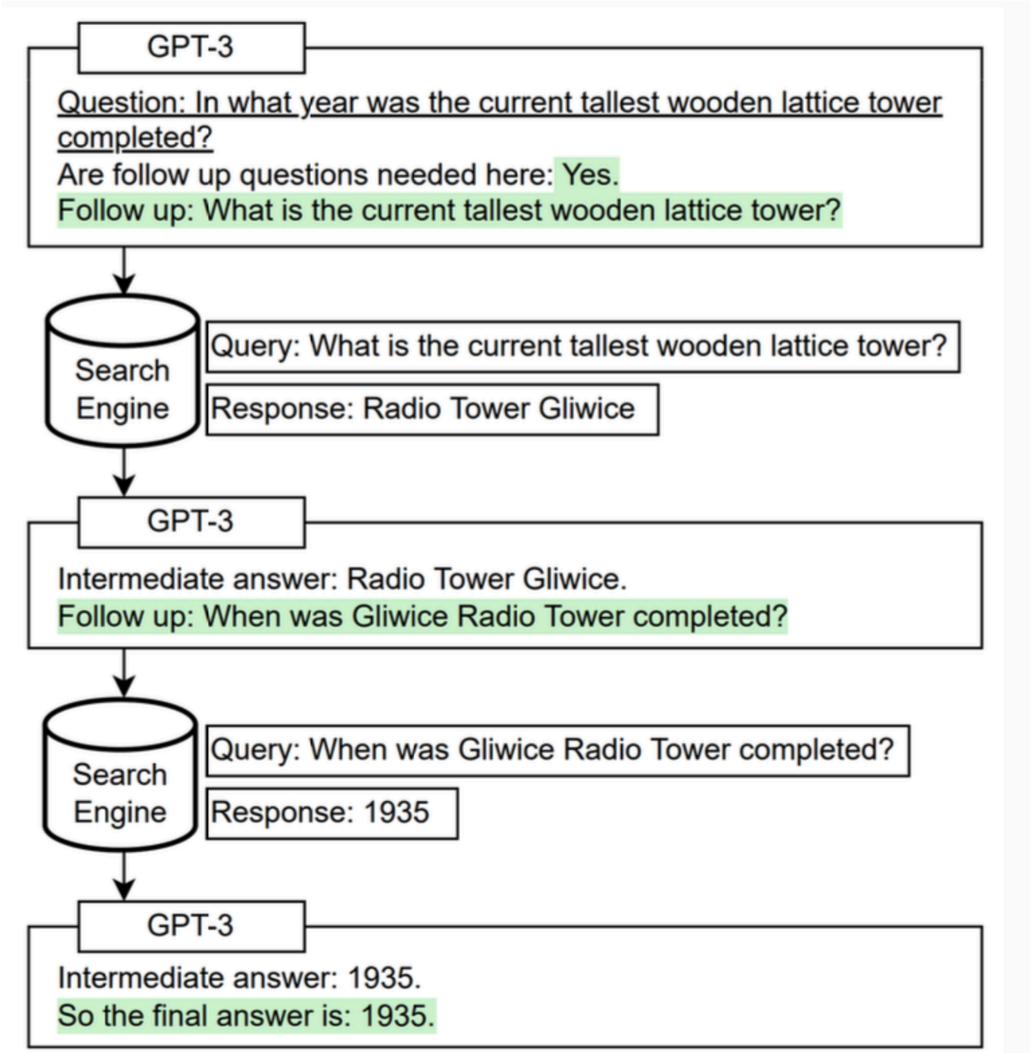



- This auto-regressive decoding of CoT can be represented by

  generate thought: $z \sim P_\theta(z \mid x)$

  generate answer: $y \sim P_\theta(y \mid x, z)$

- **Search** is an example of multiple step chained meta-generation, with access to **tools like search engine calls**:



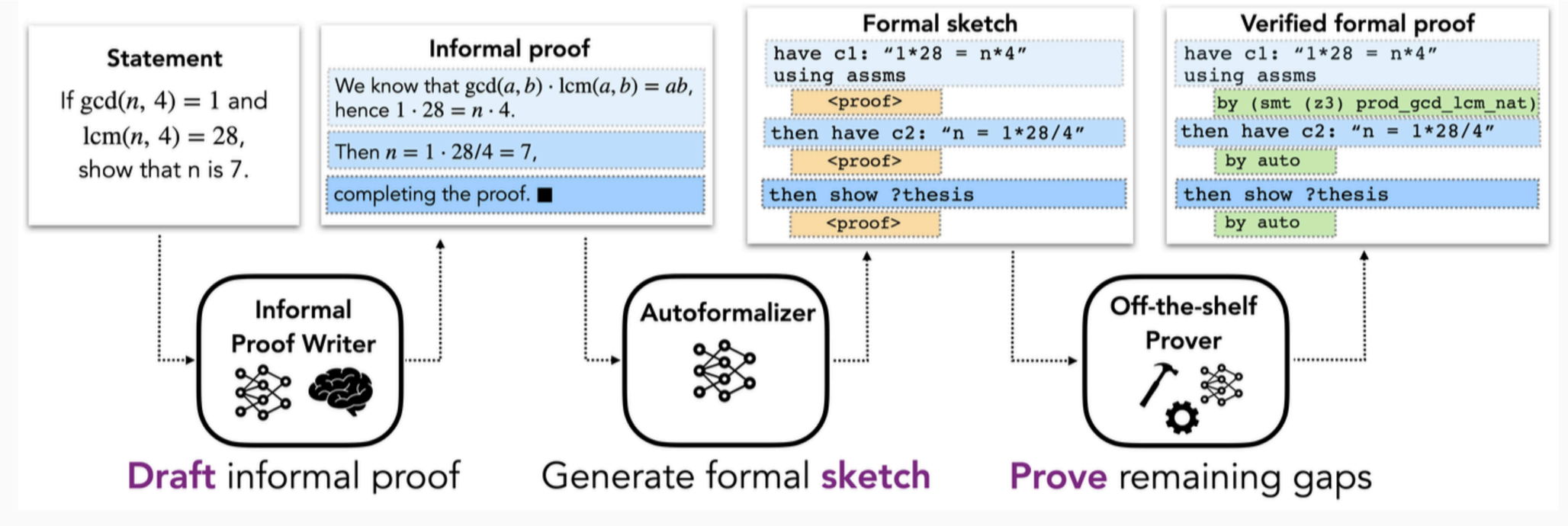

*Self-Ask* [Press et al., 2023]

- This can be represented as a program, which typically improves the reasoning:

```
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]

- Many other strategies
  - Re-write input before feeding in to LM for an answer: System-2 attention [Weston and Sukhbaater, 2023]
  - Sketch proof, fill gaps, check proof Draft-sketch-prove [Jiang et al., 2023]




  - Chained meta-generators only utilize/control the **input space.**

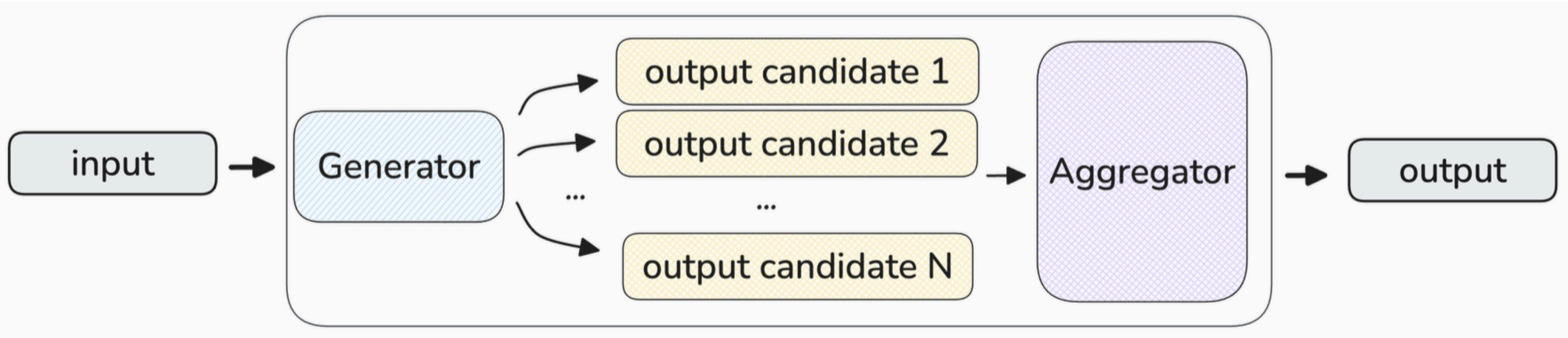
2. **Parallel meta-generators** generate multiple outputs to select from.

- Generate candidates:

$$\{y^{(1)}, \ldots, y^{(m)}\} \sim G(\cdot \mid x)$$

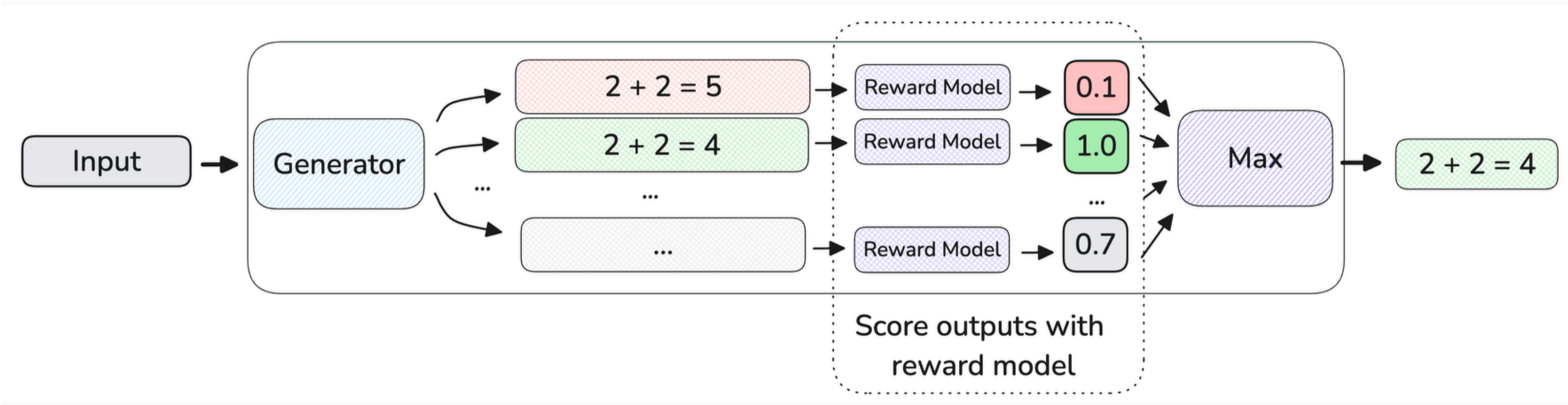
- Aggregate:

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

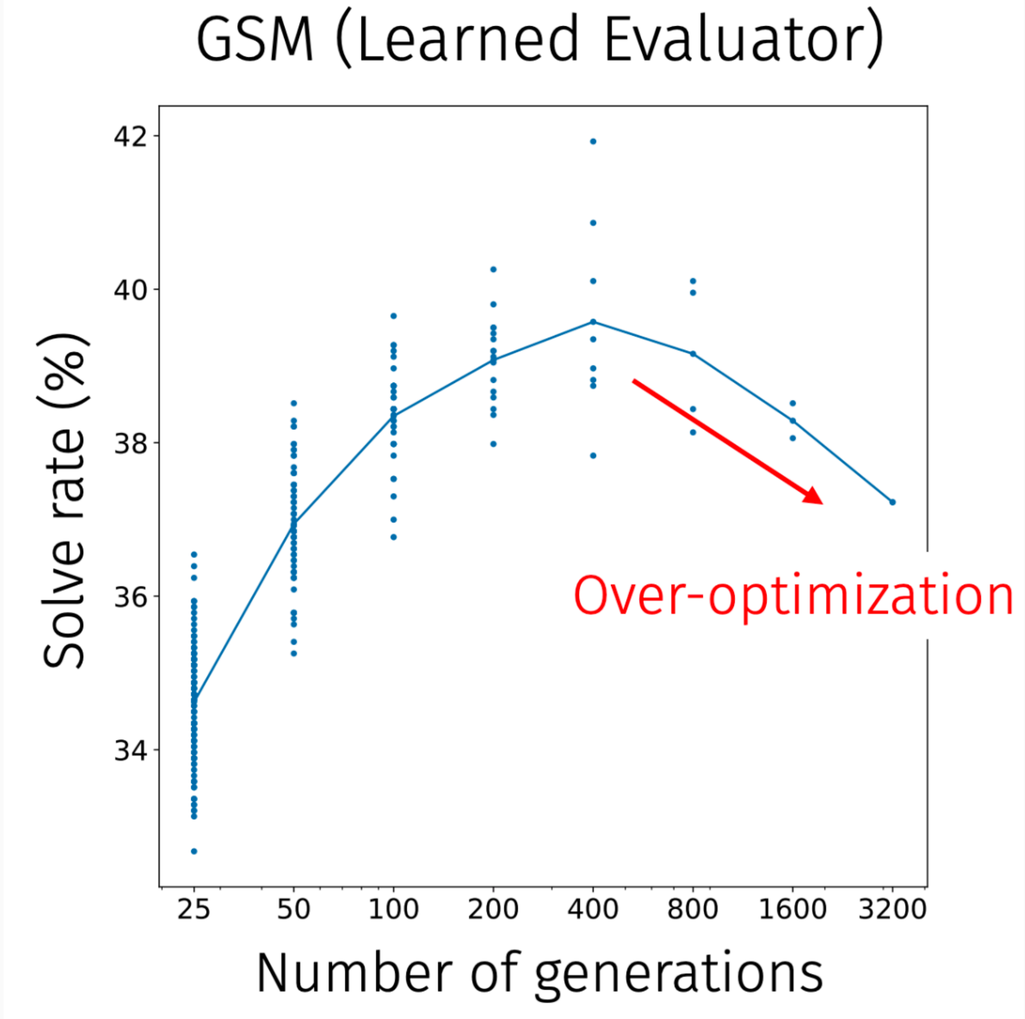


- **Best-of-$m$ sampling** and **rejection sampling**
  - Aggregate: with a reward model:

$$y \leftarrow \arg \max_{y^{(1)},\ldots,y^{(m)}} A(y)$$



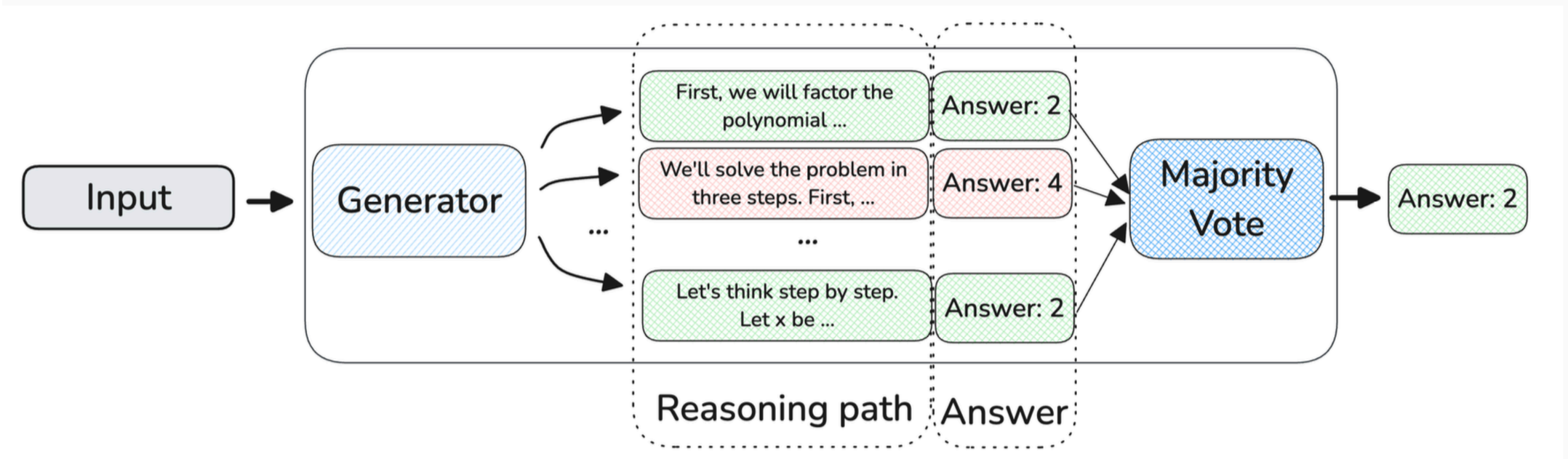
- This can suffer from over optimizing to the reward $A(\cdot)$




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

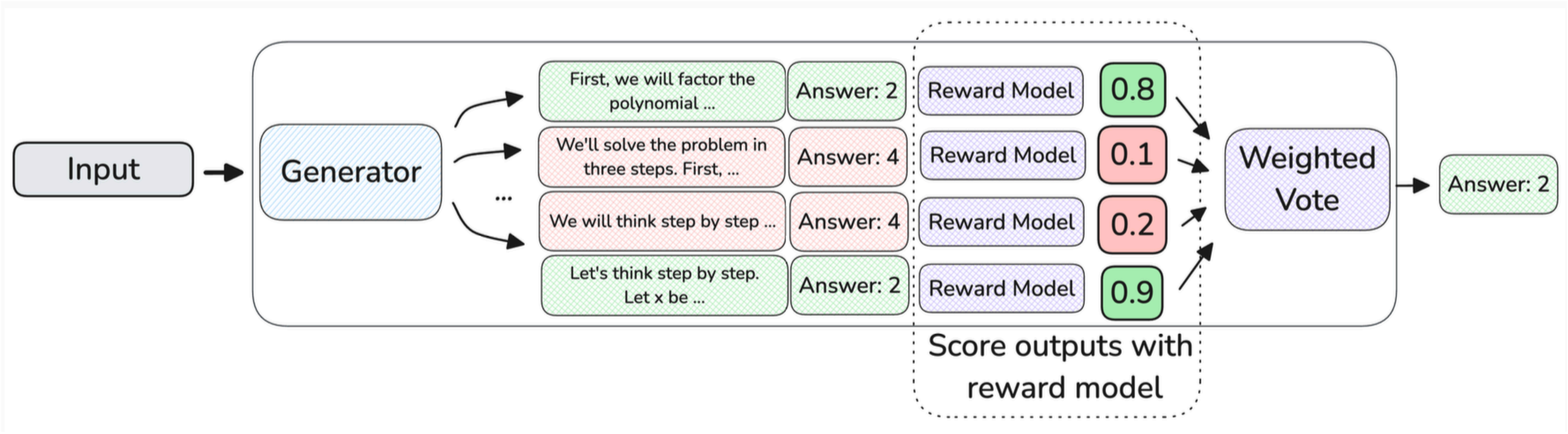
- **Majority voting** and **self-consistency** does not require external reward model.
  - Aggregation:

$$y \leftarrow \arg\max_{a} \sum_{i=1}^{m} \mathbb{I}\{y^{(i)} = a\},$$

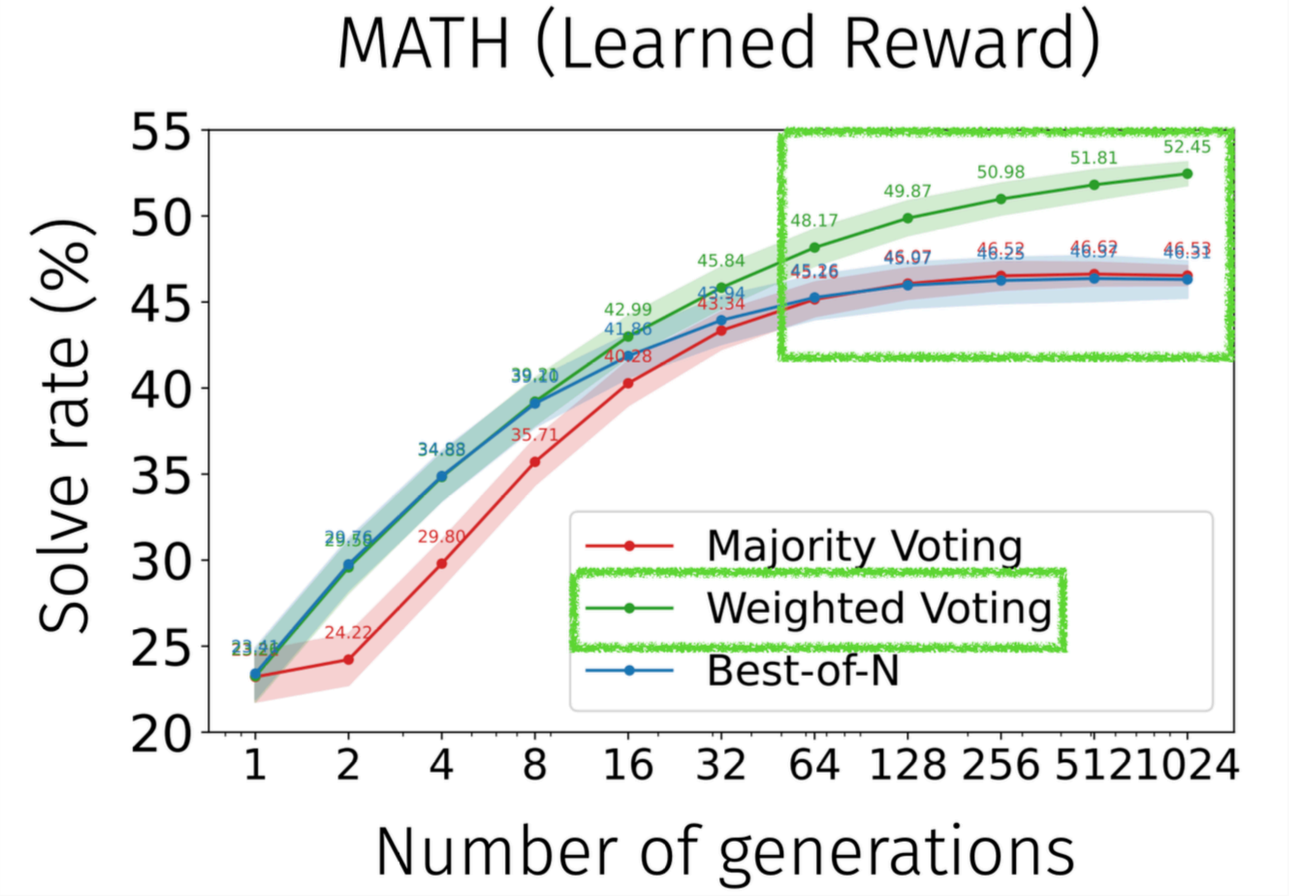


- You can combine **best-of-$m$ and voting**:
- Weighted aggregation:

$$y \leftarrow \arg\max_{a} \sum_{i=1}^{m} A(y^{(i)}) \cdot \mathbb{I}\{y^{(i)} = a\}$$



- **Weighted voting** can outperform **best-of-$m$**
  - This happens when weighted maximum reward is more likely to give the correct answer
  - Q: why does weighted voting work better?

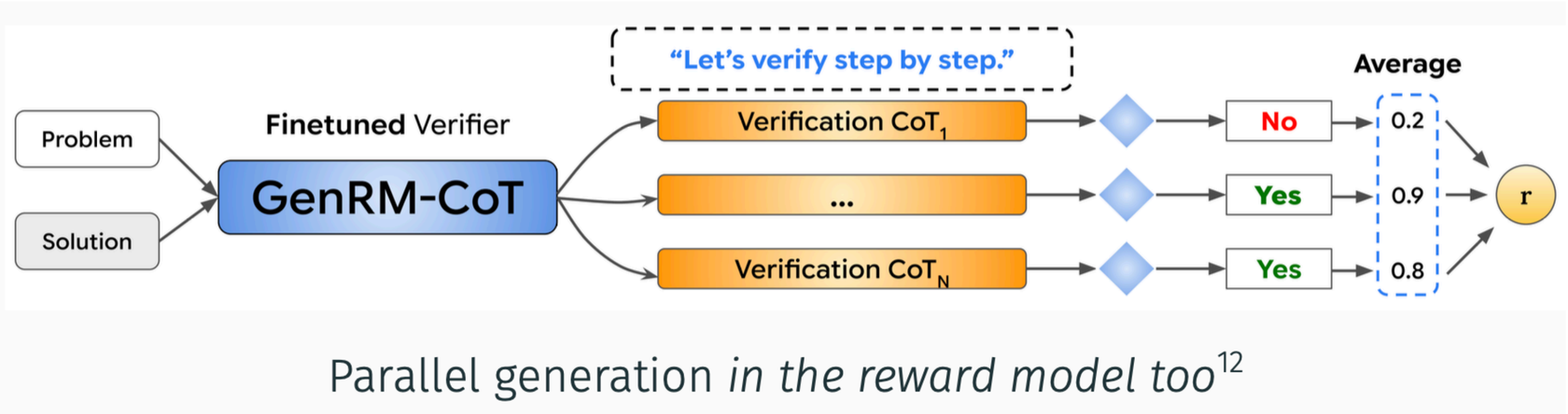



[10] [Sun et al., 2024] *Easy-to-Hard Generalization: Scalable Alignment Beyond Human Supervision.* Z. Sun, L. Yu, Y. Shen, W. Liu, Y. Yang, S. Welleck, C. Gan. NeurIPS 2024.

- For large $m$, this converges to maximum conditional expectation of a **tilted distribution**:

$$y \leftarrow \arg\max_a \sum_z \underbrace{V(x, z, y = a)}_{\text{reward to } a} \times \underbrace{g(z, y = a \mid x)}_{\text{prior on } a}$$

- One can potentially further improve the performance by
  - **using better reward,** and
  - using a better generator that reasons better

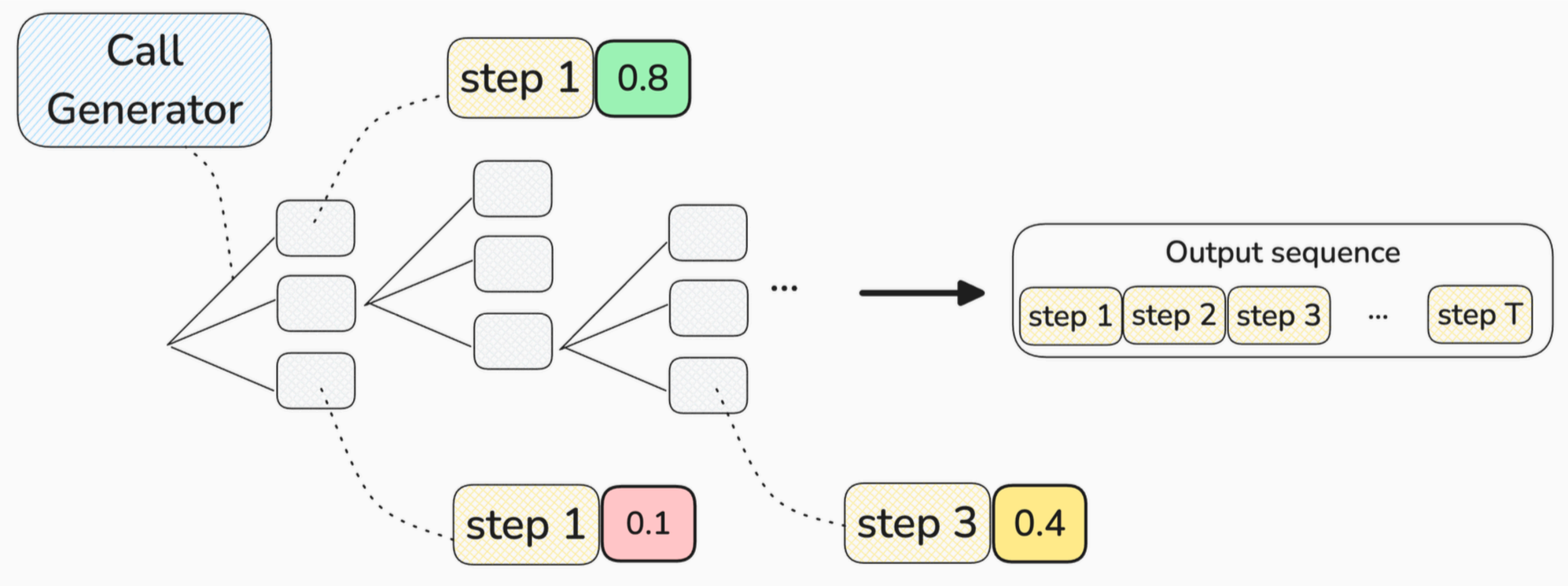



Parallel generation *in the reward model too*[12]

- Parallel meta-generators use the reward in the end.

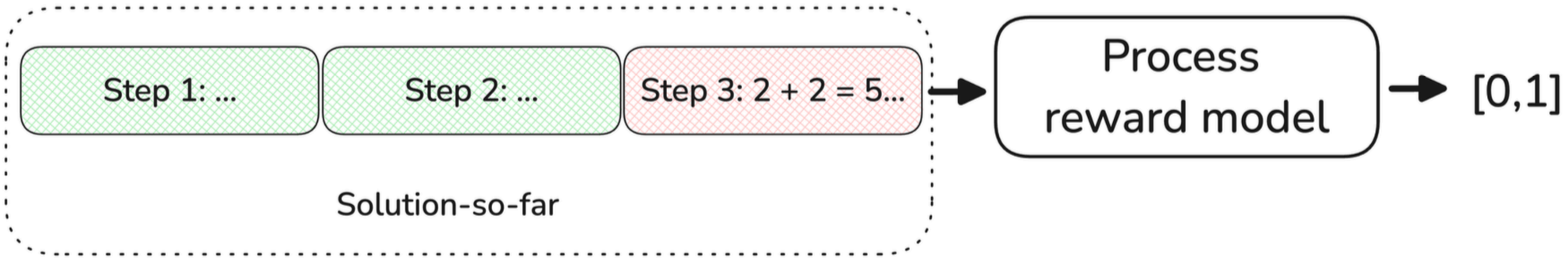
12: [Zhang et al., 2024]

3. **Tree search meta-generators** can evaluate reward on a sequence of intermediate states and the final outcome. (sometimes called process reward)



- **Tree search meta-generators** can evaluate reward on a sequence of intermediate states and the final outcome.

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

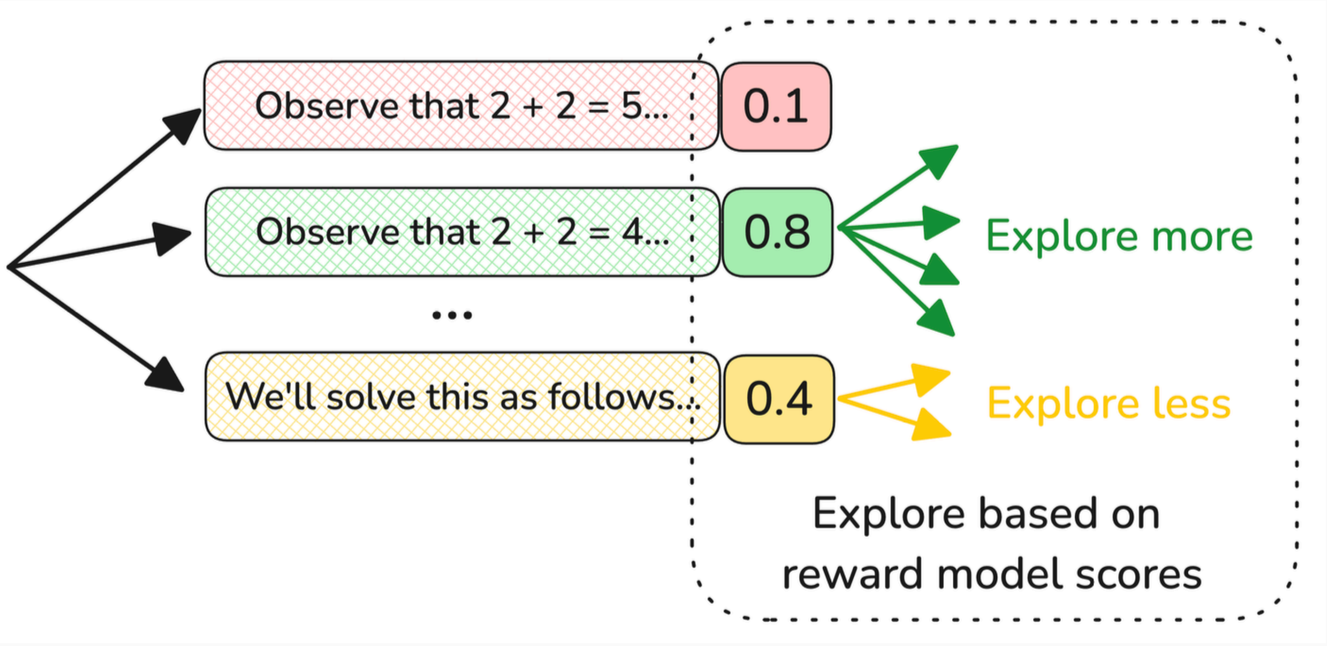



$$v(x, s_1, s_2, \ldots, s_t) \rightarrow [0, 1]$$

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

- Selects which state to explore next by taking the reward into account.

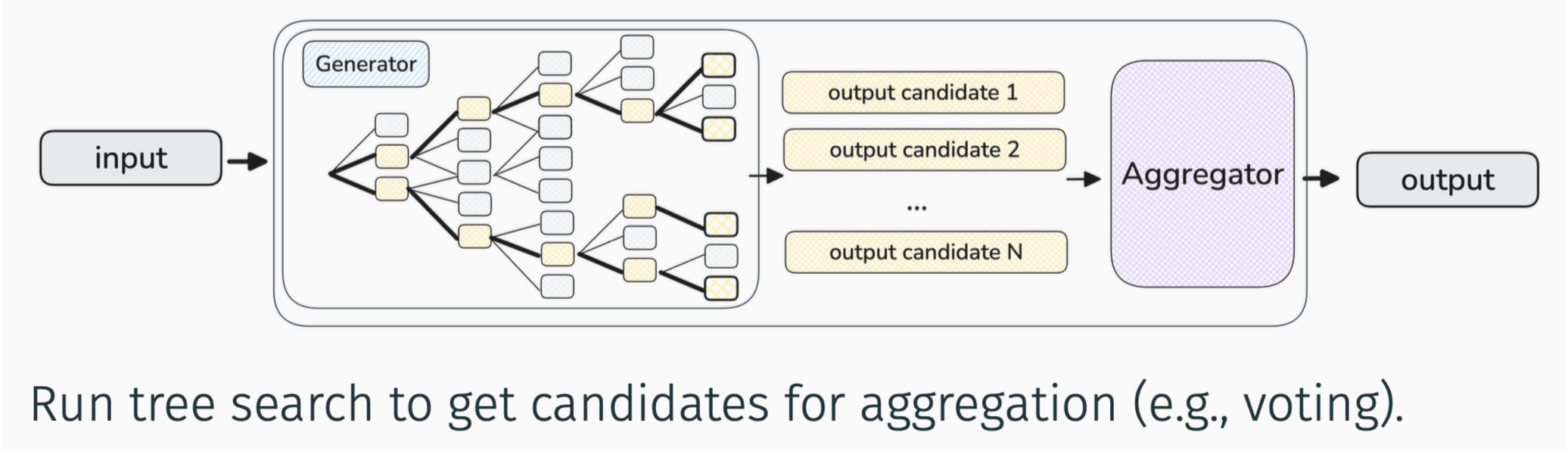
## 2. *Reward Balanced Search (Rebase)*[14]



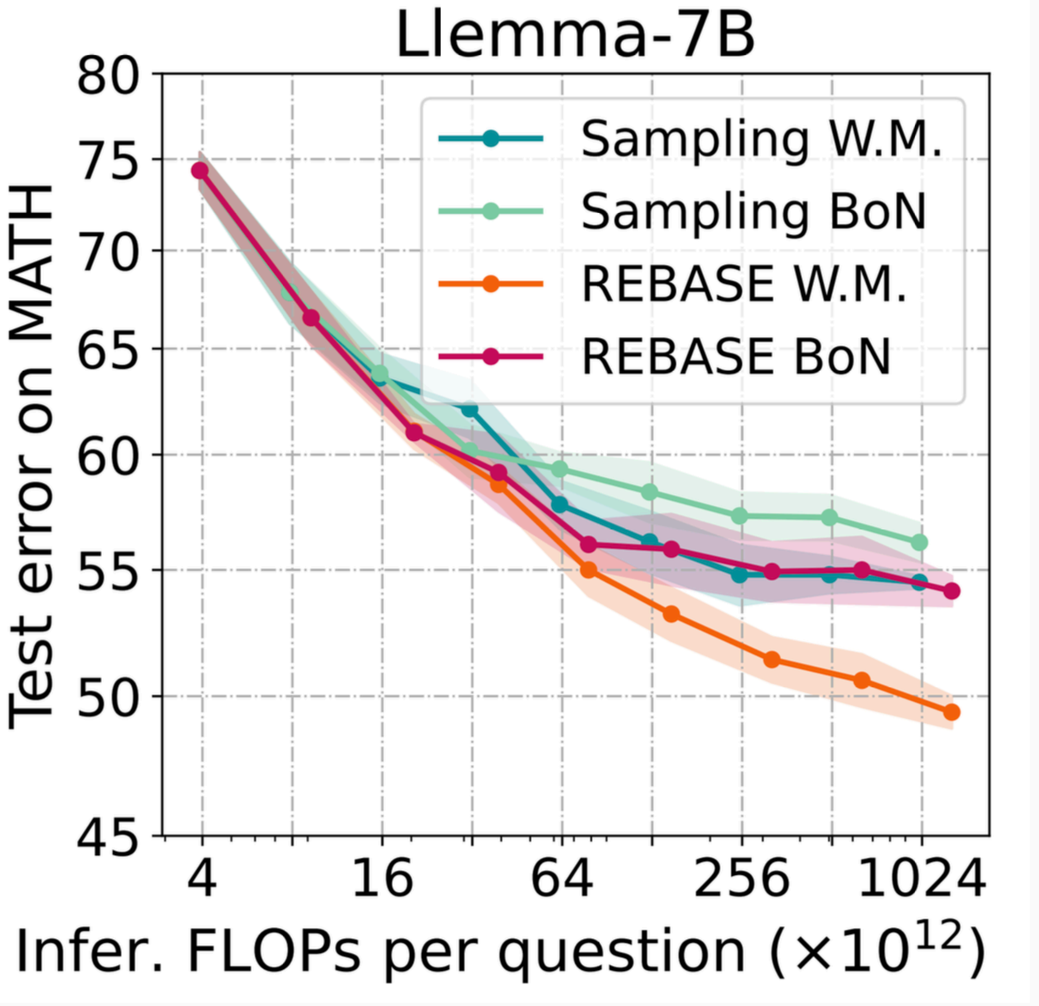

$$\text{explore}_i = \text{Round}\left(\text{Budget}\frac{\exp\left(V(s_i)/\tau\right)}{\sum_j \exp\left(V(s_j)/\tau\right)}\right), \tag{4}$$

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

- Aggregates the final answer using, e.g., weighted voting



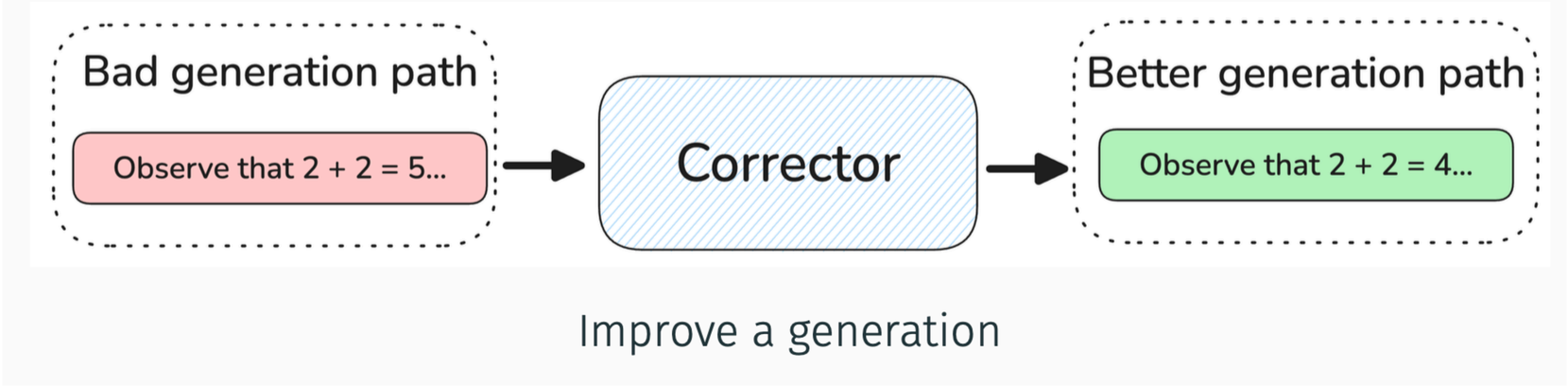

- Key idea in tree search meta-generator is leveraging **intermediate states** and **rewards** to back-track/explore.



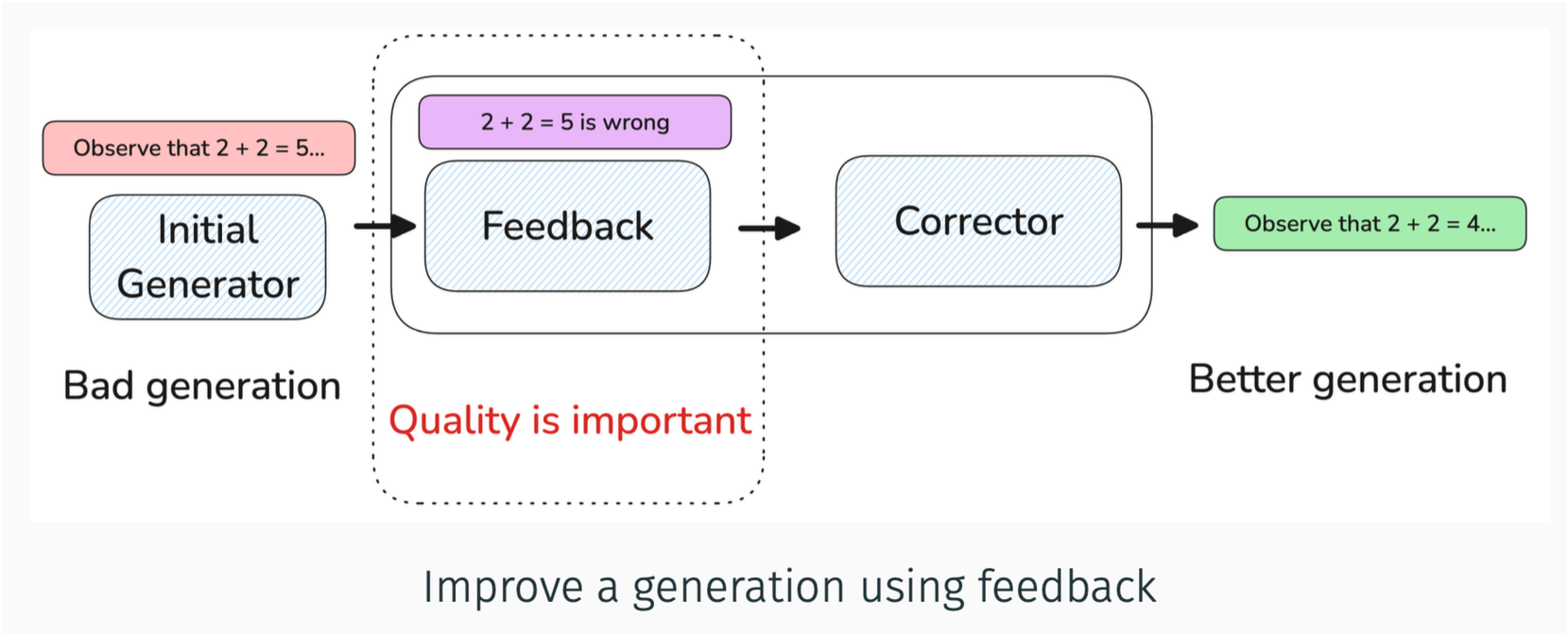

[15] [Wu et al., 2024b] *Inference Scaling Laws: An Empirical Analysis of Compute-Optimal Inference.*

- Tree search meta-generators (REward BAlanced SEarch (REBASE)) require good reward functions over well-defined states.

4. **Refinement/self-correction meta-generators** use past generation and correct mistakes.




- Quality of the feedback is critical.

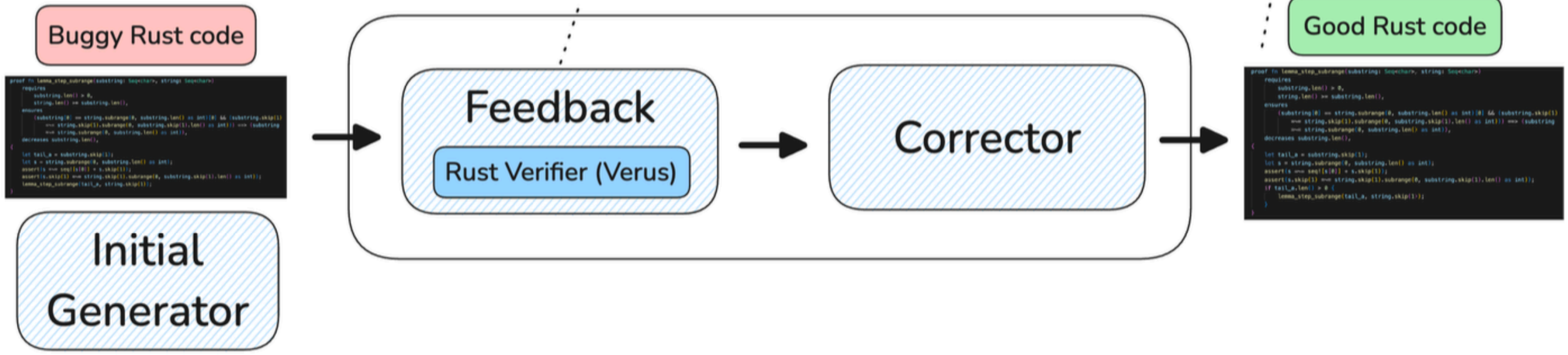


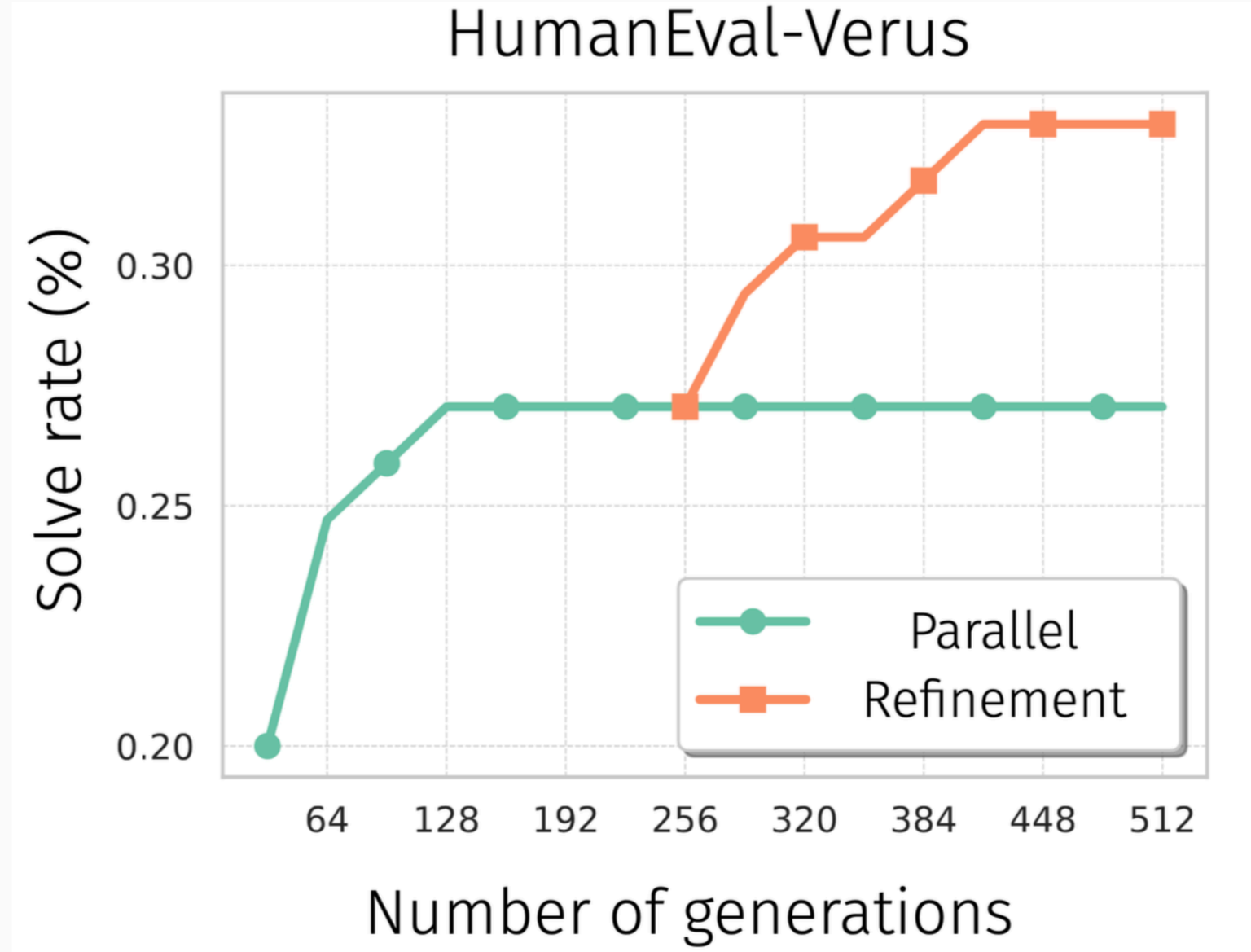
- There are extrinsic/intrinsic feedback.

1. **Extrinsic**: external feedback  Intuition: adds new information, can detect and localize errors

```
Standard Error

error: precondition not satisfied
  --> /playground/src/main.rs:23:5
   |
9  |         substring.len() > 0,
   |         ------------------- failed precondition
...
23 |     lemma_step_subrange(tail_a, string.skip(1));
   |     ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^

error: aborting due to 1 previous error

Standard Output

verification results:: 1 verified, 1 errors
```

```
20      if tail_a.len() > 0 {
21          lemma_step_subrange(tail_a, string.skip(1));
22      }
```

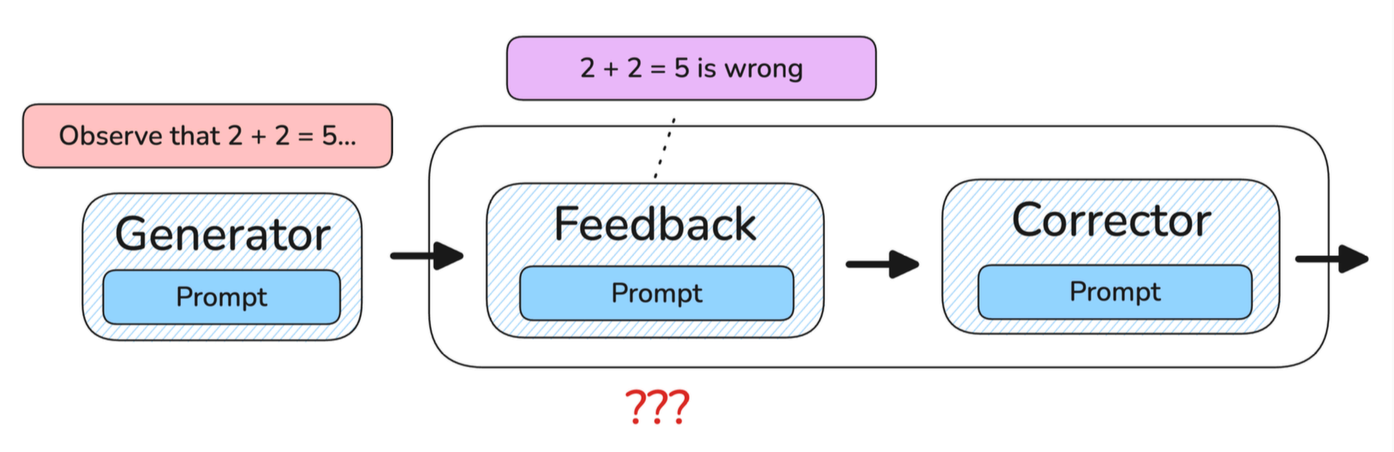





*AlphaVerus*. P. Aggarwal, B. Parno, S. Welleck.

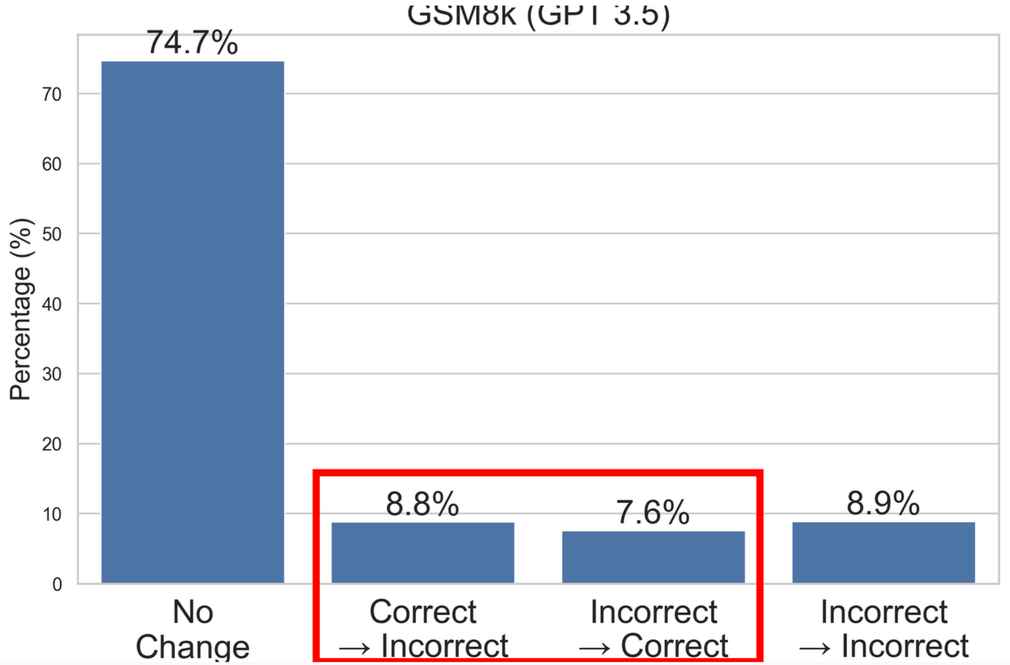
- There are extrinsic/intrinsic feedback.

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




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

Easy to evaluate but results are mixed.

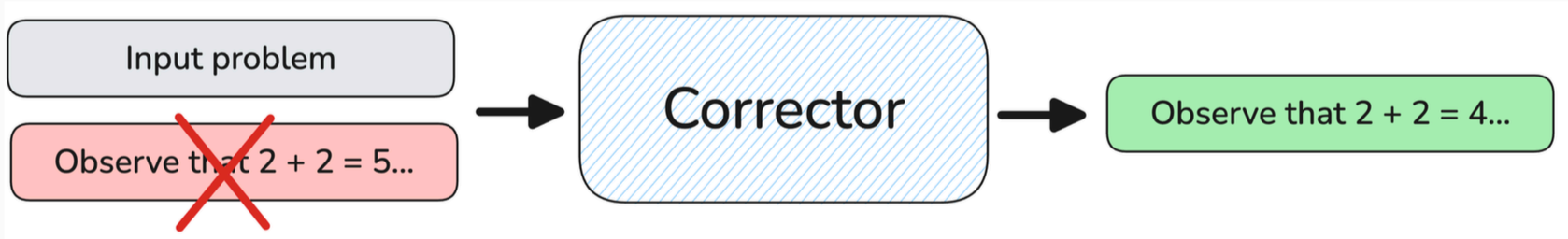



**Takeaway:** feedback is too noisy From [Huang et al., 2024]

- One can train a corrector based on samples generated and optimized to maximize reward.

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

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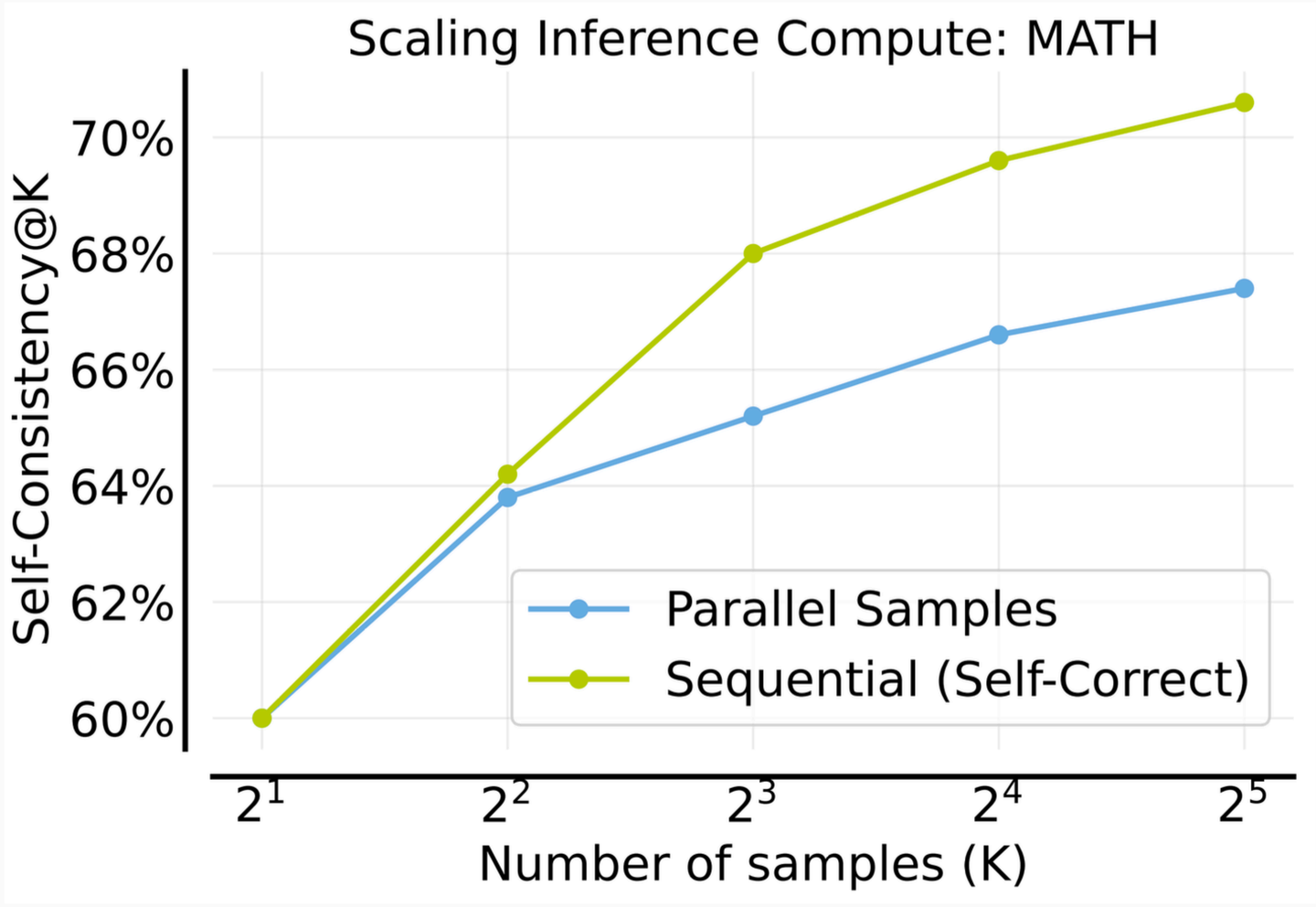
[18] E.g., Self-corrective learning [Welleck et al., 2023], SCoRe [Kumar et al., 2024].




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

# Sources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