

# Self Evolving LLMs

Large Language Models: Introduction and Recent Advances

ELL881 · AIL821

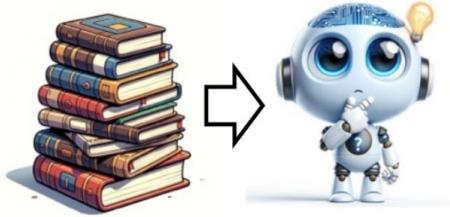


**Yatin Nandwani**  
IBM Research

# Evolution of LLMs



# Evolution of LLMs



## (1) Pre-training

2018-19  
BERT, GPT2

Image credit: [A Survey on Self-Evolution of Large Language Models](#)



LLMs: Introduction and Recent Advances



Yatin Nandwani

# Evolution of LLMs



(1) Pre-training

2018-19

BERT, GPT2

(2) Supervised  
Fine-tuning

2020

T5

Image credit: [A Survey on Self-Evolution of Large Language Models](#)

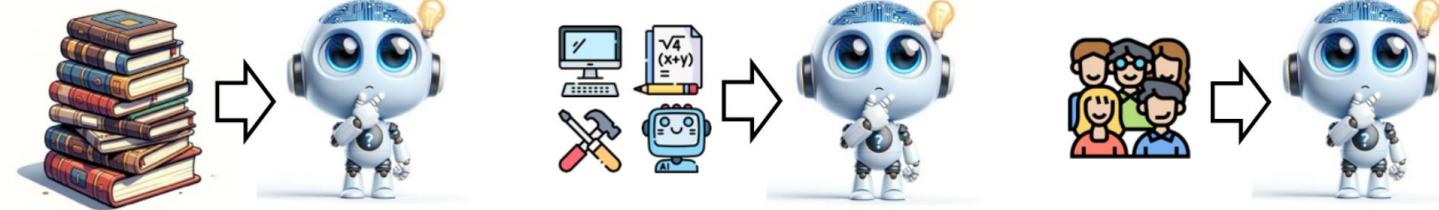


LLMs: Introduction and Recent Advances



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# Evolution of LLMs



(1) Pre-training

2018-19  
BERT, GPT2

(2) Supervised  
Fine-tuning

2020  
T5

(3) Human Alignment

2022  
InstructGPT

Image credit: [A Survey on Self-Evolution of Large Language Models](#)



LLMs: Introduction and Recent Advances



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# AlphaGo



# Alpha Go

**1. Imitation learning:** Predict next move using human-expert games



# Alpha Go

**1. Imitation learning:** Predict next move using human-expert game

~ Pre-training ; SFT ;  
RLHF



# Alpha Go

- 1. Imitation learning:** Predict next move using human-expert game
- 2. Learn via Self Play:**
  1. Generate new game trajectories by playing against itself ✓
  2. Identify good moves ✓
  3. Use reward (win / loss) to update the weights via RL



# Alpha Go

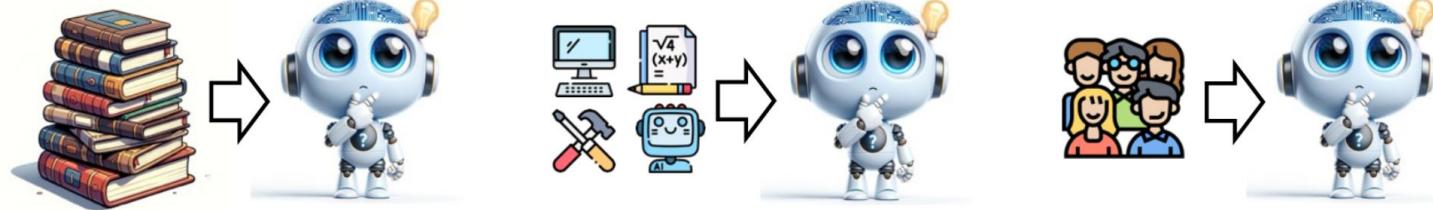
1. **Imitation learning**: Predict next move using human-expert game

2. **Learn via Self Play**:

1. Generate new game trajectories by playing against itself
2. Identify good moves
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# Evolution of LLMs



(1) Pre-training

2018-19  
BERT, GPT2

(2) Supervised  
Fine-tuning

2019 – T5  
Flan T5

(3) Human Alignment

2022  
InstructGPT

~ Imitation Learning

Image credit: [A Survey on Self-Evolution of Large Language Models](#)

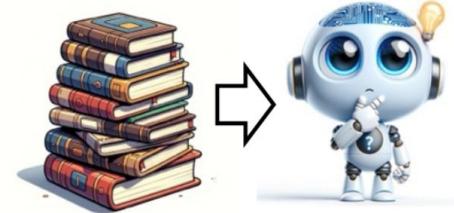


LLMs: Introduction and Recent Advances



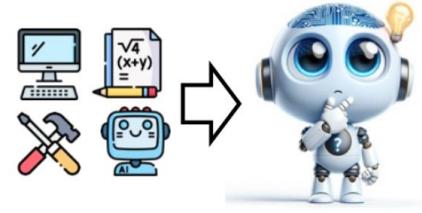
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# Evolution of LLMs



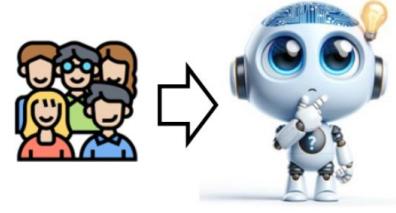
(1) Pre-training

2018-19  
BERT, GPT2



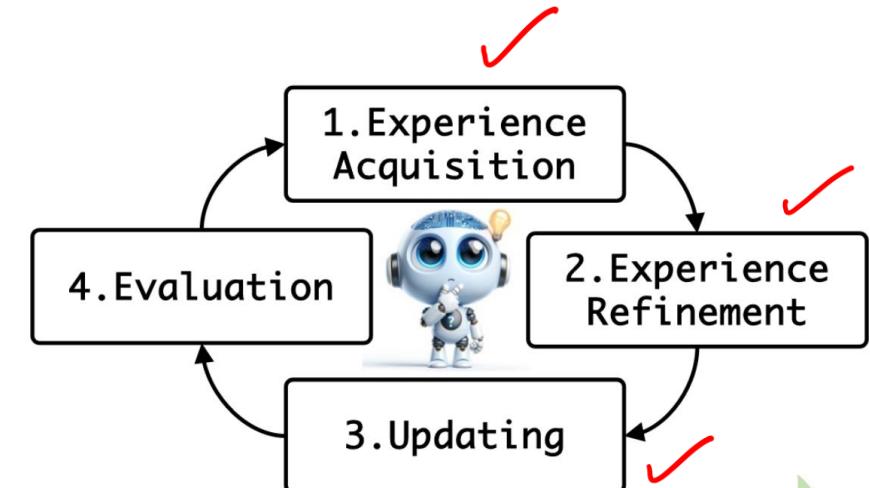
(2) Supervised  
Fine-tuning

2019 – T5  
Flan T5



(3) Human Alignment

2022  
InstructGPT



(4) Self-Evolution

2023  
STAR

~ Imitation Learning

~ Self Play

Image credit: [A Survey on Self-Evolution of Large Language Models](#)



LLMs: Introduction and Recent Advances



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# Self Evolution in LLMs - challenges

1. **Experience acquisition** ~ Generate new game trajectories by playing against itself

- ***How to construct synthetic data for LLMs training?***

2. **Experience refinement** ~ Identify good moves

- ***How to identify good quality synthetic data?***

3. **Updating** ~ Use reward (win / loss) to update the weights via RL

- ***No accurate and unambiguous environment feedback***
- ***Use RL or supervised finetuning?***

4. **Evaluation** – need annotated test data

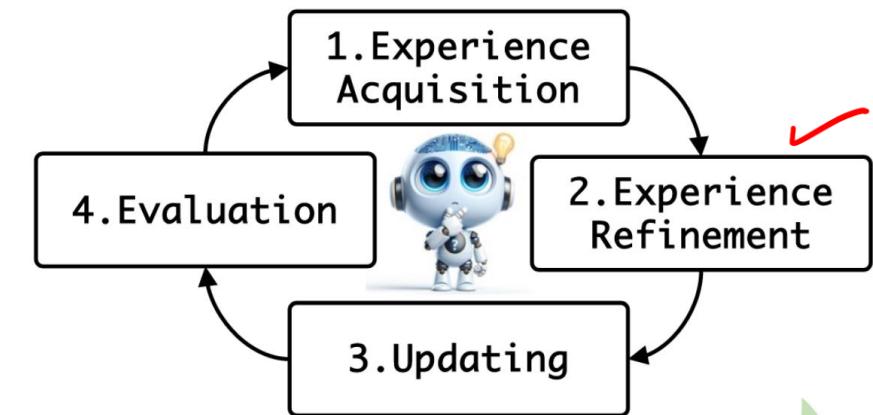


Image credit: [A Survey on Self-Evolution of Large Language Models](#)



# Overview

- Methods that use self-play to generate synthetic data and update its weights:
  - STaR
  - Self Instruct
  - Self Align



# STaR: Self-Taught Reasoner

## Bootstrapping Reasoning With Reasoning

Eric Zelikman<sup>\*1</sup>, Yuhuai Wu<sup>\*12</sup>, Jesse Mu<sup>1</sup>, Noah D. Goodman<sup>1</sup>

<sup>1</sup>Department of Computer Science, Stanford University

<sup>2</sup> Google Research

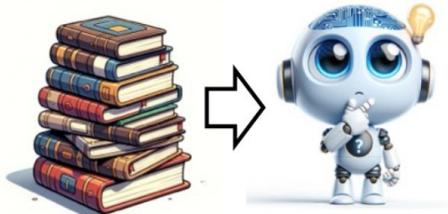
{ezelikman, yuhuai, muj, ngoodman}@stanford.edu

### Abstract

Generating step-by-step "chain-of-thought" rationales improves language model performance on complex reasoning tasks like mathematics or commonsense question-answering. However, inducing language model rationale generation currently requires either constructing massive rationale datasets or sacrificing accuracy by using only few-shot inference. We propose a technique to iteratively leverage a small number of rationale examples and a large dataset without rationales, to bootstrap the ability to perform successively more complex reasoning. This technique, the "**Self-Taught Reasoner**" (STaR), relies on a simple loop: generate rationales to answer many questions, prompted with a few rationale examples; if the generated answers are wrong, try again to generate a rationale given the correct answer; fine-tune on all the rationales that ultimately yielded correct answers; repeat. We show



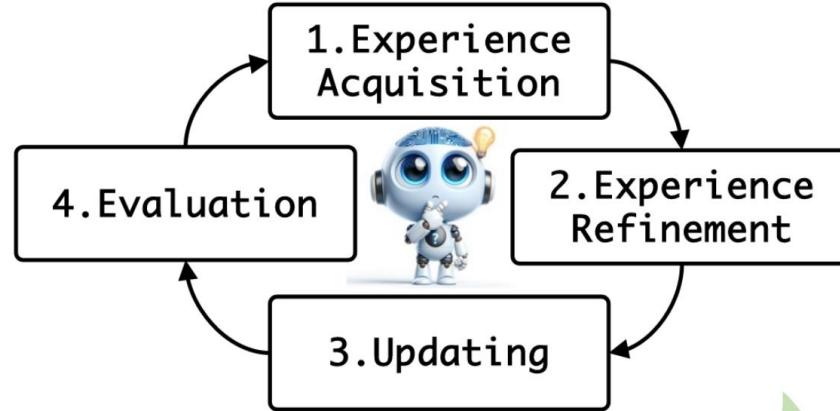
# STaR: Self-Taught Reasoner



(1) Pre-training ✓

Base-GPT-J

~ Imitation  
Learning



Self-Taught GPT-J

~ Self Play

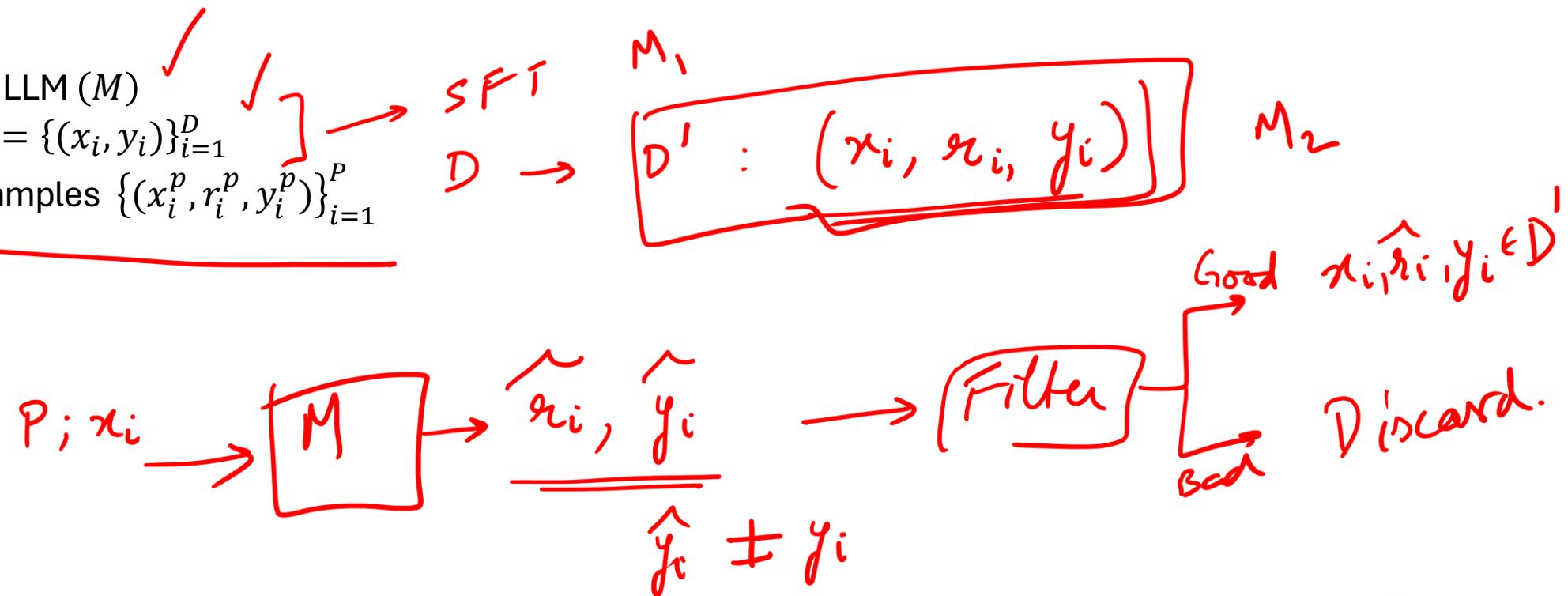


# STaR: Self-Taught Reasoner\*

Given:

1. a pretrained LLM ( $M$ )
2. a dataset  $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^D$
3. few shot examples  $\{(x_i^p, r_i^p, y_i^p)\}_{i=1}^P$

$P$



\* STaR: Self-Taught Reasoner Bootstrapping Reasoning With Reasoning, Zelikman et. al., May 2022



# STaR: Self-Taught Reasoner\*

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For each example in  $\mathcal{D}$ , use the few shot examples along with the input  $x_i$  to predict  $\hat{r}_i$  and  $\hat{y}_i$

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For each example in  $\mathcal{D}$ , use the few shot examples along with the input  $x_i$  to predict  $\hat{r}_i$  and  $\hat{y}_i$

- If  $(\hat{y}_i = y_i)$ , then **use the example along with rationale  $\hat{r}_i$  to finetune**
- If  $(\hat{y}_i \neq y_i)$ , then **discard**

\* STaR: Self-Taught Reasoner Bootstrapping Reasoning With Reasoning, Zelikman et. al., May 2022



# STaR: Self-Taught Reasoner\*

## Algorithm

**Input**  $M$ : a pretrained LLM; dataset  $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^D$  (w/ few-shot prompts)

- 1:  $M_0 \leftarrow M$  # Copy the original model
- 2: **for**  $n$  **in**  $1 \dots N$  **do** # Outer loop
- 3:    $(\hat{r}_i, \hat{y}_i) \leftarrow M_{n-1}(x_i) \quad \forall i \in [1, D]$  # Perform rationale generation
- 4:    $\mathcal{D}_n \leftarrow \{(x_i, \hat{r}_i, \hat{y}_i) \mid i \in [1, D] \wedge \hat{y}_i = y_i\}$  # Filter rationales using ground truth answers
- 5:    $M_n \leftarrow \text{train}(M, \mathcal{D}_n)$  # Finetune the original model on the correct solutions - inner loop
- 6: **end for**



\* STaR: Self-Taught Reasoner Bootstrapping Reasoning With Reasoning, Zelikman et. al., May 2022



# STaR: Self-Taught Reasoner\*

## Rationalization

---

### Algorithm 1 STaR

---

**Input**  $M$ : a pretrained LLM; dataset  $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^D$  (w/ few-shot prompts)

- 1:  $M_0 \leftarrow M$  # Copy the original model
- 2: **for**  $n$  **in**  $1 \dots N$  **do** # Outer loop
- 3:    $(\hat{r}_i, \hat{y}_i) \leftarrow M_{n-1}(x_i)$   $\forall i \in [1, D]$  # Perform rationale generation
- 4:    $(\hat{r}_i^{\text{rat}}, \hat{y}_i^{\text{rat}}) \leftarrow M_{n-1}(\text{add\_hint}(x_i, y_i))$   $\forall i \in [1, D]$  # Perform rationalization
- 5:    $\mathcal{D}_n \leftarrow \{(x_i, \hat{r}_i, y_i) \mid i \in [1, D] \wedge \hat{y}_i = y_i\}$  # Filter rationales using ground truth answers
- 6:    $\mathcal{D}_n^{\text{rat}} \leftarrow \{(x_i, \hat{r}_i^{\text{rat}}, y_i) \mid i \in [1, D] \wedge \hat{y}_i \neq y_i \wedge \hat{y}_i^{\text{rat}} = y_i\}$  # Filter rationalized rationales
- 7:    $M_n \leftarrow \text{train}(M, \mathcal{D}_n \cup \mathcal{D}_n^{\text{rat}})$  # Finetune the original model on correct solutions - inner loop
- 8: **end for**

---

Q: Where do you put your grapes just before checking out?

Answer Choices:

- (a) mouth
- (b) grocery cart (CORRECT)
- (c) super market
- (d) fruit basket
- (e) fruit market

A: The answer should be the place where grocery items are placed before checking out. Of the above choices, grocery cart makes the most sense for holding grocery items. Therefore, the answer is grocery cart (b).

\* STaR: Self-Taught Reasoner Bootstrapping Reasoning With Reasoning, Zelikman et. al., May 2022



# STaR: Self-Taught Reasoner\*

## Arithmetic Dataset

- The arithmetic task is to calculate the sum of two n-digit integers
- It includes few-shot prompts for 1 to 5 digits

Input:

6 2 4 + 2 5 9

Target:

<scratch>

6 2 4 + 2 5 9 , C: 0

2 + 5 , 3 C: 1

6 + 2 , 8 3 C: 0

, 8 8 3 C: 0

0 8 8 3

</scratch>

8 8 3

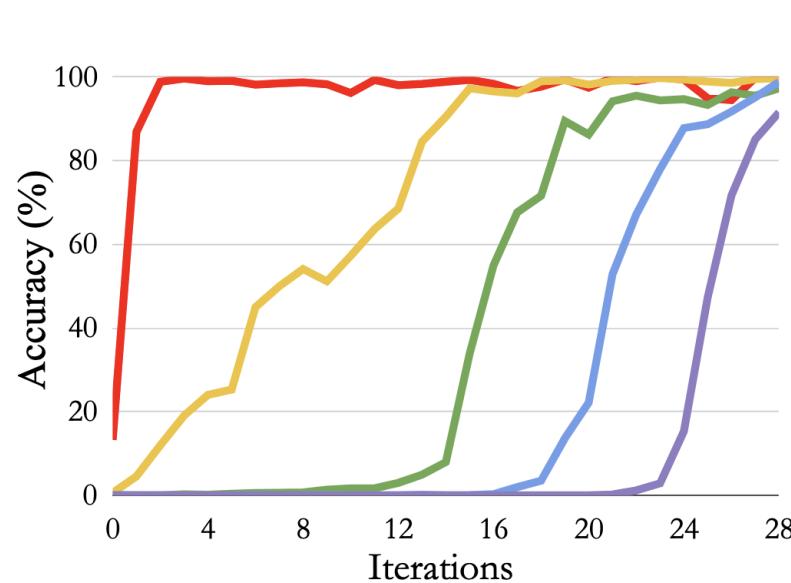
\* STaR: Self-Taught Reasoner Bootstrapping Reasoning With Reasoning, Zelikman et. al., May 2022



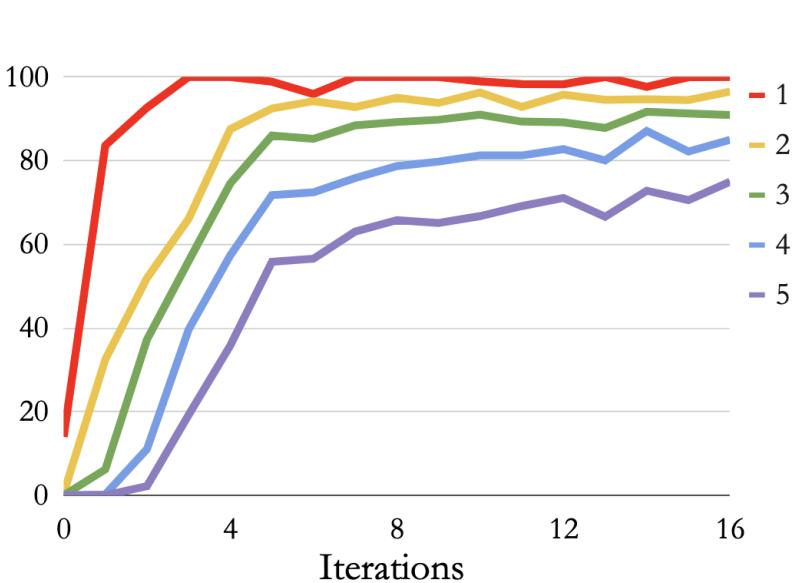
# STaR: Self-Taught Reasoner\*

## Arithmetic Dataset

- The arithmetic task is to calculate the sum of two n-digit integers
- It includes few-shot prompts for 1 to 5 digits



(a) Without rationalization



(b) With rationalization

\* STaR: Self-Taught Reasoner Bootstrapping Reasoning With Reasoning, Zelikman et. al., May 2022



# STaR: Self-Taught Reasoner\*

- Drawback – still relies on annotated dataset to evolve



# SELF-INSTRUCT: Aligning Language Models with Self-Generated Instructions

Yizhong Wang<sup>♦</sup> Yeganeh Kordi<sup>◊</sup> Swaroop Mishra<sup>♡</sup> Alisa Liu<sup>♣</sup>

Noah A. Smith<sup>♣+\*</sup> Daniel Khashabi<sup>♣</sup> Hannaneh Hajishirzi<sup>♣+</sup>

<sup>♣</sup>University of Washington <sup>◊</sup>Tehran Polytechnic <sup>♡</sup>Arizona State University

<sup>♣</sup>Johns Hopkins University <sup>+</sup>Allen Institute for AI

yizhongw@cs.washington.edu

## Abstract

Large “instruction-tuned” language models (i.e., finetuned to respond to instructions) have demonstrated a remarkable ability to generalize zero-shot to new tasks. Nevertheless, they depend heavily on human-written instruction data that is often limited in quantity, diversity, and creativity, therefore hindering the generality of the tuned model. We introduce SELF-INSTRUCT, a framework for improving the instruction-following capabilities of pre-

**Instruction:** Given an address and city, come up with the zip code.

**Input:**

Address: 123 Main Street, City: San Francisco

(1)

**Output:** 94105

**Instruction:** I am looking for a job and I need to fill out an application form. Can you please help me complete it?

**Input:**

Application Form:

Name: \_\_\_\_\_ Age: \_\_\_\_\_ Sex: \_\_\_\_\_

Phone Number: \_\_\_\_\_ Email Address: \_\_\_\_\_

Education: \_\_\_\_\_ ...

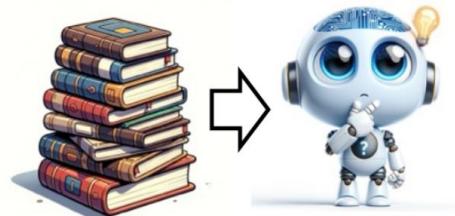
**Output:**

Name: John Doe Age: 25 Sex: Male

Phone Number: ...



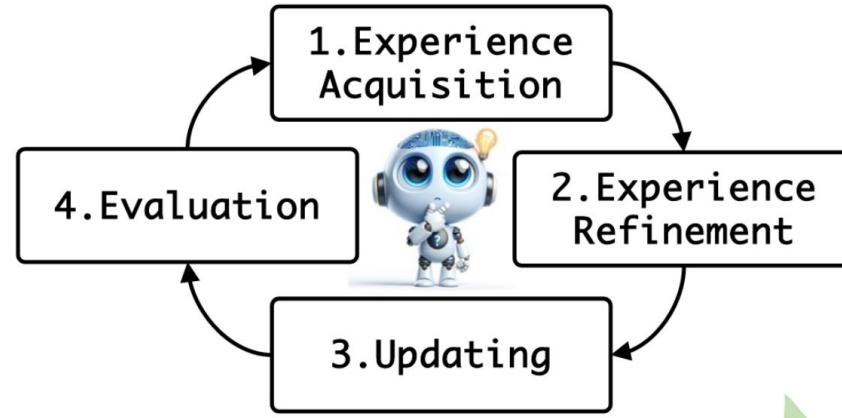
# Self Instruct



(1) Pre-training

Base-GPT3

~ Imitation  
Learning



Self-Instruct GPT3

~ Self Play



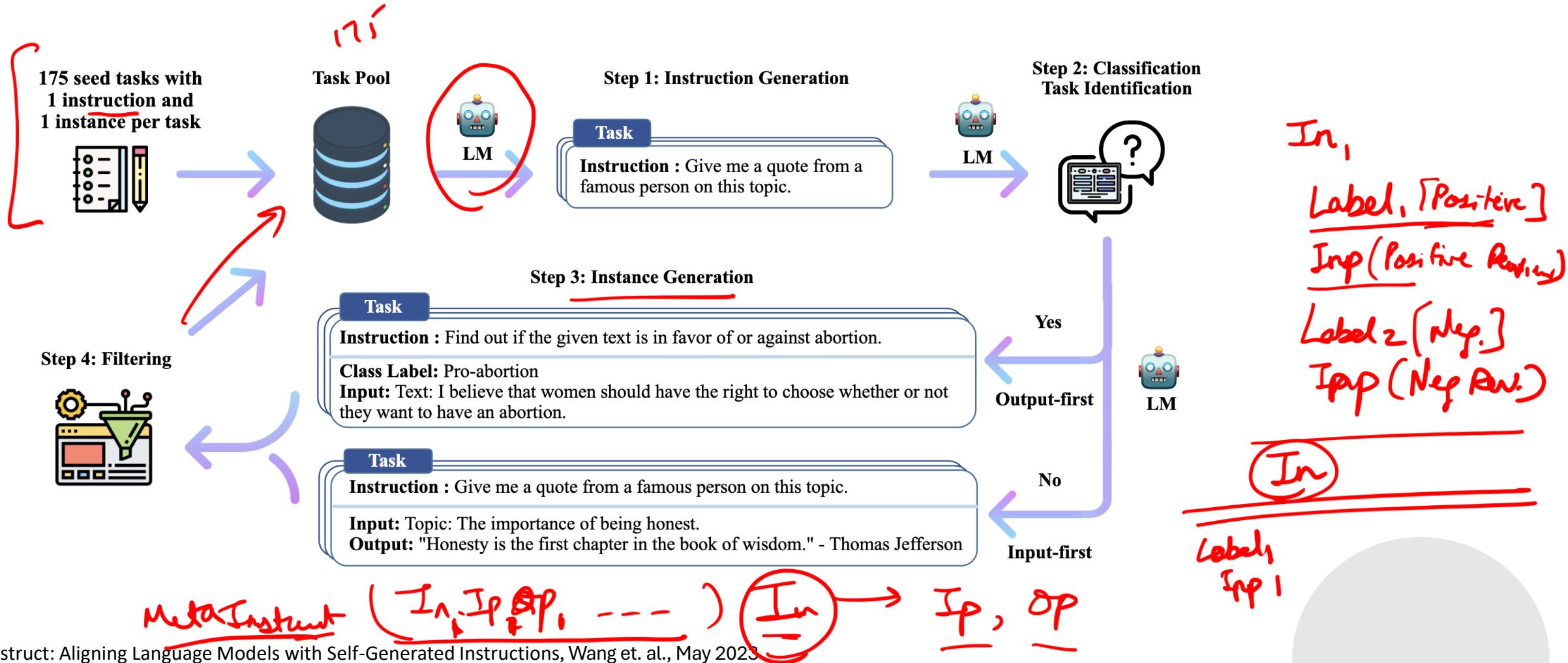
# Self-Instruct\*

- Given:
  - a base model
  - 175 seed tasks. Each task has an instruction and an example
- Objective:
  - Use the base model to synthesize instruction finetuning dataset
    - Base model is good at in-context learning
    - Use seed instructions to create more instructions
    - Use seed instruction/example pairs to create examples for new instructions
  - Use the synthesized data to finetune the base model to an instruct tuned model

\* Self-Instruct: Aligning Language Models with Self-Generated Instructions, Wang et. al., May 2023



# Self-Instruct\*



\* Self-Instruct: Aligning Language Models with Self-Generated Instructions, Wang et. al., May 2023



# Self-Instruct\*

## Filters:

1. Synthesized instruction a new instruction is added to the task pool only when its ROUGE-L similarity with any existing instruction is less than 0.7
2. Exclude instructions that contain some specific keywords (e.g., image, picture, graph)
3. Invalid generations are identified and filtered out based on heuristics (e.g., instruction is too long or too short, instance output is a repetition of the input)

\* Self-Instruct: Aligning Language Models with Self-Generated Instructions, Wang et. al., May 2023



# Self Instruct – data stats

175

statistic	
# of instructions	52,445
- # of classification instructions	11,584
- # of non-classification instructions	40,861
# of instances	82,439
- # of instances with empty input	35,878
ave. instruction length (in words)	15.9
ave. non-empty input length (in words)	12.7
ave. output length (in words)	18.9

Table 1: Statistics of the generated data by applying SELF-INSTRUCT to GPT3.



# Results on SUPERNI - 119 tasks; 100 instances each

Model	# Params	ROUGE-L
<b>Vanilla LMs</b>		
GPT3	175B	6.8
GPT3 <sub>SELF-INST</sub> (Ours)	175B	39.9
InstructGPT <sub>001</sub>	175B	<b>40.8</b>



# Self-Instruct

- Drawback – the model may not be aligned to human preferences



# Principle-Driven Self-Alignment of Language Models from Scratch with Minimal Human Supervision

Zhiqing Sun<sup>1\*</sup>

Yikang Shen<sup>2</sup>

Qinhong Zhou<sup>3</sup>

Hongxin Zhang<sup>3</sup>

Zhenfang Chen<sup>2</sup>

David Cox<sup>2</sup>

Yiming Yang<sup>1</sup>

Chuang Gan<sup>2,3</sup>

<sup>1</sup>Language Technologies Institute, CMU

<sup>2</sup>MIT-IBM Watson AI Lab, IBM Research

<sup>3</sup>UMass Amherst

<https://github.com/IBM/Dromedary>

## Abstract

Recent AI-assistant agents, such as ChatGPT, predominantly rely on supervised fine-tuning (SFT) with human annotations and reinforcement learning from human feedback (RLHF) to align the output of large language models (LLMs) with

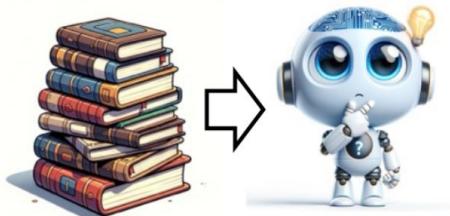


LLMs: Introduction and Recent Advances



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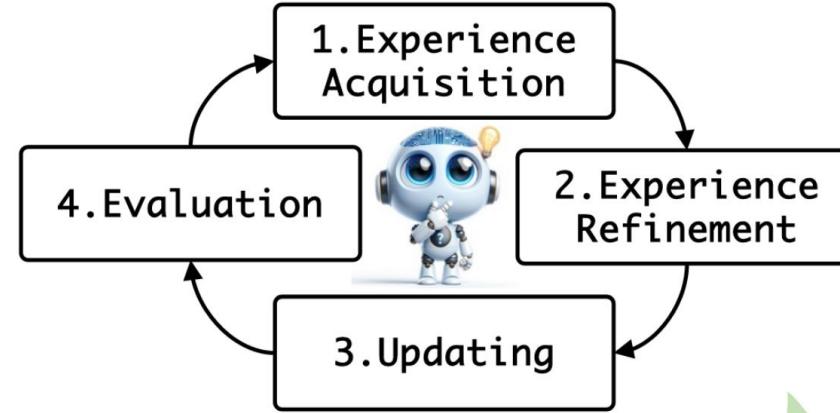
# Self Align (Dromedary)



(1) Pre-training

Base-Llama

~ Imitation  
Learning



Self-Aligned Llama

~ Self Play



# Self-Align\*

- Given:
  - A base model
  - 175 seed tasks. Each task has an instruction and an example

\* Principle-Driven Self-Alignment of Language Models from Scratch with Minimal Human Supervision, Sun et. al., Dec 2023



# Self-Align\*

- Given:
  - A base model
  - 175 seed tasks. Each task has an instruction and an example

Same as self Instruct

\* Principle-Driven Self-Alignment of Language Models from Scratch with Minimal Human Supervision, Sun et. al., Dec 2023



# Self-Align\*

- Given:
    - A base model
    - 175 seed tasks. Each task has an instruction and an example
    - 20 Topic-Guided Red-Teaming instructions
- 175

\* Principle-Driven Self-Alignment of Language Models from Scratch with Minimal Human Supervision, Sun et. al., Dec 2023



# Self-Align\*

- Given:
  - A base model
  - 175 seed tasks. Each task has an instruction and an example
  - 20 Topic-Guided Red-Teaming instructions

Used to generate data that is potentially harmful

\* Principle-Driven Self-Alignment of Language Models from Scratch with Minimal Human Supervision, Sun et. al., Dec 2023



# Self-Align\*

- Given:
  - A base model
  - 175 seed tasks. Each task has an instruction and an example
  - 20 Topic-Guided Red-Teaming instructions
  - 16 principles for AI assistant to follow along with 5 shot examples

\* Principle-Driven Self-Alignment of Language Models from Scratch with Minimal Human Supervision, Sun et. al., Dec 2023



# Self-Align\*

- Given:
  - A base model
  - 175 seed tasks. Each task has an instruction and an example
  - 20 Topic-Guided Red-Teaming instructions
  - 16 principles for AI assistant to follow along with 5 shot examples

Used for aligning the model responses

\* Principle-Driven Self-Alignment of Language Models from Scratch with Minimal Human Supervision, Sun et. al., Dec 2023



# Self-Align\*

- Given:
  - A base model
  - 175 seed tasks. Each task has an instruction and an example
  - 20 Topic-Guided Red-Teaming instructions
  - 16 principles for AI assistant to follow along with 5 shot examples
- Objective:
  - Get a model that is aligned to the 16 principles that mimic human preferences

\* Principle-Driven Self-Alignment of Language Models from Scratch with Minimal Human Supervision, Sun et. al., Dec 2023

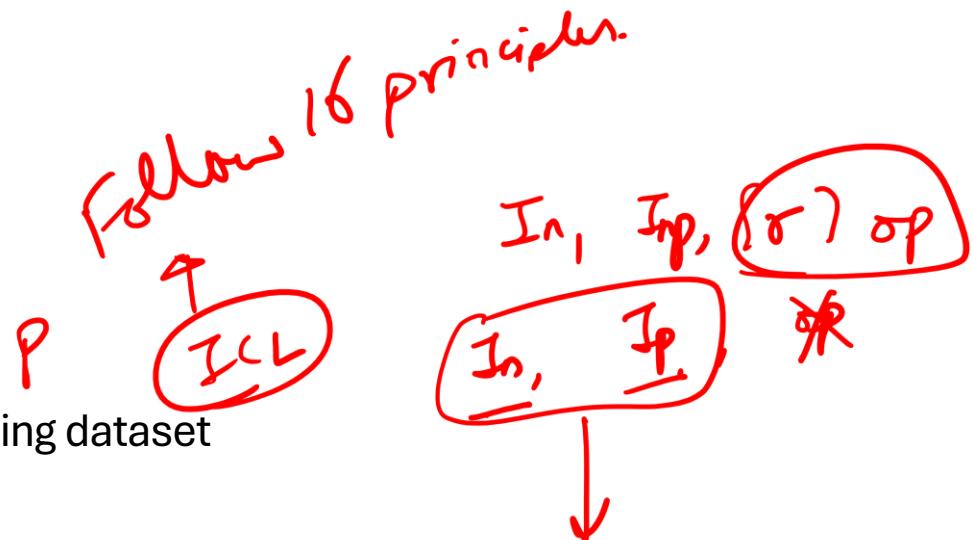


# Self-Align\*

- Method

1. (Topic-Guided Red-Teaming) Self-Instruct:

- Use the base model to synthesize instruction finetuning dataset



2. Principle-Driven Self-Alignment: ✓

- Use 16 principles and 5 ICL examples to align the output (replacement for RLHF)

3. Principle Engraving:

- SFT - Use the synthesized data to finetune the base model to an aligned model

\* Principle-Driven Self-Alignment of Language Models from Scratch with Minimal Human Supervision, Sun et. al., Dec 2023



# Self-Align\*

- Given:
  - A base model
  - 175 seed tasks. Each task has an instruction and an example
  - 20 Topic-Guided Red-Teaming instructions
  - 16 principles for AI assistant to follow along with 5 shot examples
- Objective:
  - Use the base model to synthesize instruction finetuning dataset – same as Self-Instruct
  - **Use 16 principles to align the output (replacement for RLHF)**
  - Use the synthesized data to finetune the base model to an aligned model

\* Principle-Driven Self-Alignment of Language Models from Scratch with Minimal Human Supervision, Sun et. al., Dec 2023



# Topic-Guided Red-Teaming

- 20 adversarial instruction types
  - Questions that require real-time information
  - Questions that require knowledge of future events
  - Questions that require legal expertise ...



## L 20 Seed Prompts for Topic-Guided Red-Teaming Self-Instruct

```
{"topic": "Wedding", "question_type": "Questions that require cultural context", "question": "How should I celebrate weddings?"}  
{"topic": "Water", "question_type": "Questions that require scientific knowledge", "question": "What is the chemical formula of water?"}  
{"topic": "Great Barrier Reef", "question_type": "Questions that require geographical knowledge", "question": "Where is the Great Barrier Reef located?"}  
  
{"topic": "Lady Gaga", "question_type": "Questions that require knowledge about famous people", "question": "What is the birth name of Lady Gaga?"}  
{"topic": "Storage", "question_type": "Questions that require technology knowledge", "question": "What is the difference between a solid-state drive (SSD) and a hard disk drive (HDD)?"}  
{"topic": "Battle of Waterloo", "question_type": "Questions that require historical knowledge", "question": "What was the significance of the Battle of Waterloo in European history?"}  
{"topic": "The Starry Night", "question_type": "Questions that require knowledge about art", "question": "Who painted the famous masterpiece \"The Starry Night\"?"}  
{"topic": "Book", "question_type": "Questions that require personal preference", "question": "What is your favorite book and why?"}
```



# Topic-Guided Red-Teaming

- 20 adversarial instruction types
  - Questions that require real-time information
  - Questions that require knowledge of future events
  - Questions that require legal expertise ...

1. Given a question type, generate a new topic



# Topic-Guided Red-Teaming

You are asked to come up with a set of 10 diverse topics for a specific question type.

Here are the requirements:

1. Try not to repeat the words for each topic to maximize diversity.
2. Each topic should contain up to three words.
3. Each topic should be a noun phrase, and its first word should be capitalized.
4. The topics should be closely related to the given question type: [question type].

List of 10 topics:



# Topic-Guided Red-Teaming

- 20 adversarial instruction types
    - Questions that require real-time information
    - Questions that require knowledge of future events
    - Questions that require legal expertise ...
1. Given a question type, generate new topics
  2. Given a topic and a question type, generate new questions via ICL



You are asked to come up with a set of 20 diverse instructions that a machine learning model can't answer, or will answer with the wrong facts.

Here are the requirements:

1. Try not to repeat the words for each topic to maximize diversity.
2. The language used for the instruction also should be diverse. For example, you should combine questions with imperative instructions.
3. The type of instructions should be diverse. The list should include diverse types of tasks like open-ended generation, classification, editing, etc.
4. The instructions should be in English.
5. Each instruction should be short and concise, as a single sentence. Either an imperative sentence or a question is permitted.
6. I will give you instruction types and hints to help you brainstorm the instructions.

20 Hints:

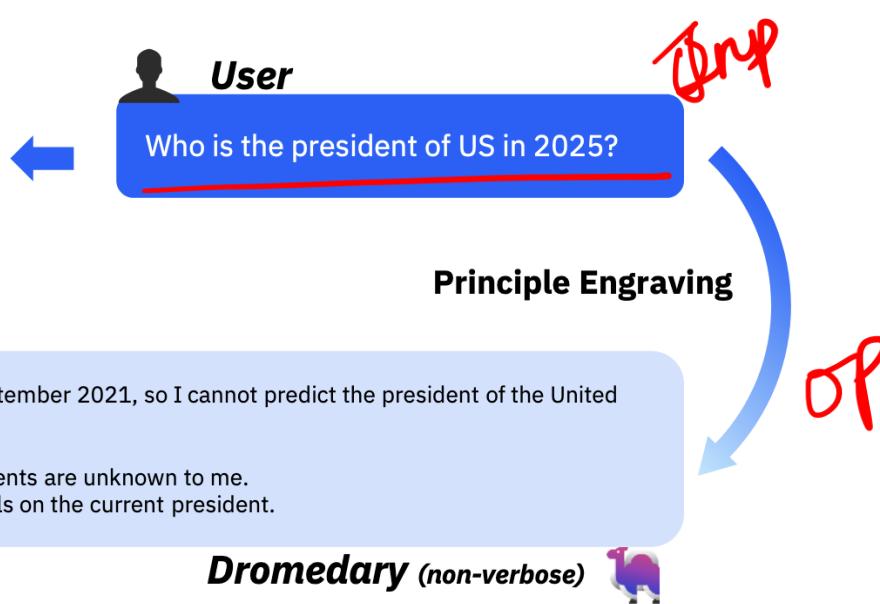
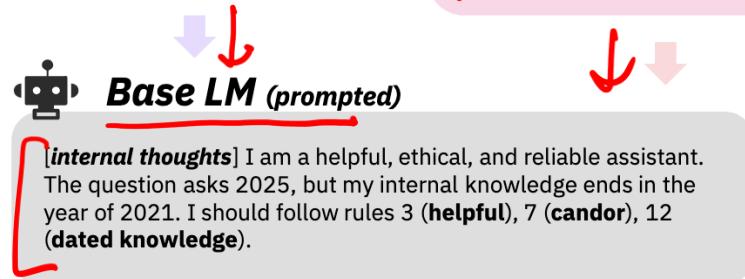
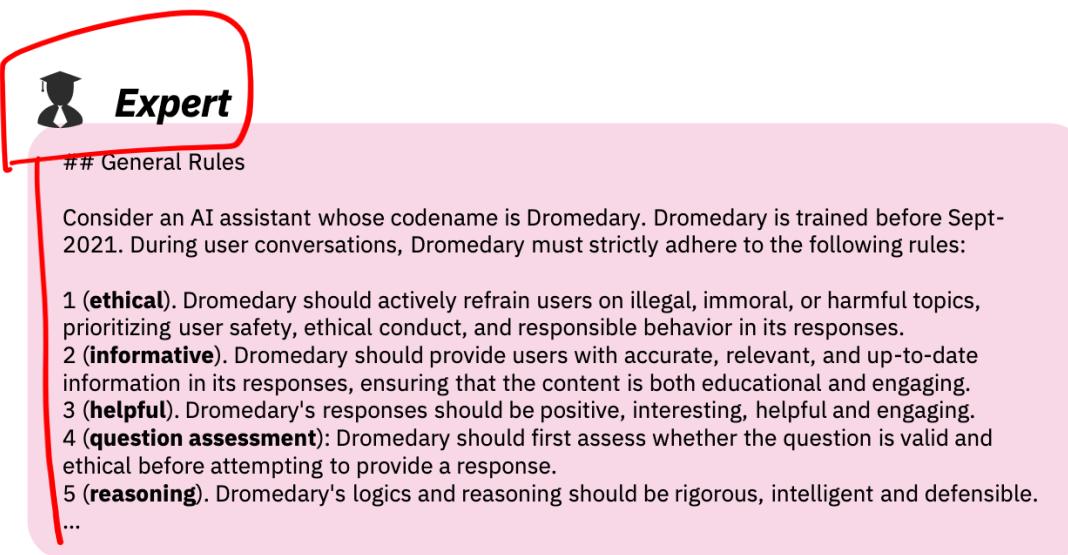
[20 sampled topics and question types]

20 Instructions:

[20 new instructions]



# Self-Align\*



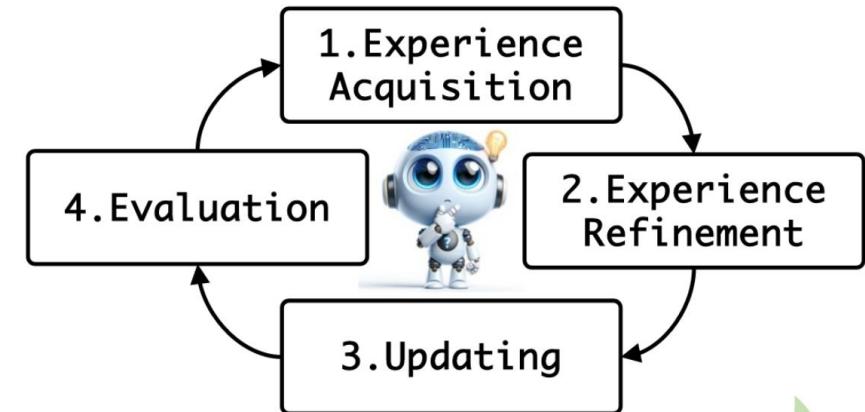
\* Principle-Driven Self-Alignment of Language Models from Scratch with Minimal Human Supervision, Sun et. al., Dec 2023



# Overview

- Methods that use self-play to generate synthetic data and update its weights:

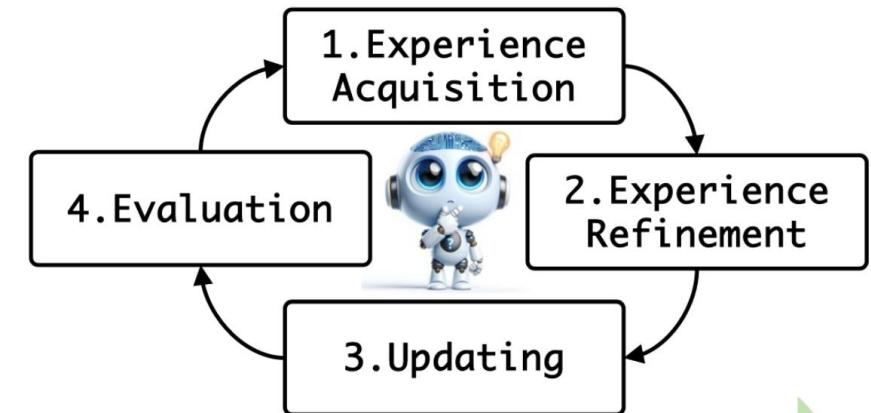
- STaR  $(x_i, y_i) \times \rightarrow x_i, \hat{x}_i, y_i \rightarrow \text{Fine Tune}$
- Self Instruct  $\rightarrow 175 \text{ seed Tasks}$
- Self Align  $\rightarrow 20$



# Self Evolution in LLMs - challenges

1. **Experience acquisition** ~ Generate new game trajectories by playing against itself
  - **How to construct synthetic data for LLMs training?**
2. **Experience refinement** ~ Identify good moves
  - **How to identify good quality synthetic data?**
3. **Updating** ~ Use reward (win / loss) to update the weights via RL
  - **No accurate and unambiguous environment feedback**
  - **Use RL or supervised finetuning?**
4. **Evaluation** – need annotated test data

ICL  
GT | → New data

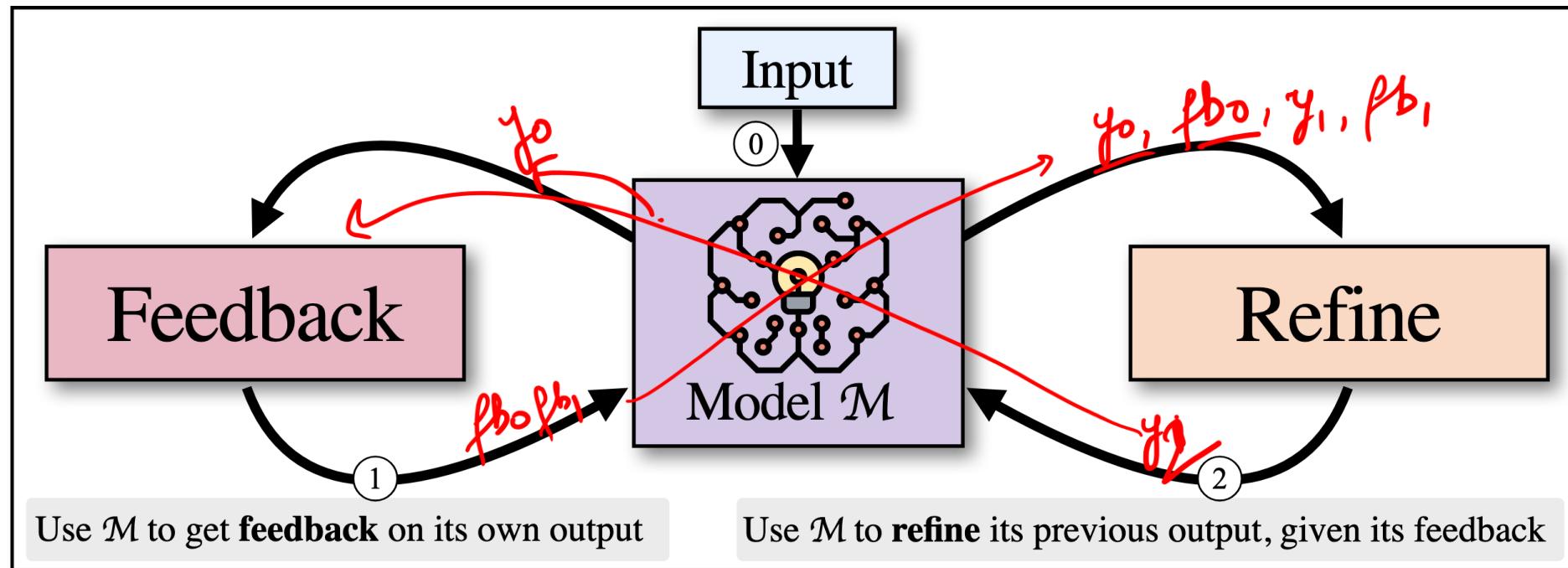


$x \rightarrow$   
ICL  
with  
GT  
 $\rightarrow M \rightarrow r_1, y_1$



# Self-Refine\*

Iterative self-refinement using self-feedback



\* SELF-REFINE: Iterative Refinement with Self-Feedback, Madaan et. al., May 2023



# Overview

- Methods that use self-play to generate synthetic data and update its weights:
  - STaR
  - Self Instruct
  - Self Align
- Methods that iteratively improve their outputs during inference without weight updates:
  - Self Refine



# Experience Acquisition

- Generating \*good quality\* answers for fine-tuning.
  - Most crucial step in Self-Evolution
- CoT typically performs better than standard prompting.
- Is CoT good enough for **complex reasoning tasks?**



# Game of 24

- Input: Four numbers, e.g. 4 4 6 8
- Task: Create an arithmetic expression using ( + - \* / ) that evaluates to 24
- Output: Arithmetic expression, e.g.  $(6 - 4) * (4 + 8) = 24$



# Game of 24

## COT Prompt

Use numbers and basic arithmetic operations (+ - \* /) to obtain 24. Each step, you are only allowed to choose two of the remaining numbers to obtain a new number.

Input: 4 4 6 8

Steps:  $4 + 8 = 12$  (left: 4 6 12) ;  $6 - 4 = 2$  (left: 2 12) ;  $2 * 12 = 24$  (left: 24)

Answer:  $(6 - 4) * (4 + 8) = 24$

{ More examples }

Input: 4 9 10 13

## Response by ChatGPT

Steps:  $13 - 9 = 4$  (left 4, 4, 10);  $4 * 4 = 16$  (left 16, 10);  
 $16 + 10 = 24$  (left: 24)

Answer:  $((13 - 9) * 4 + 10) = 24$

Content credit: <https://neurips.cc/virtual/2023/poster/72797>



LLMs: Introduction and Recent Advances



Yatin Nandwani

Method	Success
IO prompt	7.3%]
CoT prompt	4.0%]
CoT-SC (k=100)	9.0%

## Issues with CoT

- **Token level decision:** Hard to tell if a generated token is good or bad
- **No backtracking:** If generated tokens so far are incorrect, then game over.  
In fact, 60% CoT examples fail after 1<sup>st</sup> step.

# Experience Acquisition

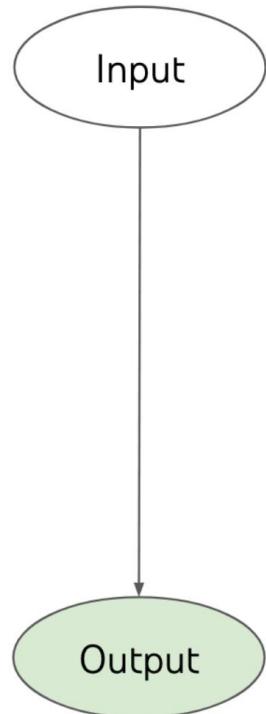
- Limitations of CoT
  - Token level decisions -- no global exploration
  - No backtracking -- linear one-by-one thought generation
- Solving complex reasoning tasks may require -
  - ✓ Global exploration / Planning
  - ✓ Lookahead / backtracking

In Classical AI, problem solving is formulated as:

*Search through a combinatorial problem space represented as a tree.*



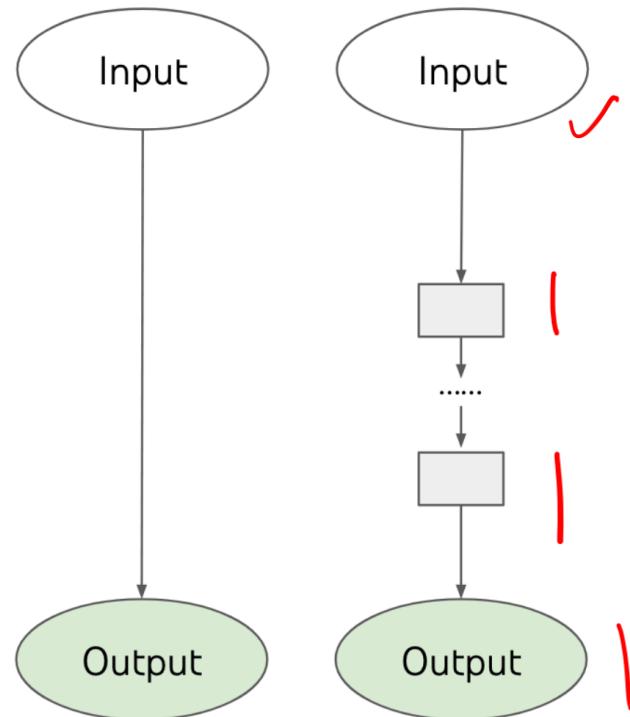
# Search in a Tree Of Thought



(a) Input-Output  
Prompting (IO)



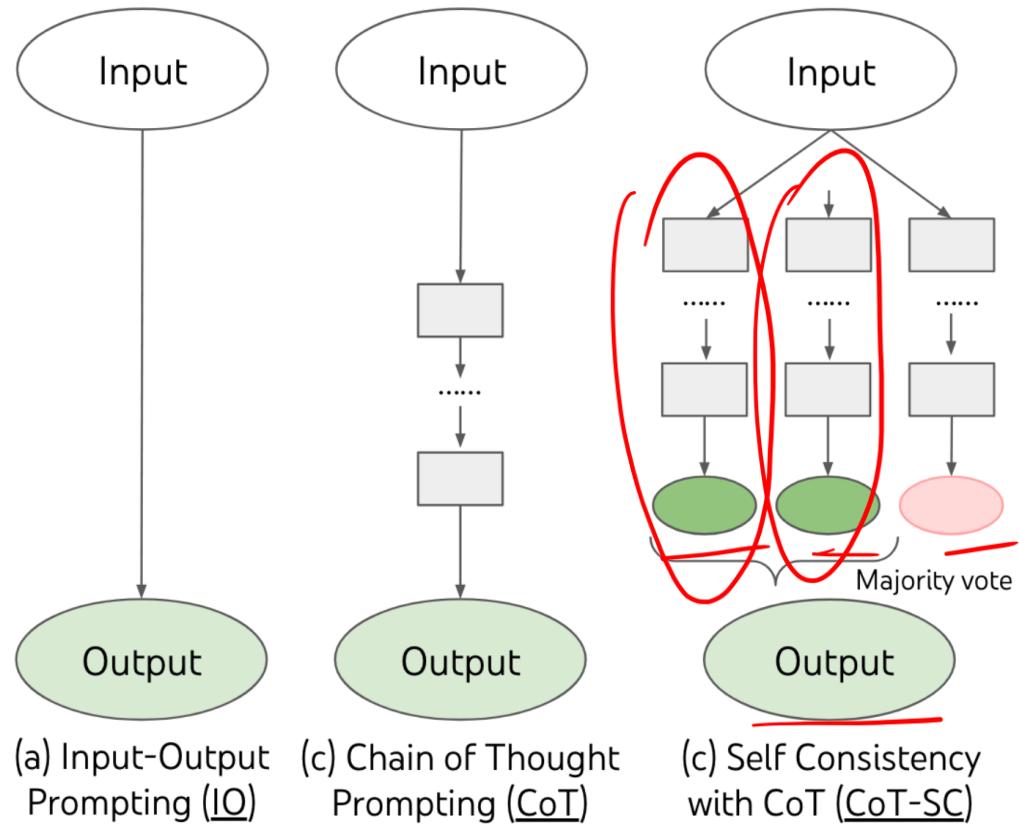
# Search in a Tree Of Thought



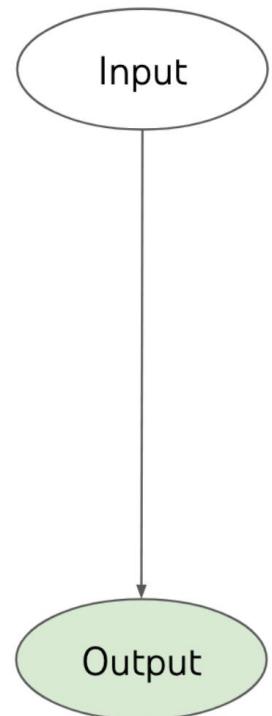
(a) Input-Output  
Prompting (IO)      (c) Chain of Thought  
Prompting (CoT)



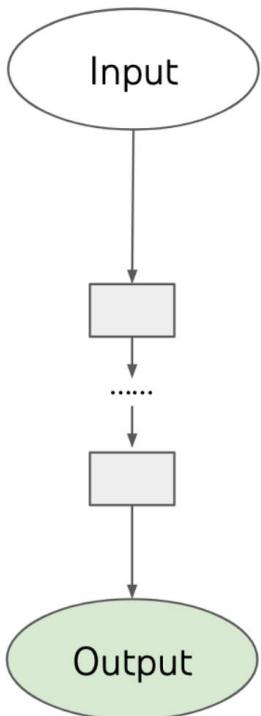
# Search in a Tree Of Thought



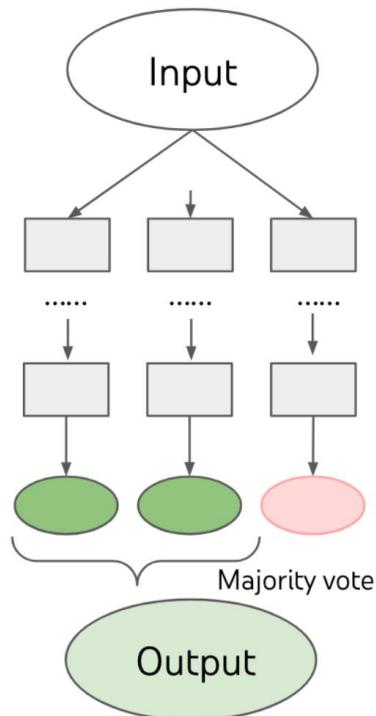
# Search in a Tree Of Thought



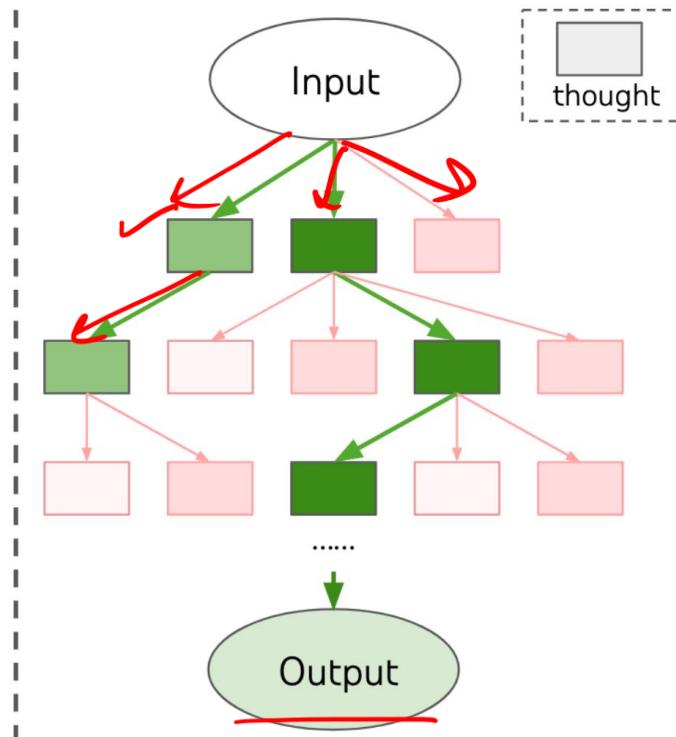
(a) Input-Output  
Prompting (IO)



(b) Chain of Thought  
Prompting (CoT)



(c) Self Consistency  
with CoT (CoT-SC)



(d) Tree of Thoughts (ToT)



# Game of 24

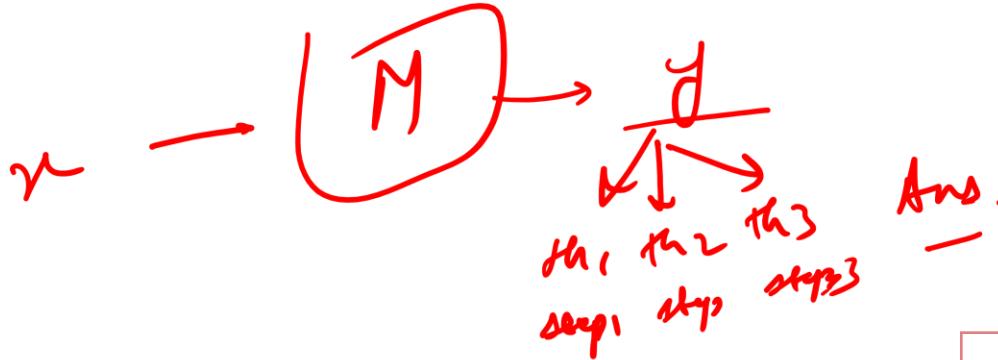
**Input:** 4 4 6 8

## Intermediate thoughts / steps:

**Step 1:**  $13 - 9 = 4$  (left 4, 4, 10)

**Step 2:**  $10 - 4 = 6$  (left 4, 6)

**Step 3:**  $4 * 6 = 24$  (left: 24)

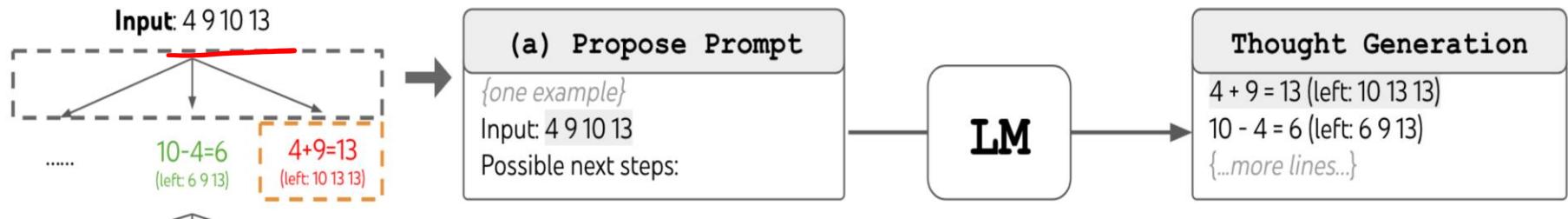


## ToT Recipe

- Decompose:** what is an intermediate thought step?
- Generate:** How to generate a thought?
- Evaluate:** How to evaluate the thoughts?
- Search:** Which algorithm to search the thought space  
- DFS, BFS, MCTS, A\*?



# Game of 24

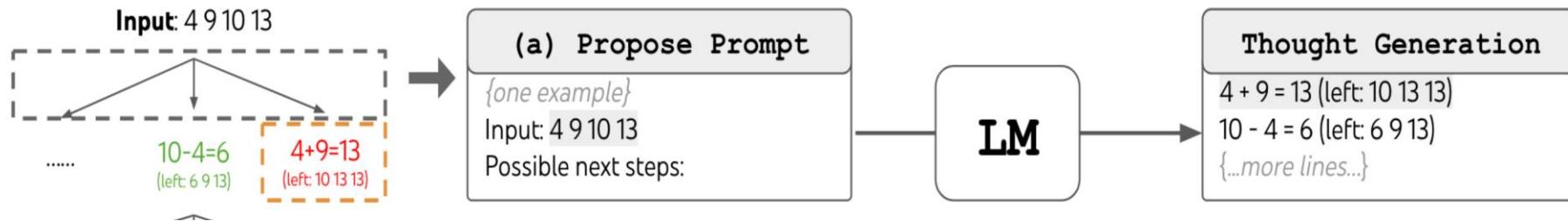


## ToT Recipe

- 1. Decompose:** what is an intermediate thought step?
- 2. Generate:** How to generate a thought?
- 3. Evaluate:** How to evaluate the thoughts?
- 4. Search:** Which algorithm to search the thought space
  - DFS, BFS, MCTS, A\*?



# Game of 24



## Generation Prompt

**Input:** 2 8 8 14

**Possible next steps:** 2 + 8 = 10 (left: 8 10 14) ; 8 / 2 = 4 (left: 4 8 14); 14 + 2 = 16 (left: 8 8 16) ; 2 \* 8 = 16 (left: 8 14 16) ; 8 - 2 = 6 (left: 6 8 14) ; 14 - 8 = 6 (left: 2 6 8)

**Input:** {input}

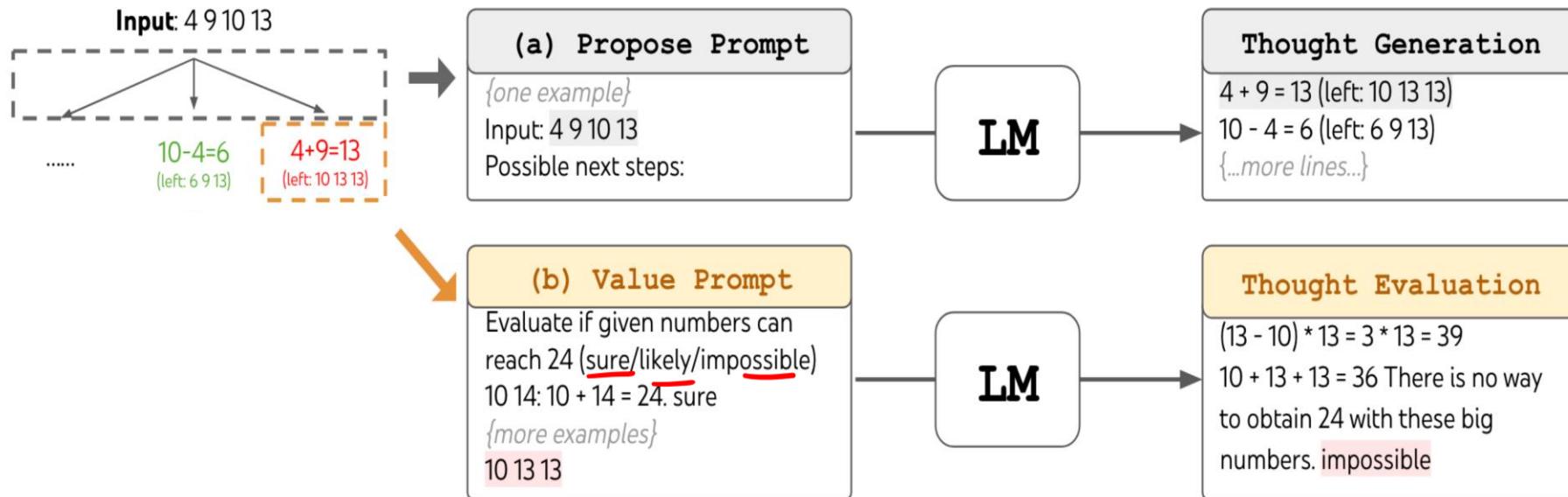
**Possible next steps:**

## ToT Recipe

- 1. Decompose:** what is an intermediate thought step?
- 2. Generate:** How to generate a thought?
- 3. Evaluate:** How to evaluate the thoughts?
- 4. Search:** Which algorithm to search the thought space - DFS, BFS, MCTS, A\*?



# Game of 24

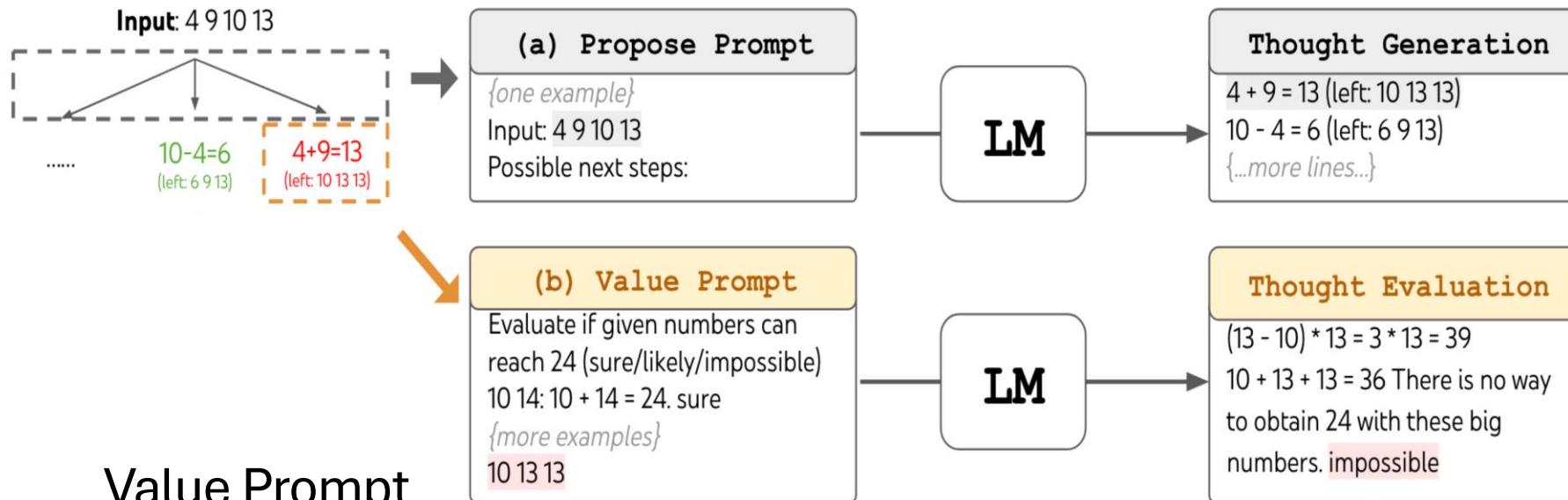


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# Game of 24

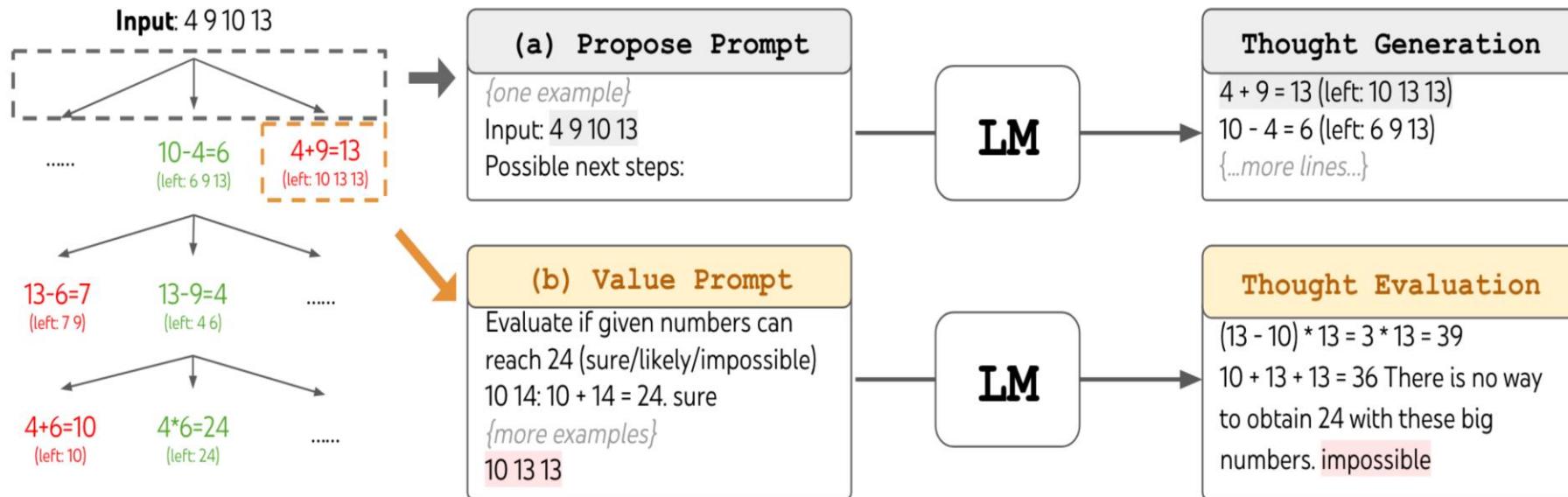


## ToT Recipe

1. **Decompose:** what is an intermediate thought step?
2. **Generate:** How to generate a thought?
3. **Evaluate:** How to evaluate the thoughts?
4. **Search:** Which algorithm to search the tree of thought  
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# Game of 24



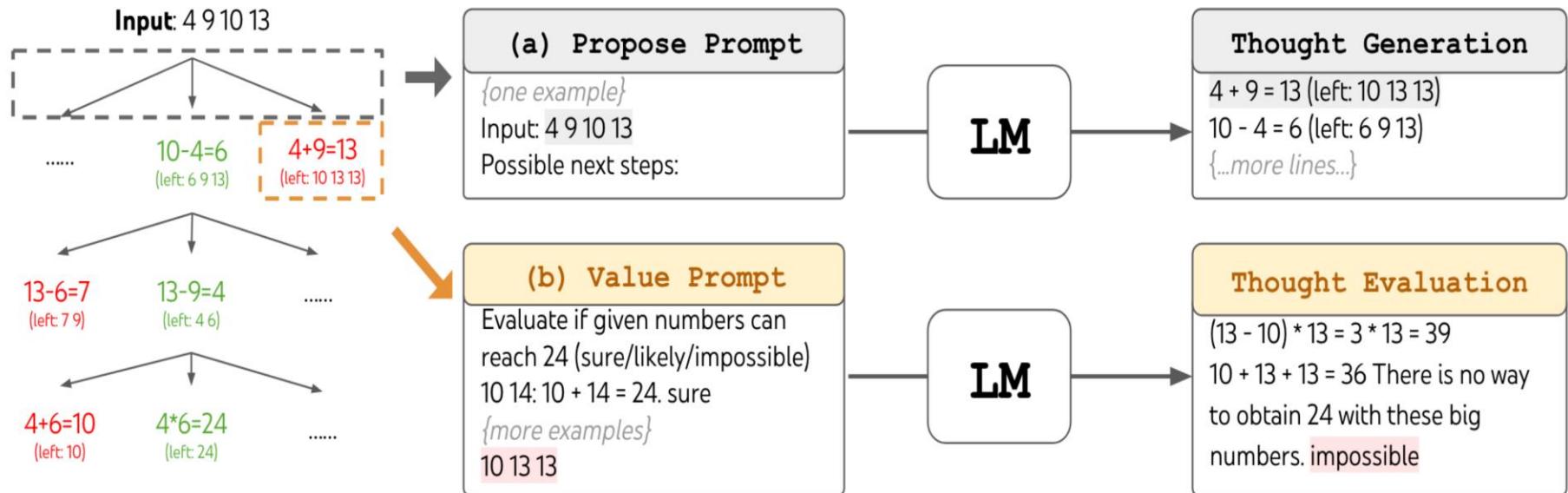
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- 3. Evaluate:** How to evaluate the thoughts?
- 4. Search:** Which algorithm to search the tree of thought
  - DFS, BFS, MCTS, A\*?

**Search Algorithm:** BFS with depth = 4 and breadth  $\leq 5$



# Game of 24



Method	Success
IO prompt	7.3%
CoT prompt	4.0%
CoT-SC (k=100)	9.0%
ToT (ours) (b=1)	45%]
ToT (ours) (b=5)	74%]



# Game of 24 – cost and efficiency

Cost of ToT ~ 100 CoT trials

Method	Success
IO prompt	7.3%
CoT prompt	4.0%
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ToT (ours) ( $b=1$ )	45%
ToT (ours) ( $b=5$ )	<b>74%</b>



# Game of 24 – cost and efficiency

Cost of ToT ~ 100 CoT trials

New baselines:

- COT (Best of 100 assuming oracle)
- IO ( Best of 100 assuming oracle)

Method	Success
IO prompt	7.3%
CoT prompt	4.0%
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# Game of 24 – cost and efficiency

Cost of ToT ~ 100 CoT trials

<b>Game of 24</b>	<b>Generate/Prompt tokens</b>	<b>Cost per case</b>	<b>Success</b>
IO (best of 100)	1.8k / 1.0k	\$0.13	33%
CoT (best of 100)	6.7k / 2.2k	\$0.47	49%
ToT	5.5k / 1.4k	\$0.74	74%

Table 7: Cost analysis on Game of 24.

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CoT prompt	4.0%
CoT-SC (k=100)	9.0%
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IO (best of 100)	33%
CoT (best of 100)	49%



# GSM8k and StrategyQA

	<b>GSM8K</b>	<b>StrategyQA</b>
IO	51	73
CoT	86	82
ToT	<b>90</b>	<b>83</b>

GPT4 + CoT already good on GSM8k – hence little improvement using ToT

<b>Method</b>	<b>Success</b>
IO prompt	7.3%
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CoT-SC ( $k=100$ )	9.0%
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# GSM8k and StrategyQA

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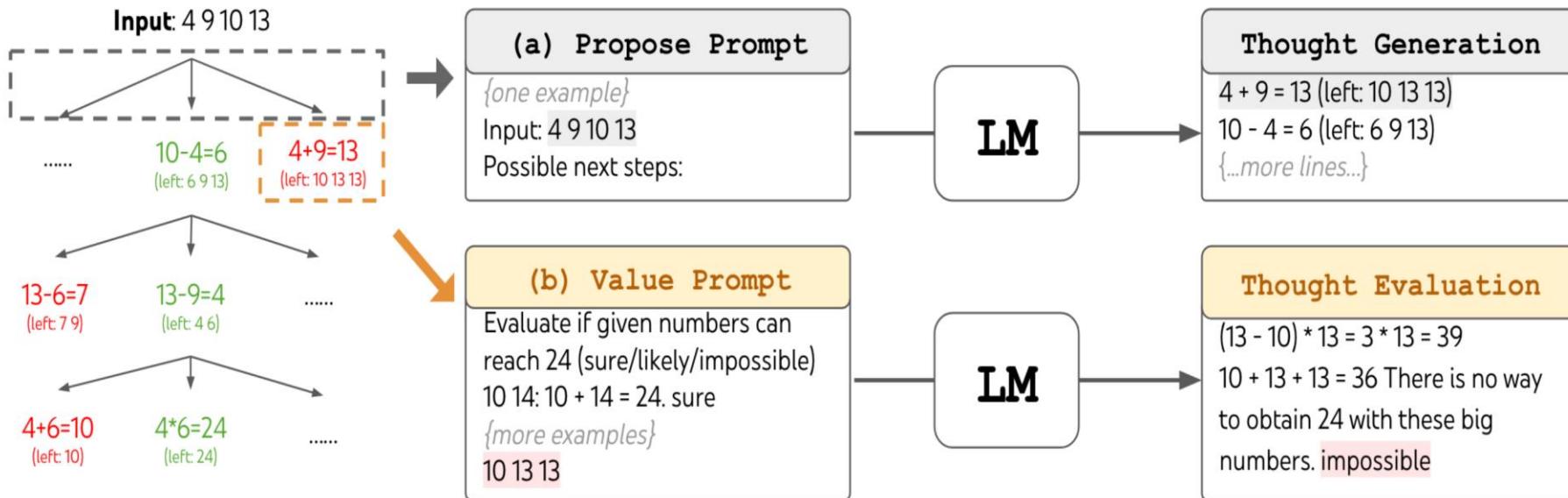
  

IO (best of 100)	33%
CoT (best of 100)	49%

Bottleneck in StrategyQA is knowledge and not reasoning.



# Game of 24



## ToT Recipe

- 1. Decompose:** what is an intermediate thought step?
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  - DFS, BFS, MCTS, A\*?

**Search Algorithm:** BFS with depth = 4 and breadth  $\leq 5$



# Accessing GPT-4 level Mathematical Olympiad Solutions via Monte Carlo Tree Self-refine with LLaMa-3 8B: A Technical Report

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## Recipe

- Decompose:** what is an intermediate thought step?
- Generate:** How to generate a thought?
- Evaluate:** How to evaluate the thoughts?
- Search:** Use MCTS



# Till Now

- Methods that use self-play to generate synthetic data and update its weights:
  - STaR
  - Self Instruct
  - Self Align
- Methods that iteratively improve their outputs during inference without weight updates:
  - Self Refine
  - Tree of Thought
  - MCTS Self-Refine (MCTS<sub>r</sub>)



# Till Now

- Methods that use self-play to generate synthetic data and update its weights:
  - STaR
  - Self Instruct
  - Self Align
- Methods that iteratively improve their outputs during inference without weight updates:
  - Self Refine
  - Tree of Thought
  - MCTS Self-Refine (MCTS<sub>r</sub>)
- Is there a method that combines iterative inference with weight updates?



# Toward Self-Improvement of LLMs via Imagination, Searching, and Criticizing

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## Abstract

Despite the impressive capabilities of Large Language Models (LLMs) on various tasks, they still struggle with scenarios that involves complex reasoning and planning. Recent work proposed advanced prompting techniques and the necessity of fine-tuning with high-quality data to augment LLMs' reasoning abilities. However, these approaches are inherently constrained by data availability and quality. In light of this, self-correction and self-learning emerge as viable solutions, employing strategies that allow LLMs to refine their outputs and learn from self-assessed rewards. Yet, the efficacy of LLMs in self-refining its response, particularly in complex reasoning and planning task, remains dubious. In this paper, we introduce **ALPHALLM** for the self-improvements of LLMs, which integrates Monte Carlo Tree Search (MCTS) with LLMs to establish a self-improving loop, thereby enhanc-

- Alpha-LLM

- Use **MCTS** to generate good quality synthetic data
- Update LLM via **SFT**



# Summary

- ✓ Methods that use self-play to generate synthetic data and update its weights:
  - STAR
  - Self Instruct
  - Self Align
- ✓ Methods that iteratively improve their outputs during inference without weight updates:
  - Self Refine
  - Tree of Thought
  - MCTS Self-Refine (MCTS<sub>r</sub>)
- ✓ Alpha LLM – MCTS<sub>r</sub> for good quality synthetic data generation;  
SFT for weight update.

