# **RL for LLM Alignment and Inference**

Sharif University 2025-05-29

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#### **Research topics**

- Machine Learning: reinforcement learning, uncertainty quantification, federated learning, inverse constraint learning
- Natural Language Processing: LLM alignment and inference, agentic LLMs, knowledge graphs, post-editing ASR error correction
- **Applications**: autonomous driving, sports analytics, material design for CO<sub>2</sub> recycling



#### Outline

- LLM Alignment
  - Reinforcement Learning from Human Feedback
  - Direct Preference Optimization
  - Reward Guided Text Generation
- LLM Reasoning
  - Search and planning
  - Group Relative Policy Optimization (GRPO)
  - Reflection: Verbalized RL





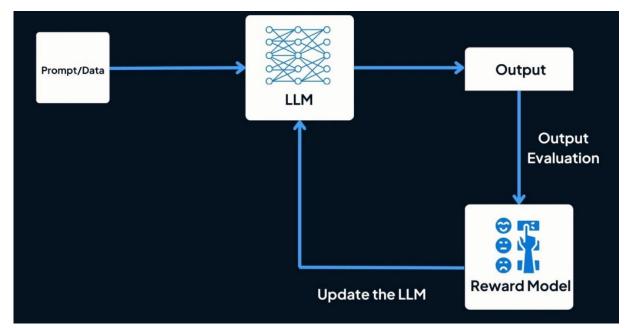
#### Large Language Models

Agent: system

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- Environment: user
- **State:** history of past utterances
- Action: system utterance
- Reward: task completion, human feedback

"We posit that the superior writing abilities of LLMs, as manifested in surpassing human annotators in certain tasks, are fundamentally driven by RLHF, as documented in Gilardi et al. (2023) and Huang et al. (2023)." Llama 2 Technical Report (Touvron et. al 2023)



Credit: https://www.twine.net/blog/what-is-reinforcement-learning-from-human-feedback-rlhf-and-how-does-it-work/

"This behavior (re-evaluation) is not only a testament to the model's growing reasoning abilities but also a captivating example of how reinforcement learning can lead to unexpected and sophisticated outcomes" Deepseek-R1 Technical Report (Guo et. al 2025)



#### **Recipe For Large Language Model Training**

#### Step 1

Collect demonstration data, and train a supervised policy.

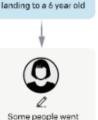
#### A prompt is sampled from our prompt dataset.

A labeler demonstrates the desired output behavior.

This data is used to fine-tune GPT-3 with supervised learning.

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to the moon..

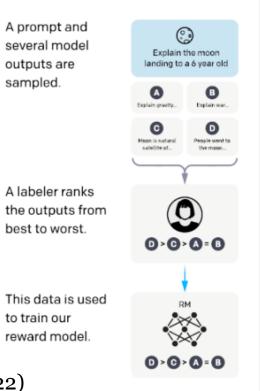
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InstructGPT (Ouyang et. al 2022)

#### Step 2

sampled.

Collect comparison data, and train a reward model.



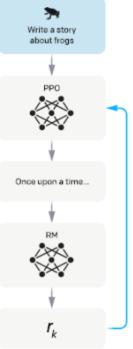
#### Step 3

Optimize a policy against the reward model using reinforcement learning.

#### A new prompt is sampled from the dataset.

The policy generates an output.

- The reward model calculates a reward for the output.
- The reward is used to update the policy using PPO.





## **Response Ranking**

Explain reinforcement learning in three sentences.

< 1 / 2 > 🏼 🌀

Reinforcement learning is a type of machine learning where an agent learns to make decisions by receiving feedback in the form of rewards or punishments. The agent's goal is to maximize its cumulative reward over time by exploring different actions and learning which actions lead to the highest rewards. Reinforcement learning has been successfully applied to a variety of tasks, including game playing, robotics, and recommendation systems.

Reinforcement learning is a type of machine learning that focuses on training an agent to make decisions based on trial and error. The agent receives feedback in the form of rewards or penalties for each decision it makes. By learning from this feedback, the agent can improve its decision-making abilities over time.





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## **RL from Human Feedback (RLHF)**

Collect a preference data set:

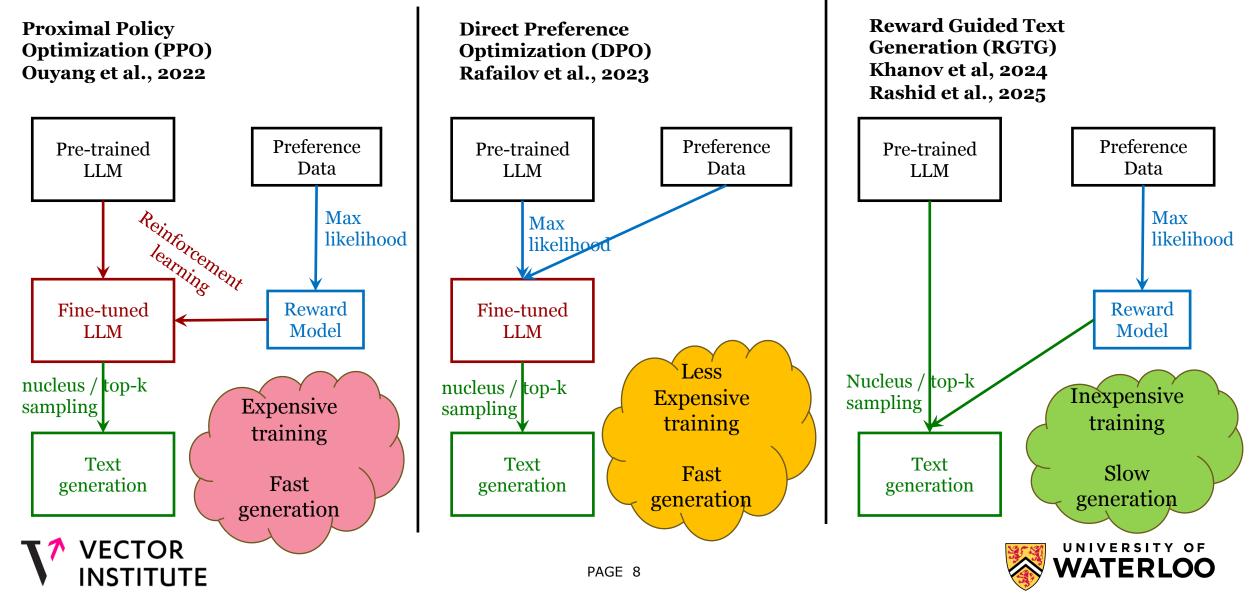
$$D = \{(s, a_+, a_-)_k\}_{k=1}^K \text{ where } a_+ > a_-$$

- Train a reward model according to the Bradley Terry Model:  $\max_{\theta} E_D[\log \sigma(r_{\theta}(s, a_{+}) - r_{\theta}(s, a_{-}))]$
- Make a copy of the LLM and finetune it to maximize:  $\max_{\phi} E_{D,\pi_{\phi}}[r_{\phi}(s, a)] - \beta KL[\pi_{\phi}(a|s)||\pi_{pretrained}(a|s)]$





#### **RLHF Improvements**



## **LLM Alignment with Preference Data**

• Collect preference data:  $D = \{(s, a_+, a_-)_k\}_{k=1}^K$ where *s*: user prompt *a*: system response  $a_+$  is preferred to  $a_-$  (i.e.,  $a_+ > a_-$ ) Domain data Instruction Client data LLM Toxicit airness prevention data PAGE 9

#### **Reward Model**

Stiennon, Ouyang, Wu, Ziegler, Lowe Voss, Radford, Amodei, Christiano (2020) Learning to summarize from human feedback, *NeurIPS*.

- Reward function:  $r_{\theta}(s, a) = real number$
- Consider several possible responses  $a_1 \ge a_2 \ge \cdots \ge a_k$  ranked by annotator
- Training reward function to be consistent with the ranking:

$$Loss(\theta) = -\frac{1}{\binom{k}{2}} E_{(s,a_i,a_j) \in Dataset} \log \sigma \left( r_{\theta}(s, a_i) - r_{\theta}(s, a_j) \right)$$



## **Reinforcement Learning**

Ouyang, Wu, Jiang, Wainwright, et al. (2022) **Training language models to follow instructions with human feedback**, *NeurIPS*.

- Pretrain language model (GPT-3)
- Fine-Tune GPT-3 by RL to obtain InstructGPT
  - Policy (language model):  $\pi_{\phi}(a|s)$
  - Optimize  $\pi_{\phi}(s)$  by Proximal Policy Iteration (PPO)

$$\max_{\phi} E_{s \in Dataset} \left[ E_{a \sim \pi_{\phi}(a|s)} [r_{\theta}(s,a)] - \beta \, KL \big( \pi_{\phi}(\cdot|s) \big| \pi_{ref}(\cdot|s) \big) \right]$$



# **Policy Optimization**

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Stochastic policy  $\pi_{\phi}(a|s) = \Pr(a|s; \phi)$  parametrized by  $\phi$ .

	<b>Supervised</b> Fine-Tuning	<b>Reinforcement Learning</b>
Data	{ $(s_1, a_1^*), (s_2, a_2^*), \dots$ } ( $a^*$ denotes optimal action)	$\{(s_1, a_1, r_1), (s_2, a_2, r_2),\}$ ( <i>r</i> denotes reward for s,a pair)
Objective	Maximum likelihood $\max_{\phi} \sum_{n} \log \pi_{\phi}(a_{n}^{*} s_{n})$	Maximum expected rewards $\max_{\phi} \sum_{n} \gamma^{n} E_{\pi_{\phi}}[r_{n} s_{n}, a_{n}]$
Policy update	$\phi \leftarrow \phi + \alpha  \nabla_{\phi} \log \pi_{\phi}(a_n^*   s_n)$	$\phi \leftarrow \phi + \alpha  \mathbf{G}_n  \nabla_\phi \log \pi_\phi(a_n   s_n)$ where $G_n = \sum_{t=n}^{\infty} \gamma^t r_t$

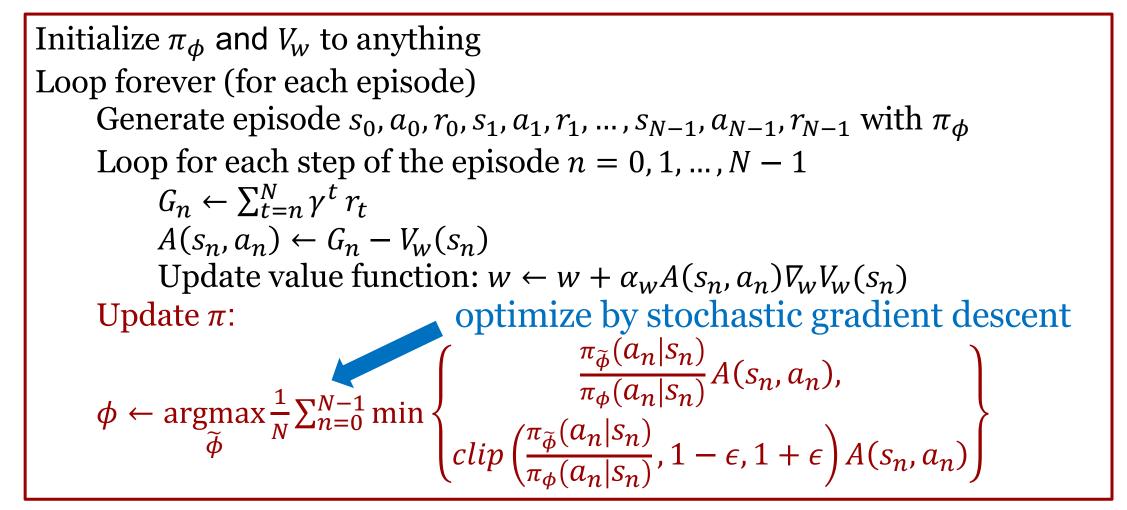


### **REINFORCE Algorithm**

**REINFORCE**( $s_0$ ) Initialize  $\pi_{\phi}$  to anything Loop forever (for each episode) Generate episode  $s_0, a_0, r_0, s_1, a_1, r_1, \dots, s_T, a_T, r_T$  with  $\pi_{\phi}$ Loop for each step of the episode  $n = 0, 1, \dots, T$   $G_n \leftarrow \sum_{t=n}^T \gamma^t r_t$ Update policy:  $\phi \leftarrow \phi + \alpha \ G_n \nabla_{\theta} \log \pi_{\phi}(a_n | s_n)$ Return  $\pi_{\phi}$ 



# **Proximal Policy Optimization (PPO)**

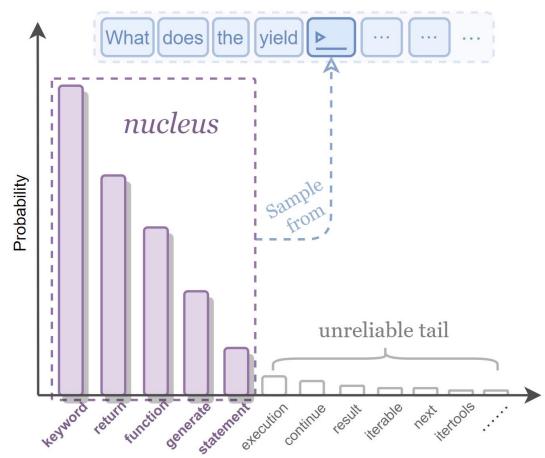




## Inference: Nucleus sampling

Sample from nucleus (top tokens only) to avoid unreliable responses while ensuring diversity

Holtzman, Ari; Buys, Jan; Du, Li; Forbes, Maxwell; Choi, Yejin (2019). **The Curious Case of Neural Text Degeneration**, arxiv.

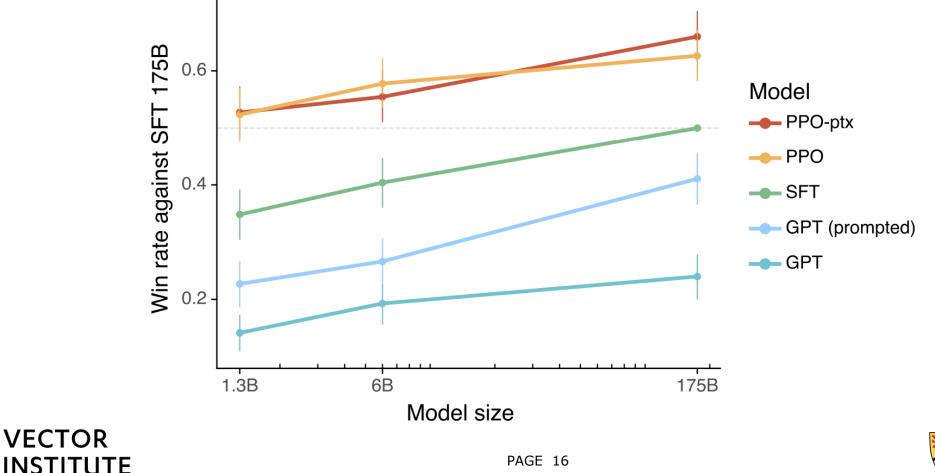


Credit: https://ar5iv.labs.arxiv.org/html/2208.11523



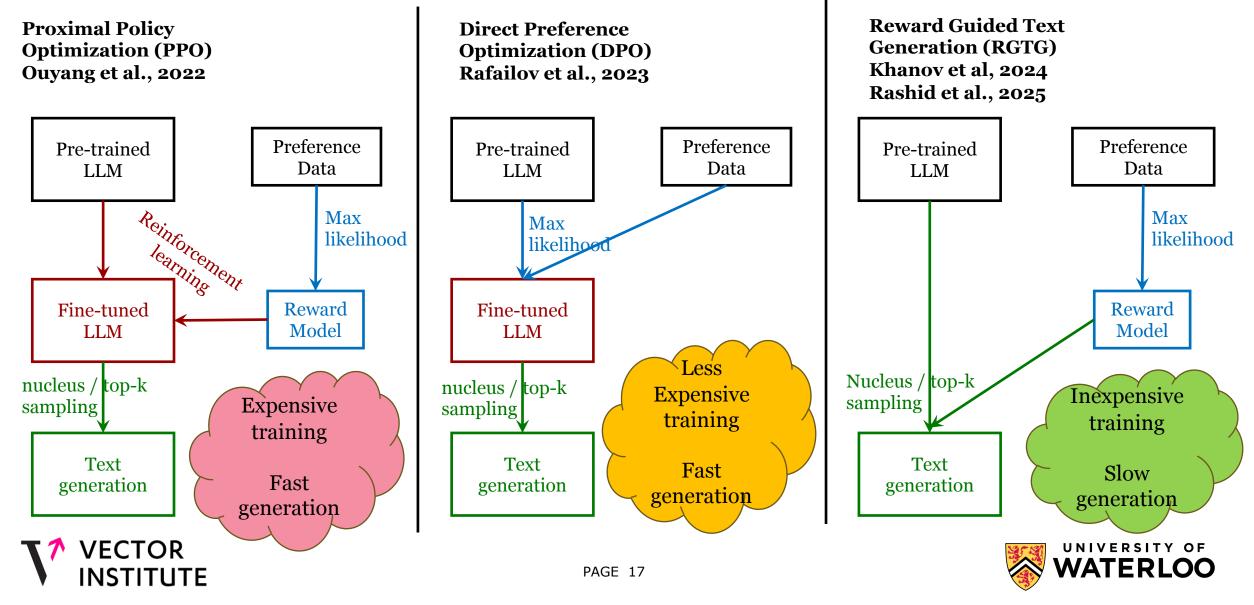
#### **InstructGPT Results**

Ouyang, Wu, Jiang, Wainwright, et al. (2022)



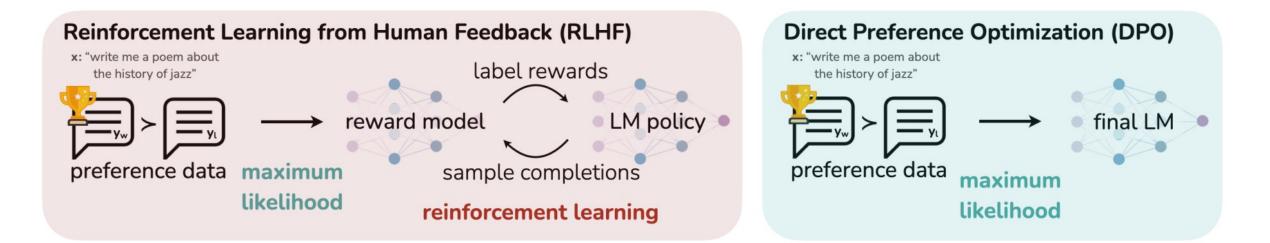


#### **RLHF Improvements**



## **Direct Preference Optimization**

#### Rafailov, Sharma, Mitchell, Ermon, Manning, Finn (2023) **Direct Preference Optimization: Your Language Model is Secretly a Reward Model**, *NeurIPS*.





# **Bypassing RL**

- Recall RL objective:  $\max_{\phi} E_{s \in Dataset} \left[ E_{a \sim \pi_{\phi}(a|s)} [r_{\theta}(s,a)] - \beta KL(\pi_{\phi}(\cdot|s) | \pi_{ref}(\cdot|s)) \right]$
- Closed form solution (based on maximum entropy RL):  $\pi_{\phi}(a|s) = \frac{1}{Z(s)}\pi_{ref}(a|s)\exp\left(\frac{r_{\theta}(s,a)}{\beta}\right)$
- Isolate reward:  $r_{\theta}(s, a) = \beta \log \frac{\pi_{\phi}(a|s)}{\pi_{ref}(a|s)} + \beta \log Z(s)$
- Plug into preference objective:

$$Loss(\theta) = -\frac{1}{\binom{k}{2}} E_{(s,a_i,a_j) \in Dataset} \log \sigma \left( r_{\theta}(s,a_i) - r_{\theta}(s,a_j) \right)$$
$$= -\frac{1}{\binom{k}{2}} E_{(s,a_i,a_j) \in Dataset} \log \sigma \left( \beta \log \frac{\pi_{\phi}(a_i|s)}{\pi_{ref}(a_i|s)} - \beta \log \frac{\pi_{\phi}(a_j|s)}{\pi_{ref}(a_j|s)} \right)$$



## **Optimal Policy Derivation**

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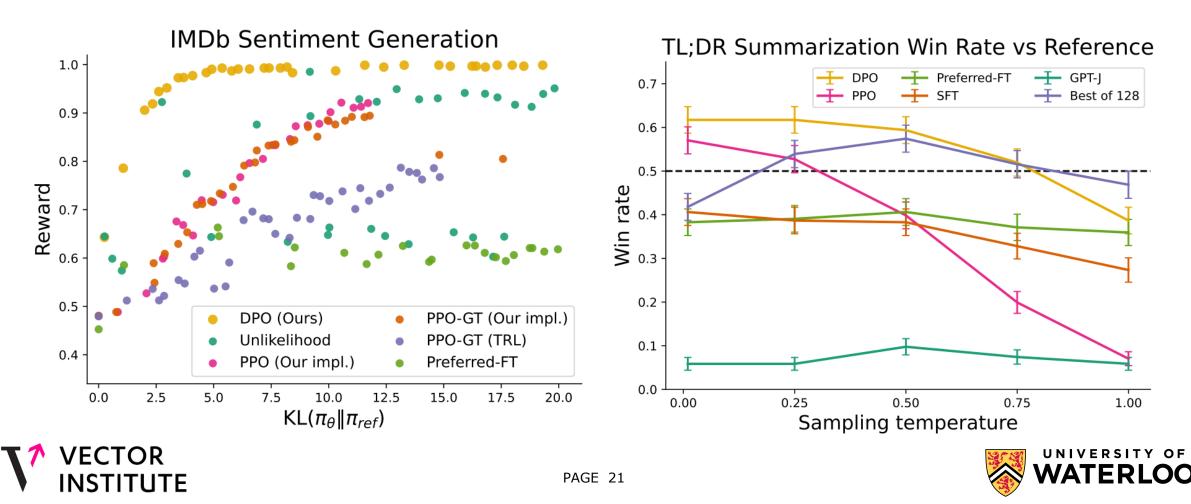
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$$\begin{aligned} \arg\max_{\phi} E_{s\in Dataset} \left[ E_{a \sim \pi_{\phi}(a|s)} [r_{\theta}(s,a)] - \beta \ KL(\pi_{\phi}(\cdot|s)|\pi_{ref}(\cdot|s)) \right] \\ &= \arg\max_{\phi} E_{s\in Dataset} \left[ E_{a \sim \pi_{\phi}(a|s)} \left[ r_{\theta}(s,a) - \beta \log \frac{\pi_{\phi}(a|s)}{\pi_{ref}(a|s)} \right] \right] \\ &= \arg\min_{\phi} E_{s\in Dataset} \left[ E_{a \sim \pi_{\phi}(a|s)} \left[ \log \frac{\pi_{\phi}(a|s)}{\pi_{ref}(a|s)} - \frac{1}{\beta} r_{\theta}(s,a) \right] \right] \\ &= \arg\min_{\phi} E_{s\in Dataset} \left[ E_{a \sim \pi_{\phi}(a|s)} \left[ \log \frac{\pi_{\phi}(a|s)}{\frac{1}{Z(s)} \pi_{ref}(a|s)} \exp \left( \frac{r_{\theta}(s,a)}{\beta} \right) - \log Z(s) \right] \right] \\ &= \arg\min_{\phi} E_{s\in Dataset} \left[ E_{a \sim \pi_{\phi}(a|s)} \left[ \log \frac{\pi_{\phi}(a|s)}{\frac{1}{Z(s)} \pi_{ref}(a|s)} \exp \left( \frac{r_{\theta}(s,a)}{\beta} \right) - \log Z(s) \right] \right] \\ &= \arg\min_{\phi} E_{s\in Dataset} \left[ E_{a \sim \pi_{\phi}(a|s)} \left[ \log \frac{\pi_{\phi}(a|s)}{\frac{1}{Z(s)} \pi_{ref}(a|s)} \exp \left( \frac{r_{\theta}(s,a)}{\beta} \right) \right] \right] \\ &= \arg\min_{\phi} E_{s\in Dataset} \left[ E_{a \sim \pi_{\phi}(a|s)} \left[ \log \frac{\pi_{\phi}(a|s)}{\frac{1}{Z(s)} \pi_{ref}(a|s)} \exp \left( \frac{r_{\theta}(s,a)}{\beta} \right) \right] \right] \\ &= \arg\min_{\phi} E_{s\in Dataset} \left[ E_{a \sim \pi_{\phi}(a|s)} \left[ \log \frac{\pi_{\phi}(a|s)}{\frac{1}{Z(s)} \pi_{ref}(a|s)} \exp \left( \frac{r_{\theta}(s,a)}{\beta} \right) \right] \right] \\ &= \arg\min_{\phi} E_{s\in Dataset} \left[ E_{a \sim \pi_{\phi}(a|s)} \left[ \log \frac{\pi_{\phi}(a|s)}{\frac{1}{Z(s)} \pi_{ref}(a|s)} \exp \left( \frac{\pi_{\theta}(s)}{\beta} \right) \right] \\ &= \arg\min_{\phi} E_{s\in Dataset} \left[ E_{a \sim \pi_{\phi}(a|s)} \left[ \log \frac{\pi_{\phi}(a|s)}{\frac{1}{Z(s)} \pi_{ref}(a|s)} \exp \left( \frac{\pi_{\theta}(s)}{\beta} \right) \right] \\ &= \arg\min_{\phi} E_{s\in Dataset} \left[ KL(\pi_{\phi}(\cdot|s)) ||\pi_{\phi}(\cdot|s) \right] \\ &= \arg\min_{\phi} E_{s\in Dataset} \left[ KL(\pi_{\phi}(\cdot|s)) ||\pi_{\phi}(\cdot|s) \right] \\ &= \varphi^{*} \end{aligned}$$

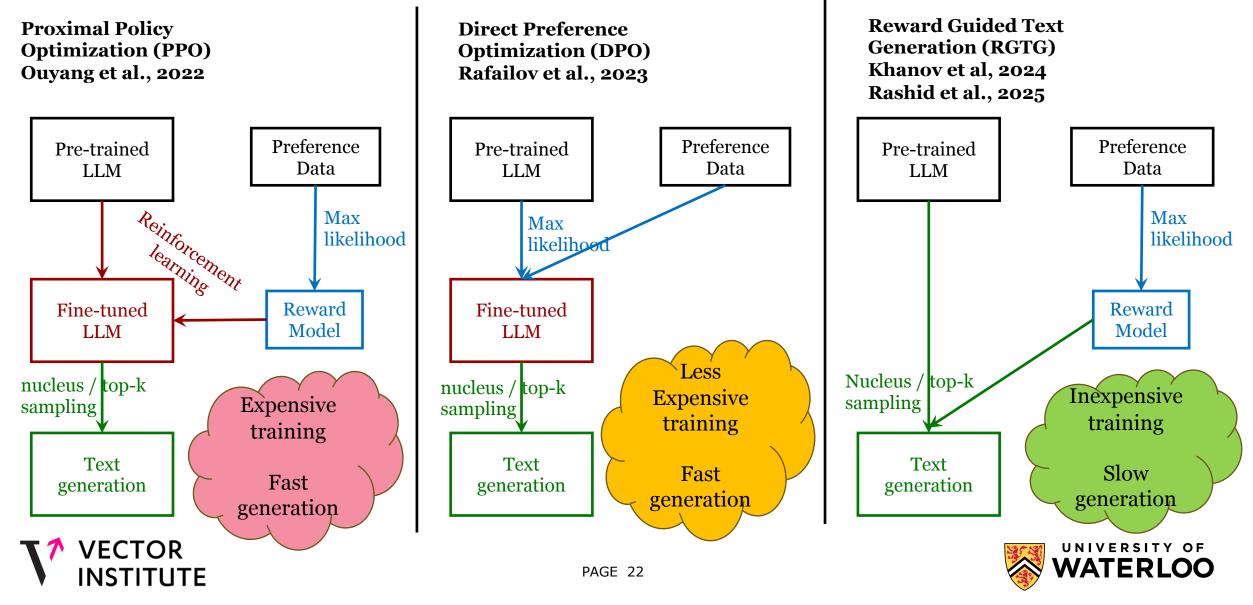


#### **Empirical Results**

#### Rafailov et al. 2023



#### **RLHF Improvements**



#### **Sequence Generation**

Recall closed form solution

$$\pi_{\phi}(\boldsymbol{a}|\boldsymbol{s}) = \frac{1}{Z(\boldsymbol{s})} \pi_{ref}(\boldsymbol{a}|\boldsymbol{s}) \exp\left(\frac{r_{\theta}(\boldsymbol{s},\boldsymbol{a})}{\beta}\right)$$
$$= softmax\left(\log \pi_{ref}(\boldsymbol{a}|\boldsymbol{s}) + \frac{r_{\theta}(\boldsymbol{s},\boldsymbol{a})}{\beta}\right)$$

• Text generation:

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$$\boldsymbol{a} \sim softmax \left( \log \begin{pmatrix} \pi_{ref}(\boldsymbol{a}_1 | \boldsymbol{s}) \\ \pi_{ref}(\boldsymbol{a}_2 | \boldsymbol{s}) \\ \pi_{ref}(\boldsymbol{a}_3 | \boldsymbol{s}) \\ \dots \\ \pi_{ref}(\boldsymbol{a}_n | \boldsymbol{s}) \end{pmatrix} + \begin{pmatrix} r_{\theta}(\boldsymbol{s}, \boldsymbol{a}_1) \\ r_{\theta}(\boldsymbol{s}, \boldsymbol{a}_2) \\ r_{\theta}(\boldsymbol{s}, \boldsymbol{a}_3) \\ \dots \\ r_{\theta}(\boldsymbol{s}, \boldsymbol{a}_n) \end{pmatrix} / \beta \right)$$



#### **Token Generation**

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Token-wise LLM modeling

$$\pi_{\phi}(a^{i}|s, a^{1:i-1}) = \frac{1}{Z(s)}\pi_{ref}(a^{i}|s, a^{1:i-1})\exp\left(\frac{r_{\theta}(s, a^{1:i})}{\beta}\right)$$
$$= softmax\left(\log \pi_{ref}(a^{i}|s, a^{1:i-1}) + \frac{r_{\theta}(s, a^{1:i})}{\beta}\right)$$

$$\begin{array}{l} \text{ Token generation:} \\ a^{i} \sim softmax \left( \log \begin{pmatrix} \pi_{ref}(a_{1}^{i} | \boldsymbol{s}, \boldsymbol{a}^{1:i-1}) \\ \pi_{ref}(a_{2}^{i} | \boldsymbol{s}, \boldsymbol{a}^{1:i-1}) \\ \pi_{ref}(a_{3}^{i} | \boldsymbol{s}, \boldsymbol{a}^{1:i-1}) \\ \dots \\ \pi_{ref}(a_{n}^{i} | \boldsymbol{s}, \boldsymbol{a}^{1:i-1}) \end{pmatrix} + \begin{pmatrix} r_{\theta}(\boldsymbol{s}, \boldsymbol{a}^{1:i-1}, a_{1}^{i}) \\ r_{\theta}(\boldsymbol{s}, \boldsymbol{a}^{1:i-1}, a_{2}^{i}) \\ r_{\theta}(\boldsymbol{s}, \boldsymbol{a}^{1:i-1}, a_{3}^{i}) \\ \dots \\ r_{\theta}(\boldsymbol{s}, \boldsymbol{a}^{1:i-1}, a_{n}^{i}) \end{pmatrix} / \beta \end{array} \right)$$





# FaRMA: Faster Reward Model for Alignment

- Rashid, Wu, Fan, Li, Kristiadi, Poupart (2025) Towards Cost-Effective Reward Guided Text Generation, *ICML*.
- Optimization problem:

$$\max_{\theta} E_{(s,a_+,a_-)\in Dataset} \log \sigma \left( r_{\theta}(s,a_+) - r_{\theta}(s,a_-) \right)$$
  
Subject to  $r_{\theta}(s, a^{1:i}) = \max_{a^{i+1:|a|}} r_{\theta}(s, [a^{1:i}, a^{i+1:|a|}]) \forall s, a, i$ 

• In practice: alternate between minimizing two loss functions

• 
$$L_1(\theta) = -E_{(s,a_+,a_-)\in Dataset} \log \sigma(r_{\theta}(s,a_+) - r_{\theta}(s,a_-))$$

• 
$$L_2(\theta) = \frac{1}{2} E_{(s,a) \in Dataset, i \le |a|} \left( r_{\theta}(s, a^{1:i}) - \max_{a^{i+1:|a|}} r_{\theta}(s, [a^{1:i}, a^{i+1:|a|}]) \right)^2$$



#### FaRMA Pseudocode

Repeat

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Repeat for each 
$$(s, a_+, a_-)$$
 in minibatch  
 $L_1(\theta) = \log \sigma (r_{\theta}(s, a_+) - r_{\theta}(s, a_-))$   
 $\theta \leftarrow \theta - \alpha \nabla L_1(\theta)$   
Repeat for each  $(s, a, i)$  in minibatch

$$L_{2}(\theta) = \frac{1}{2} \left( r_{\theta}(\boldsymbol{s}, \boldsymbol{a}^{1:i}) - \max_{a^{i+1}} r_{\theta}(\boldsymbol{s}, \boldsymbol{a}^{1:i+1}) \right)^{2}$$
$$\theta \leftarrow \theta - \alpha \nabla L_{2}(\theta)$$





## **Empirical Results**

total generation time for the TL;DR summarization task.

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TL;DR Summarization				80 -	TLDR Summarization							
Method	LLM	$r\pm{ m SE}$	Time(min)									
$\pi_{ m ref}$	frozen	$0.98{\pm}0.18$	2	_ 60 -								
ARGS	frozen	$1.46 {\pm} 0.16$	32	(%)		)						
PARGS	frozen	$1.56 {\pm} 0.19$	31	$^{ m Bate}$ $40$ -								
CD	frozen	$1.15 {\pm} 0.16$	29	а 10 а								
FaRMA	frozen	$2.05 {\pm} 0.15$	5	Win								
CARDS	frozen	$1.73 {\pm} 0.16$	17	20 -								
DPO	trained	$2.08 {\pm} 0.18$	2									
PPO	trained	$2.05{\pm}0.14$	2	0 -	Fal	RMA A	RGS PA	RGS CD	DPO	PPO	CARDS	
				(	)	10	20	30	40	50	6	
2. Avg. reward (over 100 samples) $\pm$ standard error				or	Inference Time (mins)							

Figure 2. GPT4 evaluation on TLDR



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# **Reasoning LLMs**

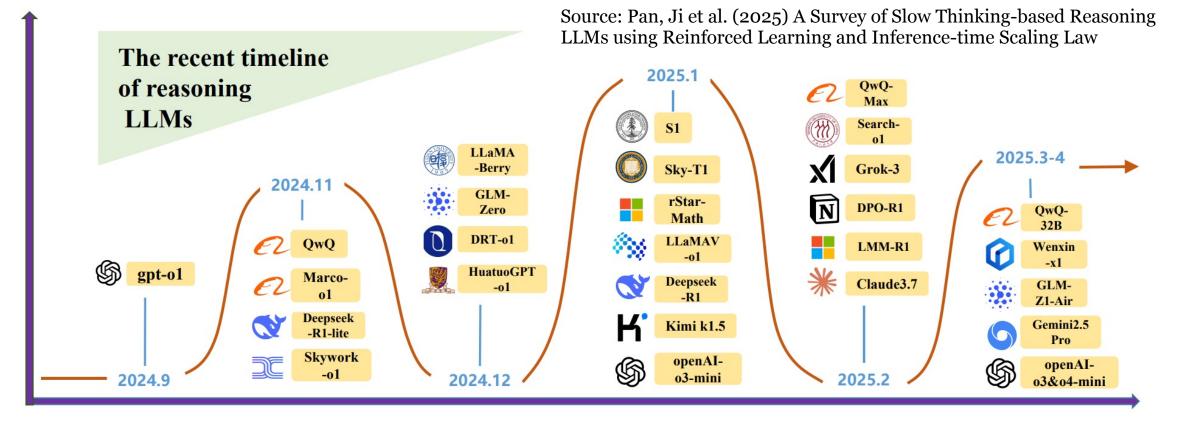
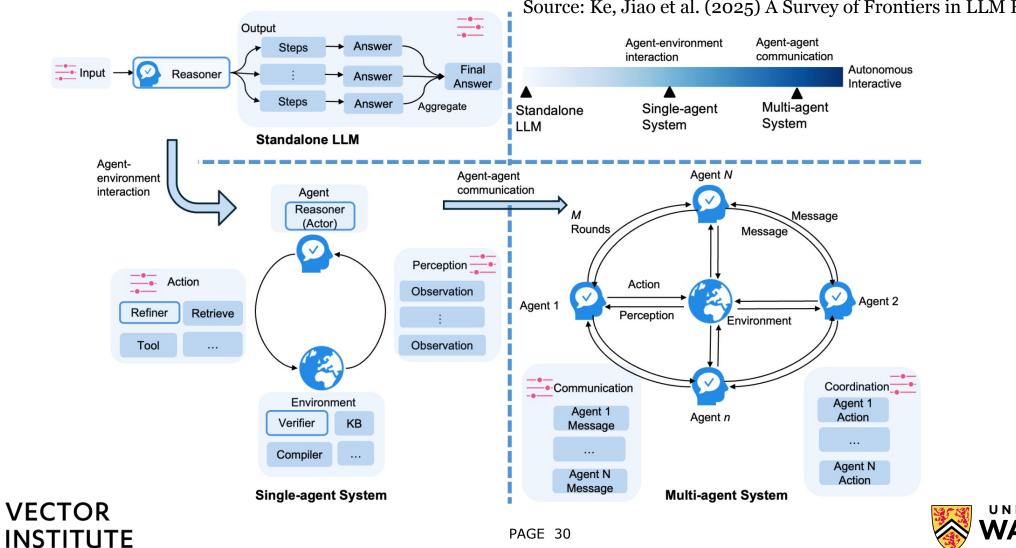


Fig. 1. The timeline of main reasoning LLMs.





## **Inference Time Reasoning**



Source: Ke, Jiao et al. (2025) A Survey of Frontiers in LLM Reasoning



# **Reasoning by Searching**

Source: Pan, Ji et al. (2025) A Survey of Slow Thinking-based Reasoning LLMs using Reinforced Learning and Inference-time Scaling Law

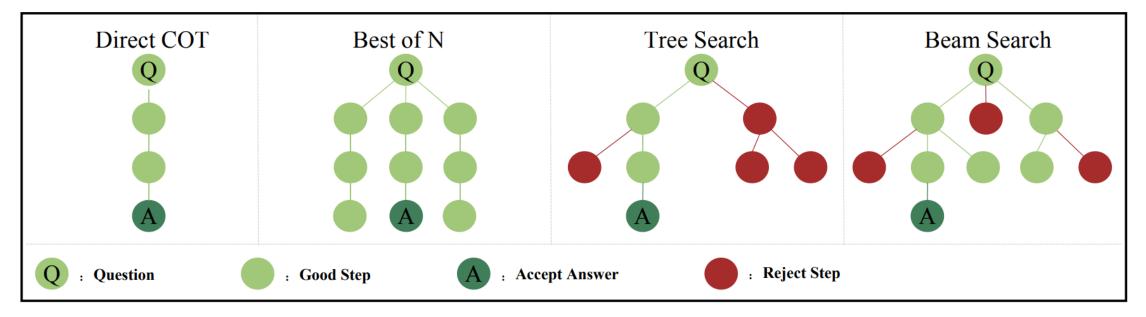


Fig. 3. The search algorithms for test-time scaling

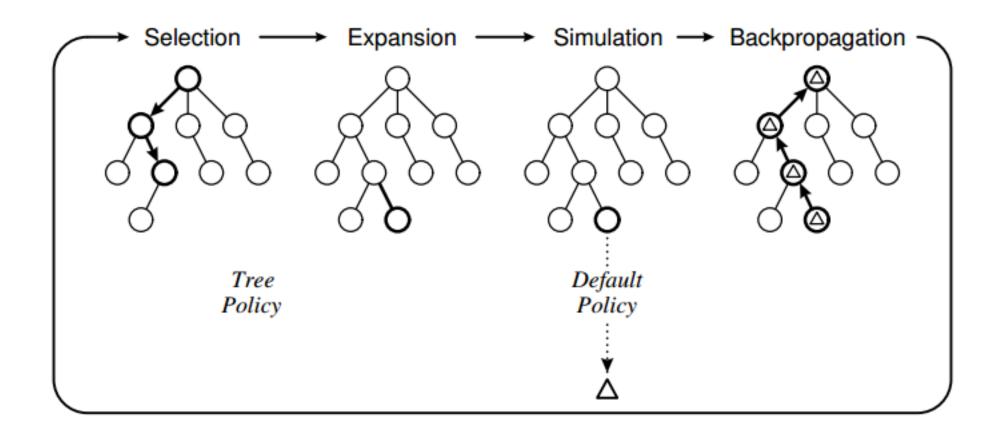




#### **Monte Carlo Tree Search**

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# Learning to Reason

Source: Pan, Ji et al. (2025) A Survey of Slow Thinking-based Reasoning LLMs using Reinforced Learning and Inference-time Scaling Law

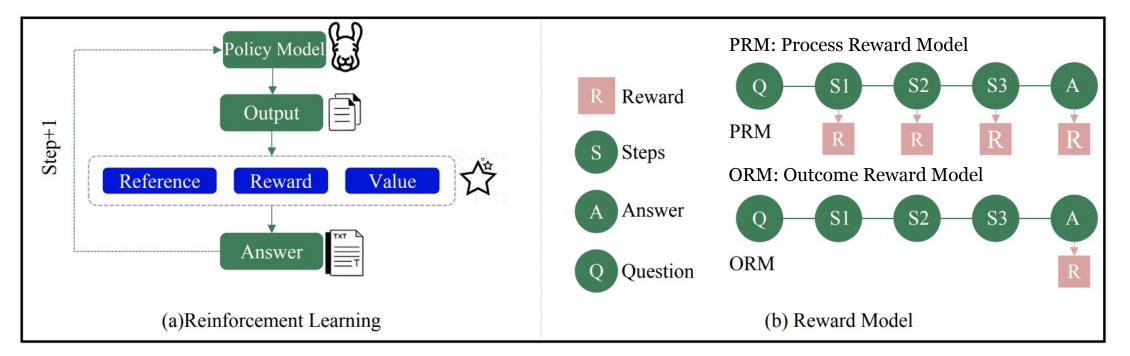


Fig. 4. The reinforcement learning framework and reward model





# **Simplifying PPO**

Source: Shao, Wang et al. (2024) DeepSeekMath: Pushing the Limits of Mathematical Reasoning in Open Language Models

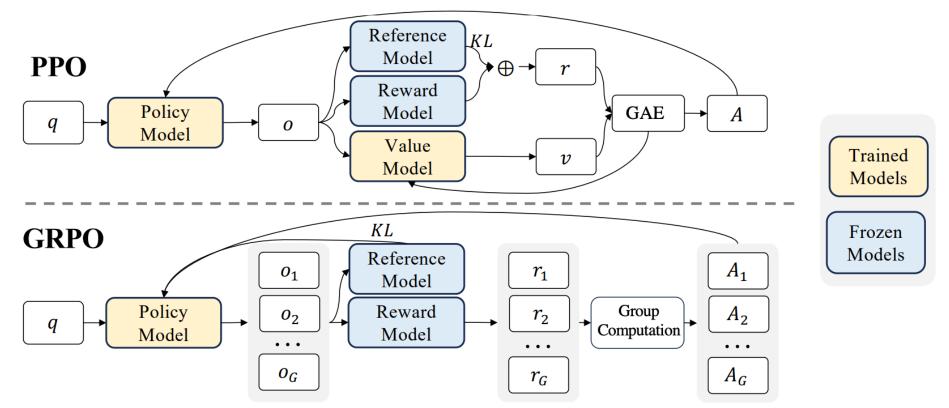


Figure 4 | Demonstration of PPO and our GRPO. GRPO foregoes the value model, instead estimating the baseline from group scores, significantly reducing training resources. VECTOR TITUTE



# **Group Relative Policy Optimization (GRPO)**

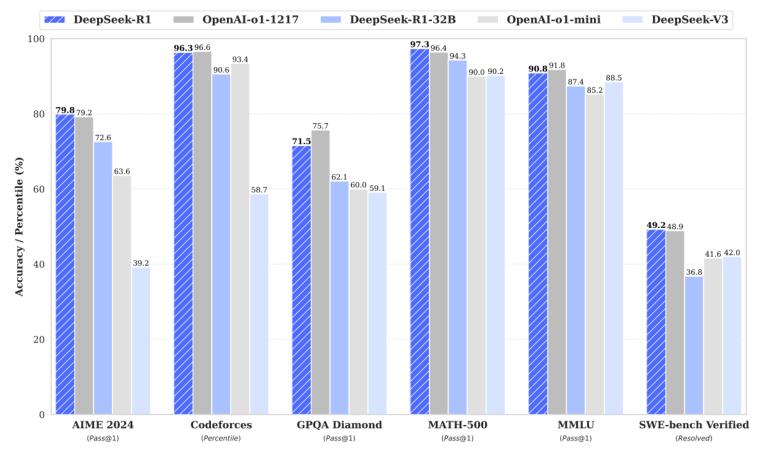
Initialize 
$$\pi_{\phi}$$
 and  $V_{w}$  to anything  
Loop forever  
Generate set of episodes  $\{\tau_{0}, ..., \tau_{G-1}\}$ :  
Sample  $\tau_{g} = (s_{0}^{g}, a_{0}^{g}, r_{0}^{g}, s_{1}^{g}, a_{1}^{g}, r_{1}^{g}, ..., s_{N-1}^{g}, a_{N-1}^{g}, r_{N-1}^{g})$  with  $\pi_{\phi}$   
Evaluate:  $R_{n}^{g} \leftarrow \sum_{t=n}^{N} \gamma^{t} r(s_{t}^{g}, a_{t}^{g}) \forall n$   
Loop for each episode  $g$  and step  $n$   
 $A_{n}^{g} \leftarrow (R_{n}^{g} - mean(\{R_{n}^{0}, ..., R_{n}^{G-1}\}))/std(\{R_{n}^{0}, ..., R_{n}^{G-1}\})$   
Update  $\pi$ :  
 $\phi \leftarrow \operatorname{argmax} \frac{1}{G} \sum_{g=0}^{G-1} \frac{1}{N} \sum_{n=0}^{N-1} \min \left\{ \begin{cases} \frac{\pi_{\tilde{\phi}}(a_{n}^{g}|s_{n}^{g})}{\pi_{\phi}(a_{n}^{g}|s_{n}^{g})} A_{n}^{g} \\ clip \left(\frac{\pi_{\tilde{\phi}}(a_{n}^{g}|s_{n}^{g})}{\pi_{\phi}(a_{n}^{g}|s_{n}^{g})}, 1 - \epsilon, 1 + \epsilon\right) A_{n}^{g} \end{cases} \right\}$ 

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#### **DeepSeek-R1**

Source: DeepSeek-R1: Incentivizing Reasoning Capability in LLMs via Reinforcement Learning (2025)



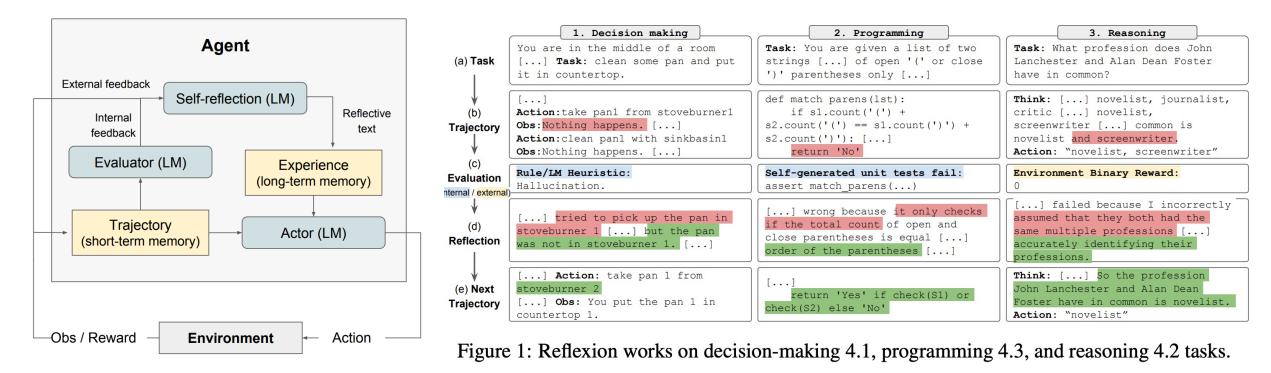




# **Reflexion: Verbalized Reinforcement Learning**

Source: Shinn, Cassano et al. (2023) Reflexion: Language Agents with Verbal Reinforcement Learning

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# Improved Reasoning by Self-Reflection

Source: Shinn, Cassano et al. (2023) Reflexion: Language Agents with Verbal Reinforcement Learning

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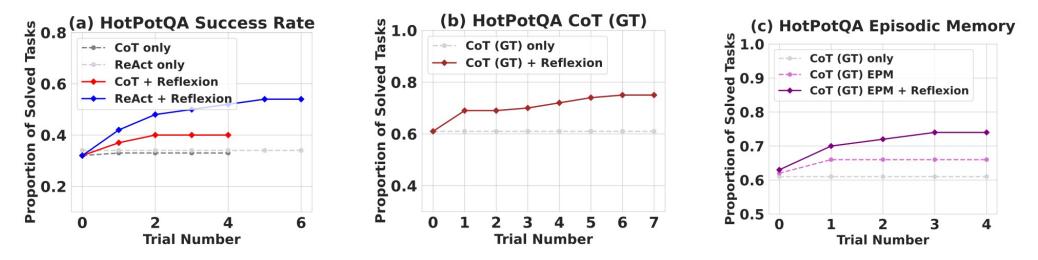


Figure 4: Chain-of-Thought (CoT) and ReAct. Reflexion improves search, information retrieval, and reasoning capabilities on 100 HotPotQA questions. (a) Reflexion ReAct vs Reflexion CoT (b) Reflexion CoT (GT) for reasoning only (c) Reflexion vs episodic memory ablation.



# Conclusion

• RL key to

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- LLM Alignment
- LLM Reasoning
- Current Frontier:
  - Multi-agent RL for agentic orchestration

Tools Agents Memory (10)رحى Feedback Short-term Long-term Chat Objective Memory Retrieval 实 – Planning Machine Rethink Action LLM Observation C,O  $\mathbf{\nabla}$ Environment APIs Reward Impact Crawler Simulation Real-Word Computer Game Code



