Inverse Reinforcement Learning Meets LLM Alignment

AAAI 2025 Tutorial

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sites.google.com/view/irl-llm

Content

- Part 0: Motivations
- Part 1: Reinforcement Learning: Forward and Inverse
- Part 2: Learning Reward Models from Data
- Part 3: Infra for IRL-LLM Research
- Part 4: Lessons from Sparse Reward RL

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Content

- Part 0: Motivations
  - 0.1 How to extend the success of DeepSeek-R1
- Part 1: Reinforcement Learning: Forward and Inverse
- Part 2: Learning Reward Models from Data
- Part 3: Infra for IRL-LLM Research
- Part 4: Lessons from Sparse Reward RL

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- Part 0: Motivations
- Part 1: Reinforcement Learning: Forward and Inverse
  - 1.1 RL, MDP; Inverse RL, MDP\R
  - 1.2 LLM alignment as Inverse RL
  - 1.3 Why do we (always) need RMs?
- Part 2: Learning Reward Models from Data
- Part 3: Infra for IRL-LLM Research
- Part 4: Lessons from Sparse Reward RL

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- Part 1: Reinforcement Learning: Forward and Inverse
- Part 2: Learning Reward Models from Data
  - 2.1 Reward Modeling in the Wild
  - 2.2 Challenges and Opportunities
- Part 3: Infra for IRL-LLM Research
- Part 4: Lessons from Sparse Reward RL

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Content

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- Part 1: Reinforcement Learning: Forward and Inverse
- Part 2: Learning Reward Models from Data
- Part 3: Infra for IRL-LLM Research
  - 3.1 Design Principles: Reproducible, Controllable, Scalable
  - 3.2 Efficiency v.s. Performance
  - 3.3 Demonstrative Use Cases
- Part 4: Lessons from Sparse Reward RL

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- Part 4: Lessons from Sparse Reward RL
  - 4.1 Hindsight Knowledge
  - 4.2 Reward Shaping, Credit Assignment
  - 4.3 Tradeoffs between Dense Reward (PRM) and Sparse Reward (ORM)
  - 4.4 Power from Self-Play

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Part 0:

Motivations

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Success of Data-Driven Large Models

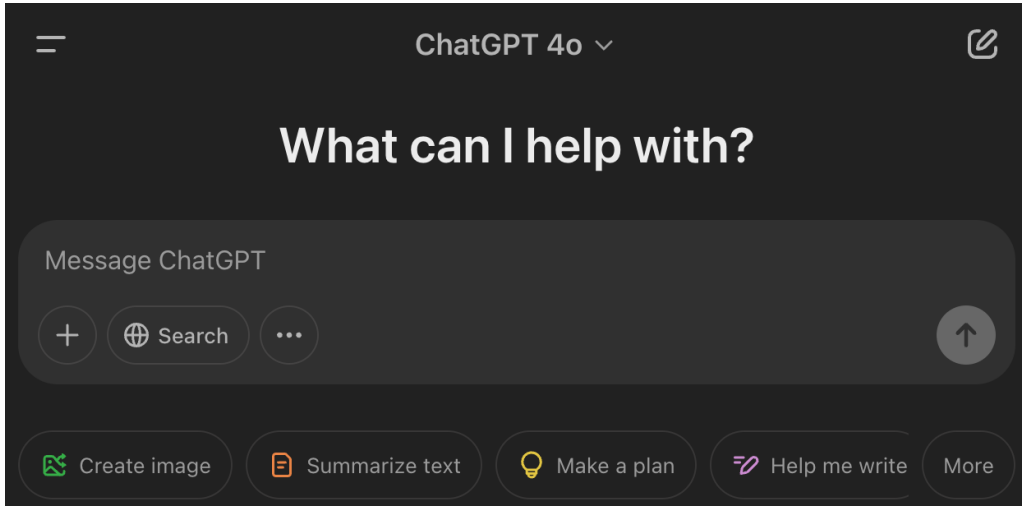
- *Realistic* contents generated by data-driven large models

[Zhang et al., 2025]

Success of Data-Driven Large Models

- Video
- Large Language Models

Video source: openai.com/sora/



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Success of Large-Scale RL

- Alpha-Go/Zero/Star/Tensor/Chip/Dev
- OpenAI-Five

Reward ⬆️⬆️

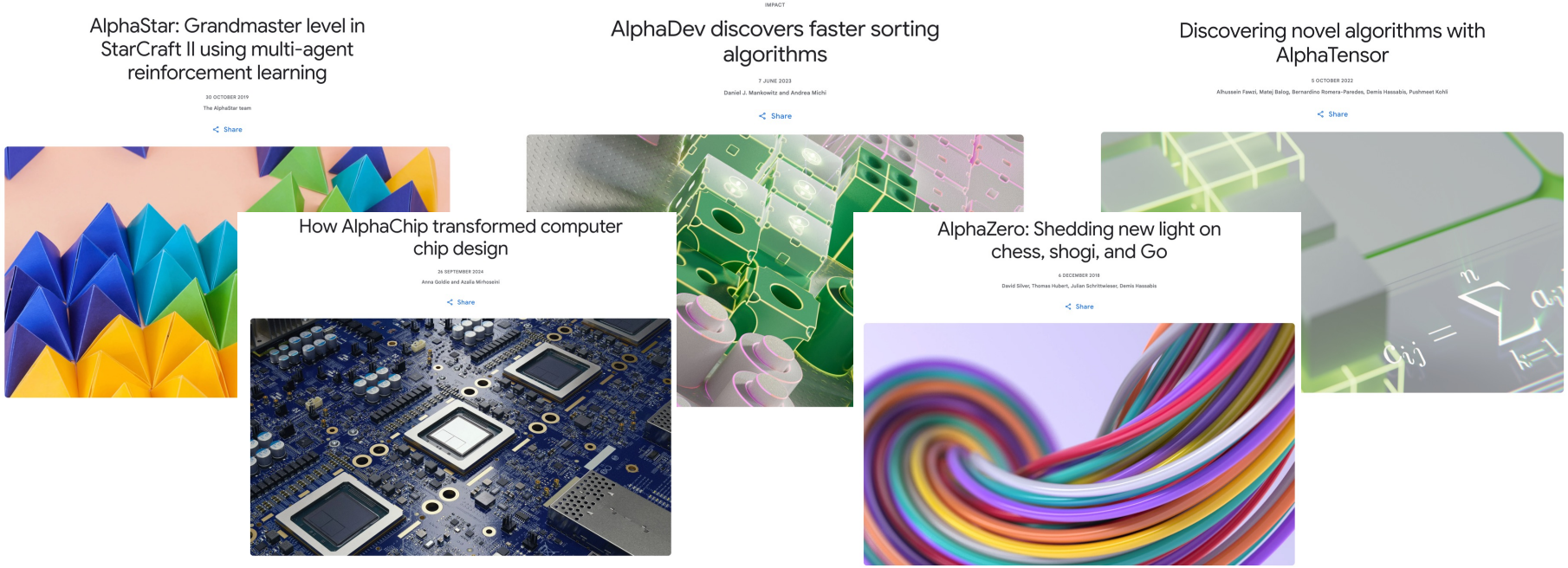

Image source: deepmind.google/discover

openai.com/index/openai-five/

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Success from Both Sides

Language (generative) Models

- Understanding and generating
- Fast adaptation to new tasks

RL

- Explore new knowledge
- Super-human (expert) performance
- Keep improving

[1] Talk: David Silver - Towards Superhuman Intelligence - RLC 2024

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Success from Both Sides

Language (generative) Models

- Understanding and generating
- Fast adaptation to new tasks

Impressive because those contents look like human might generate --- [2](rephrased)

RL

- Explore new knowledge
- Super-human (expert) performance
- Keep improving

Impressive because no person had thought of it --- [2]

[1] Talk: David Silver - Towards Superhuman Intelligence - RLC 2024
[2] Talk: Sergey Levine - Reinforcement Learning in the Age of Foundation Models - RLC 2024

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Combining the Success?

Language Models	*RL*

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Combining the Success?

Language Models | ***RL***

- RL agents can be the best Go/StarCraft/Dota2 player
- But learning from RL agents is non-trivial

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Combining the Success?

Language Models | ***RL***

- RL agents can be the best Go/StarCraft/Dota2 player
- But learning from RL agents is non-trivial

- LLM + RL:
  More interpretable, assist, empower and inspire human

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Combining the Success?

Language Models *RL*

- Use RL to improve performance of LLMs
- *LLM Alignment: to ensure its outputs are aligned with human intent, ethical principles, and task-specific requirements.*

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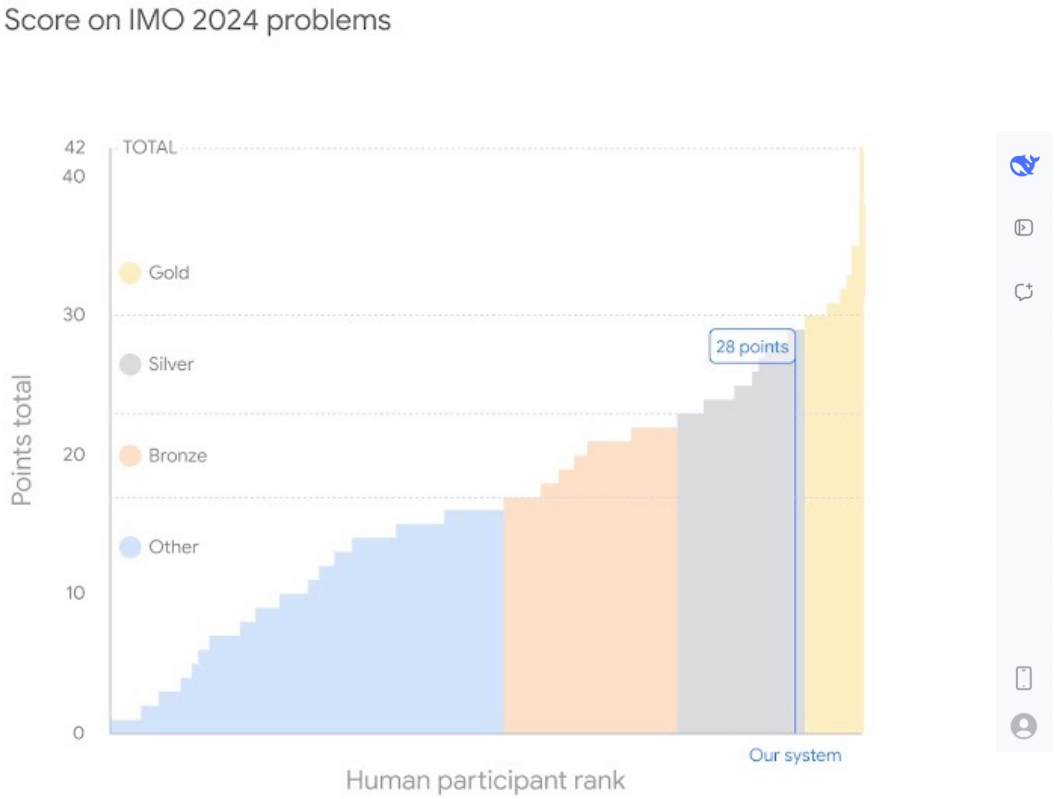
Success on Math

- AlphaProof & AlphaGeometry 2 LLM – o1/ DeepSeek-R1



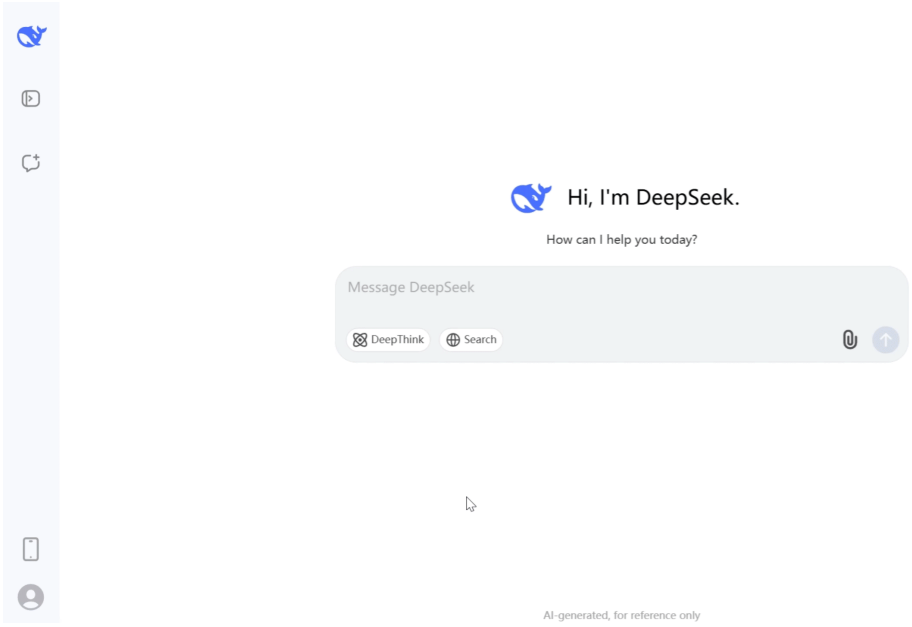


Image source: deepmind.google/discover/blog/ai-solves-imo-problems-at-silver-medal-level/

Extending Such Success?

- Opportunities
  - Improvement of LLM abilities directly helps human
  - Inspirations from the RL world
- Challenges
  - Reward signals
  - Sufficient compute for simulation and optimization
  - Scalable & efficient algorithms: no silver bullet in RL
- Next Section:
  - RL, IRL, and RL in LLMs
  - LLM Alignment as Inverse RL --- RL w/ Data Driven Reward Function

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Part 1:

Reinforcement Learning: Forward and Inverse

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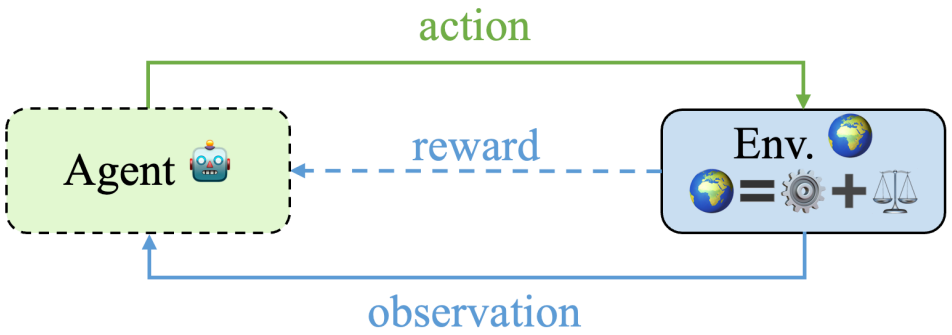
RL: Learning through Interactions

- Learning a policy to maximize the long-term return by interacting with the environment.



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RL: Learning through Interactions

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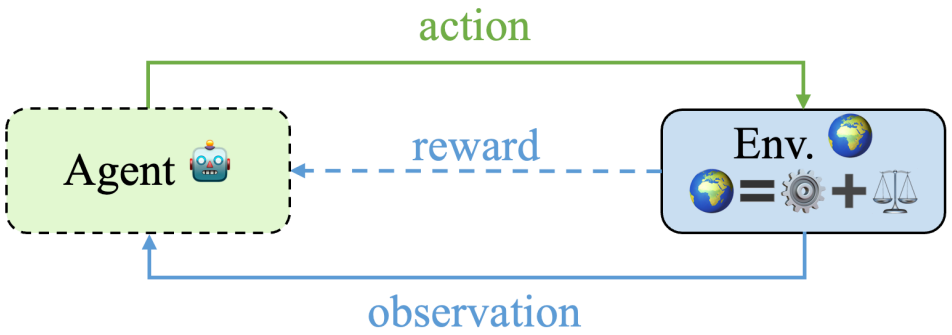

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RL: Learning through Interactions

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$$\mathcal{J}(\pi(a|s))$$

RL: Learning through Interactions

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$\mathcal{J}(\pi(a|s))$ $\sum_t \gamma^t r(s_t, a_t)$

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RL: Learning through Interactions

- Learning a policy to maximize the long-term return by interacting with the environment.
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RL: Learning through Interactions

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- Markov Decision Process: $\mathcal{M} = (S, A, P, \rho_0, R, \gamma)$
- $\max_{\pi} \mathcal{J}(\pi(a|s)) = \max_{\pi} \mathbb{E}_{\rho_0, P, \pi}[\sum_t \gamma^t r(s_t, a_t)]$

RL: Learning through Interactions

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Formal Objective of RL

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RL: Learning through Interactions

- How to optimize?

$$\max_{\pi} \mathcal{J}(\pi(a|s)) = \max_{\pi} \mathbb{E}_{\rho_0, P, \pi}[\sum_t \gamma^t r(s_t, a_t)]$$

- The core idea is “simple”:

discover and repeat successful trajectories/actions

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RL: Learning through Interactions

- How to optimize?

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- The core idea is "simple":

discover and repeat successful trajectories/actions

explore *exploit*

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RL: Learning through Interactions

- *Some* RL algorithms can be better than others in *some* tasks
- There is ***no silver bullet in RL***

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RL: Learning through Interactions

- *Some* RL algorithms can be better than others in *some* tasks
- There is ***no silver bullet in RL***
- e.g.,

Atari:	DQN
AlphaZero:	MCTS, Self-Play
OpenAI Five:	PPO, Self-Play
Robotics:	SAC, DPG
Multi-Goal:	Hindsight Methods
DeepSeek-r1:	GRPO
RLHF:	PPO, DPO, REINFORCE

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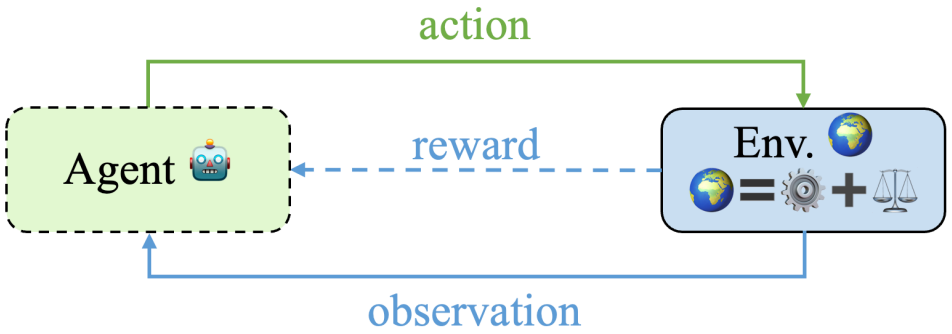
LLM Generation as an MDP?

- Markov Decision Process: $\mathcal{M} = (S, A, P, \rho_0, R, \gamma)$



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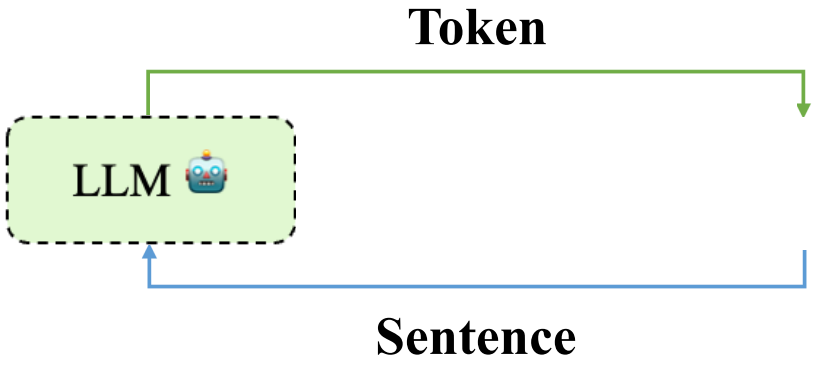
LLM Generation as an MDP?

- Markov Decision Process: $\mathcal{M} = (S, A, P, \rho_0, R, \gamma)$
- S: Current sentence
- A: Tokens (or their combinations)



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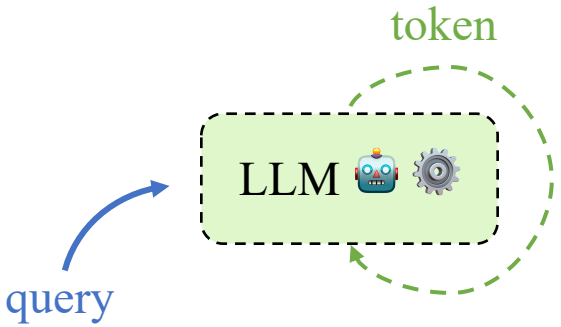

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LLM Generation as an MDP\R

- Markov Decision Process: $\mathcal{M} = (S, A, P, \rho_0, R, \gamma)$
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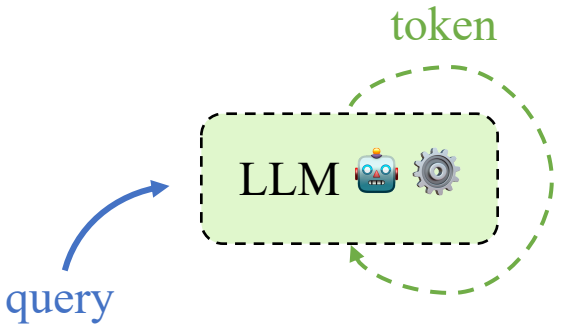
- ρ_0: Prompt/Query distribution
- ? R: *(Data-Driven)*



LLM Generation as an MDP\R

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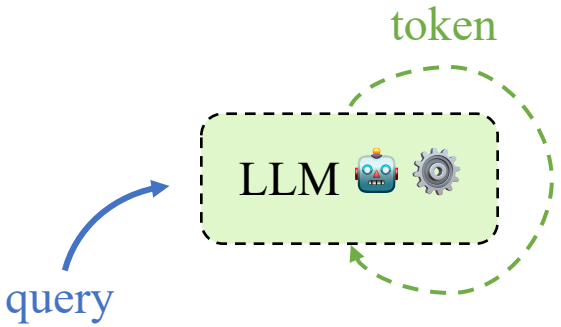
- S: Current sentence
- A: Tokens (or their combinations)
- P: Concatenation of tokens
- ρ_0: Prompt/Query distribution
- ? R: *(Data-Driven)*
- γ: ≤ 1 (e.g., =1: correct is enough / <1: correct in short answer)



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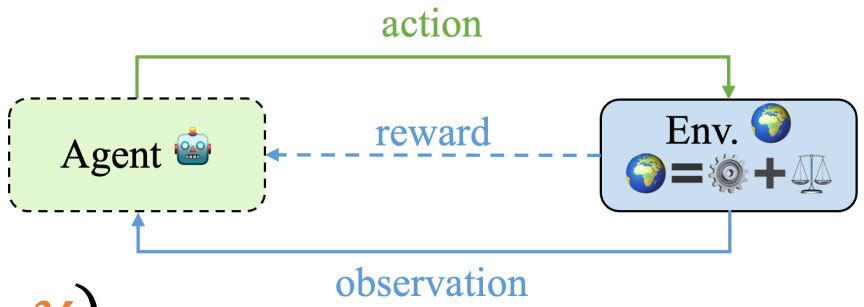
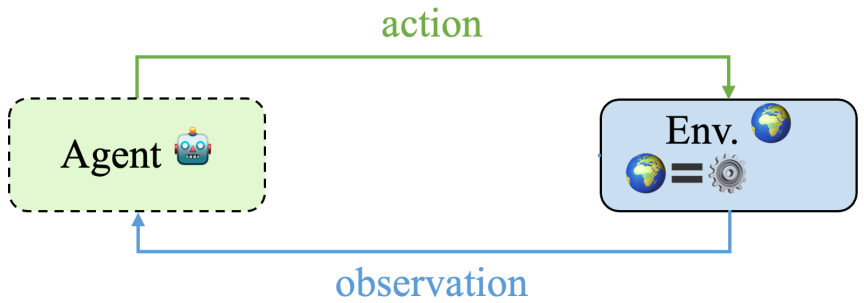
What is MDP\R

- In MDPs ($S, A, P, \rho_0, R, \gamma$), we maximize cumulative return



- In MDP\Rs (S, A, P, ρ_0, γ), how (what) to learn?



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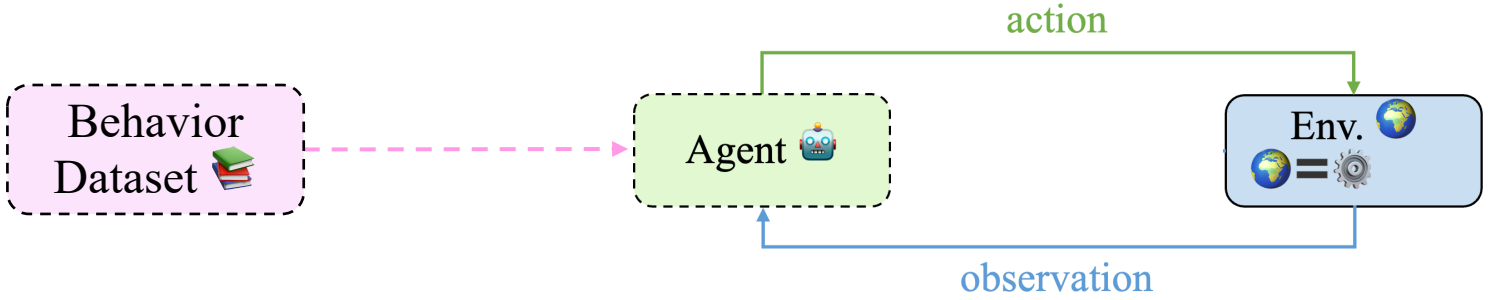
Learning from Behavior Datasets

- MDP\R (S, A, P, ρ_0, γ), how (what) to learn?



- Learning from a *behavior dataset*

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Examples

- Learning from a *behavior dataset*
  - 1. Reward function is hard to define

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Examples

- Learning from a *behavior dataset*
  - 1. Reward function is hard to define
    - ALVINN [Pomerleau, 1988]

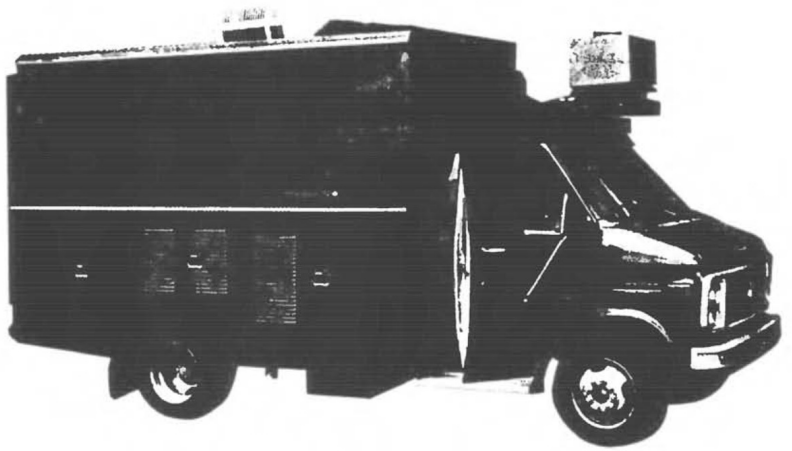

Figure 3: NAVLAB, the CMU autonomous navigation test vehicle.

Examples

- Learning from a *behavior dataset*
  - 1. Reward function is hard to define
    - ALVINN [Pomerleau, 1988]
    - Imitating behaviors [Hayes & Demiris, 1994]

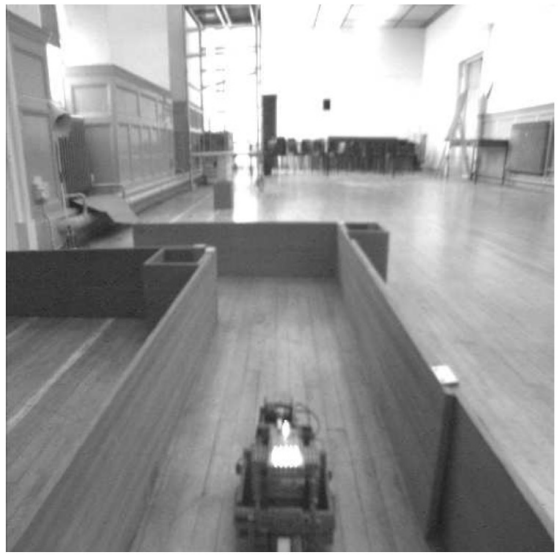

Fig. 3.: View of the teacher and part of the maze as seen by Ben Hope.

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Examples

- Learning from a *behavior dataset*
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    - ALVINN [Pomerleau, 1988]
    - Imitating behaviors [Hayes & Demiris, 1994]
    - Complex skills [Peng et al., 2016]

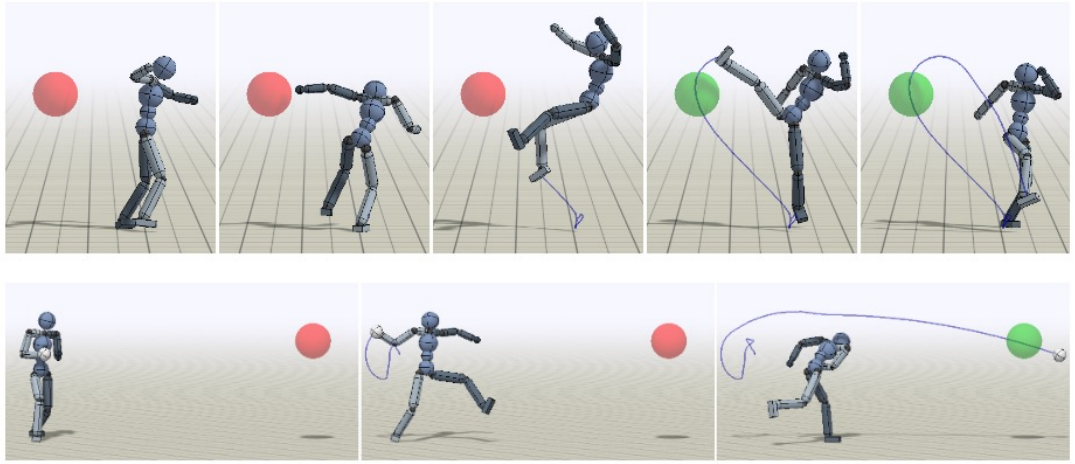

Fig. 7. **Top:** Spinkick policy trained to strike a target with the character's right foot. **Bottom:** Baseball pitch policy trained to throw a ball to a target.

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Examples

- Learning from a *behavior dataset*
  - 1. Reward function is hard to define
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    - RLHF: metrics are hard to quantify otherwise [Stiennon et al., 2020] [Bai et al., 2022]

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Examples

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  - 2. Reward signal is too sparse (e.g., win a game of Go/StarCraft/Dota2)
    - AlphaGo/AlphaStar/OpenAI Five

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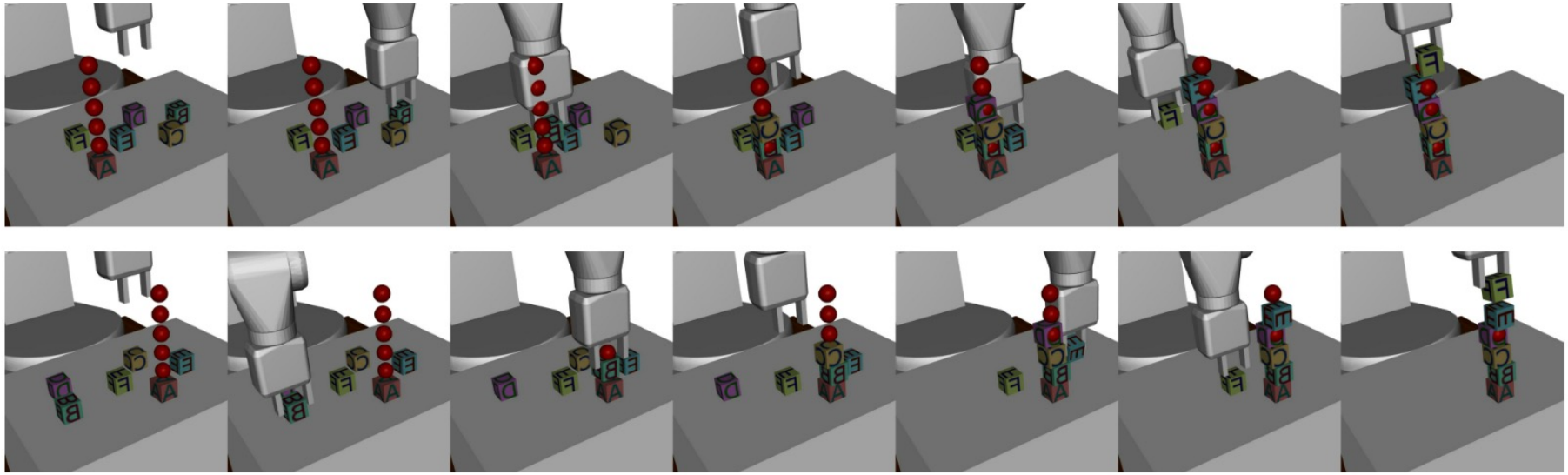
Examples



- 2. Reward signal is too sparse (e.g., win a game of Go/StarCraft/Dota2)
  - AlphaGo/AlphaStar/OpenAI Five
  - Robotics Control [Nair et al., 2017]

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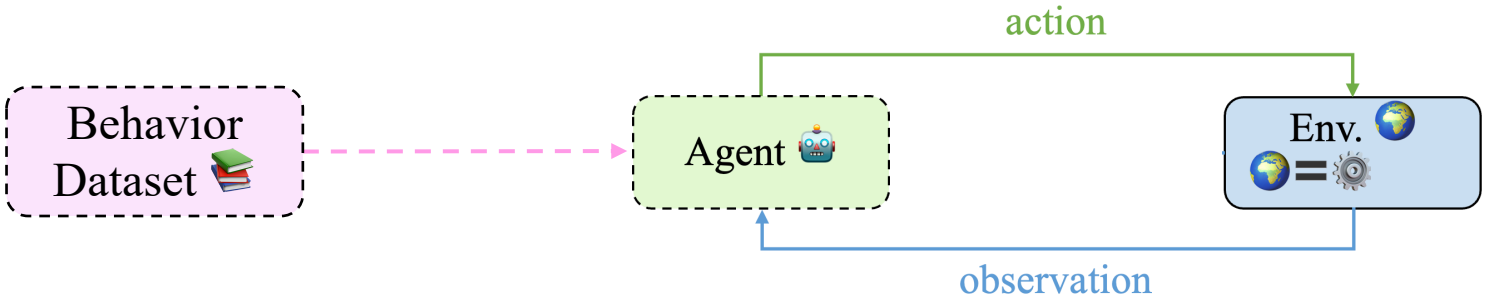
Methods for Learning from Behavior

- Learning from a *behavior dataset*
  - Imitation Learning: recover π^* given behavior generated by π^*



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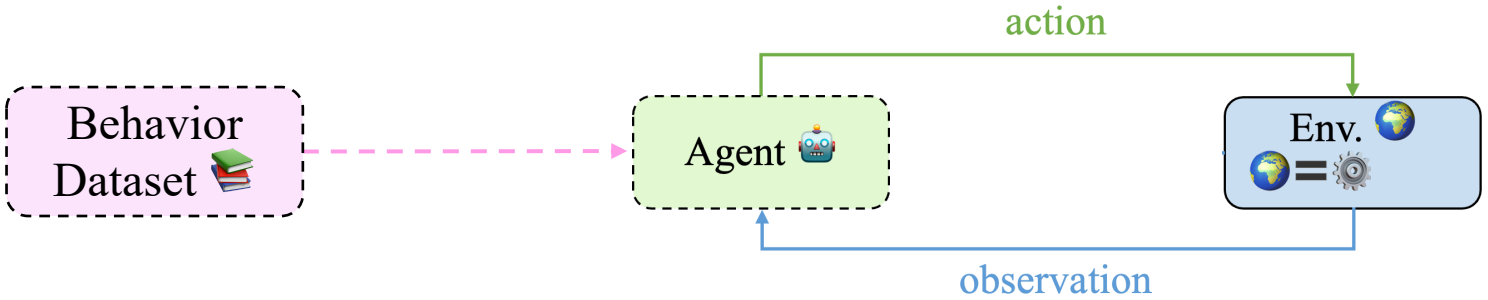
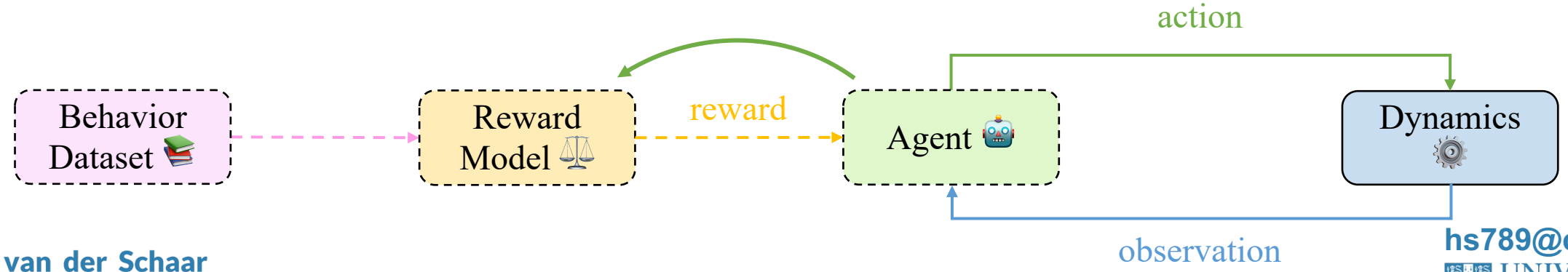


  - Inverse RL: recover R that induces π^* given behavior generated by π^*



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Imitation Learning

- Imitation Learning: recover π^* given behavior generated by π^*

  - IL 1. Behavior Clone
    [Hayes & Demiris, 1994] [Pomerleau, 1988]

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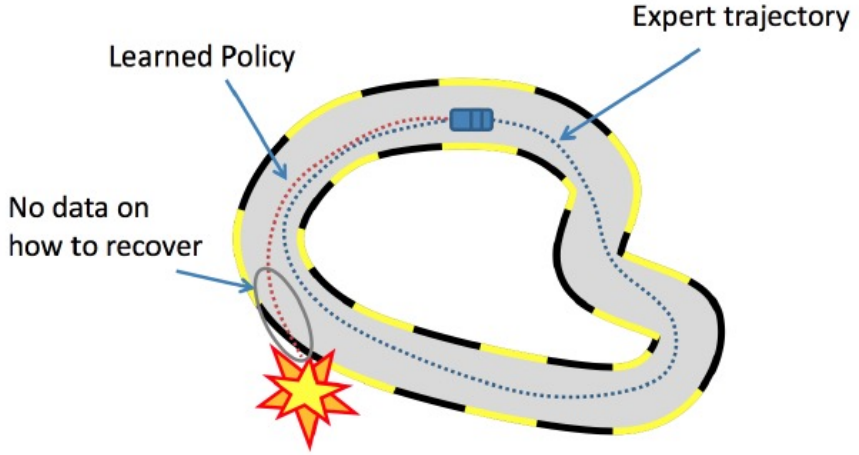
Imitation Learning

- Imitation Learning: recover π^* given behavior generated by π^*

  - IL 1. Behavior Clone "*Compounding Error*" [Hayes & Demiris, 1994] [Pomerleau, 1988]



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Imitation Learning

- Imitation Learning: recover π^* given behavior generated by π^*

- IL 1. Behavior Clone
  [Hayes & Demiris, 1994; Pomerleau, 1988]
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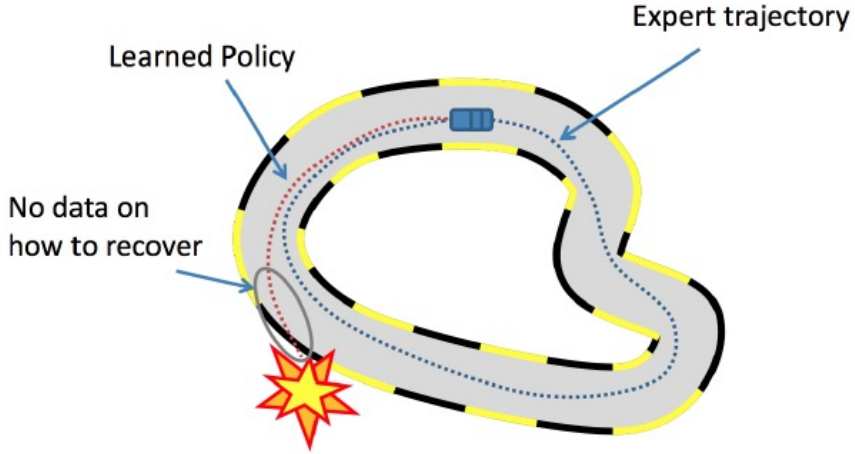

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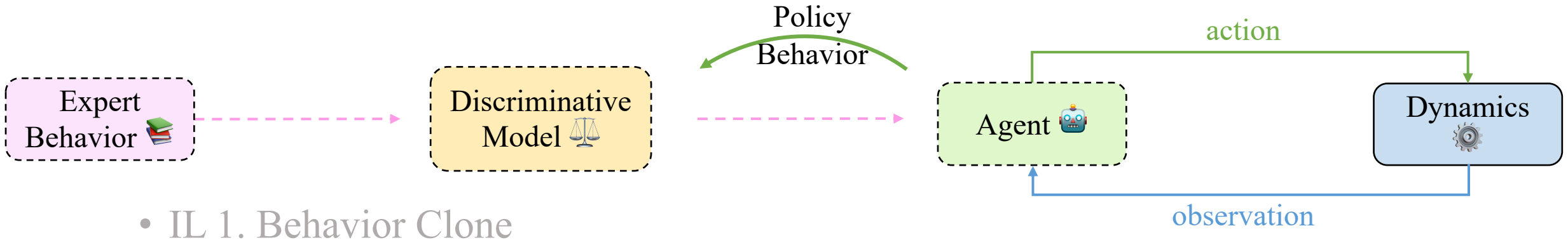

  - IL 1. Behavior Clone
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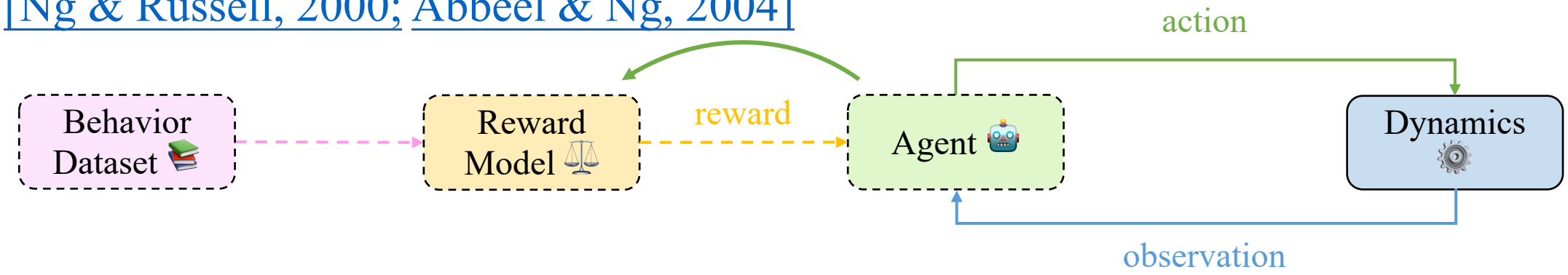
  - IL 2. Expert Engagement
    [Ross et al. 2011; Li et al., 2022; Peng et al. 2023]
  - IL 3. Adversarial Imitation
    [Ho & Ermon, 2016]

Inverse Reinforcement Learning

- Inverse RL: recover R that induces π^* given behavior generated by π^*
  [Ng & Russell, 2000; Abbeel & Ng, 2004]



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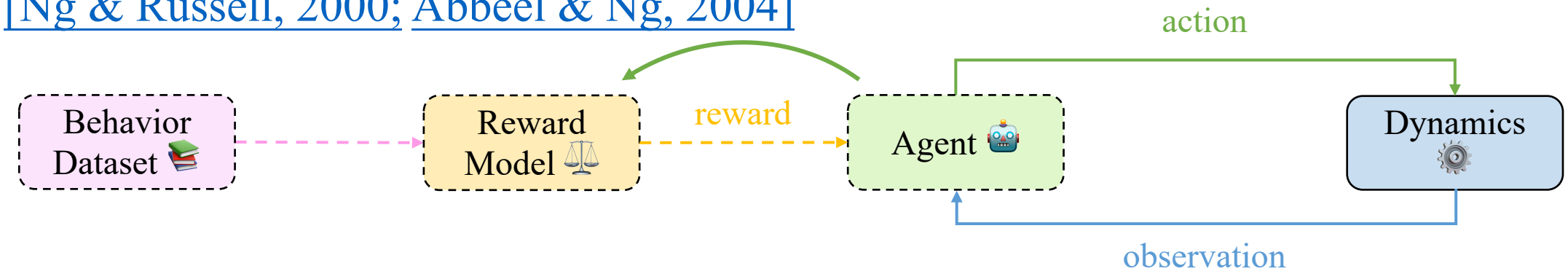

  - Max-Ent IRL [Ziebart et al., 2008]
  - Adversarial IRL [Fu et al., 2017]
  - T-REX [Brown et al., 2019]

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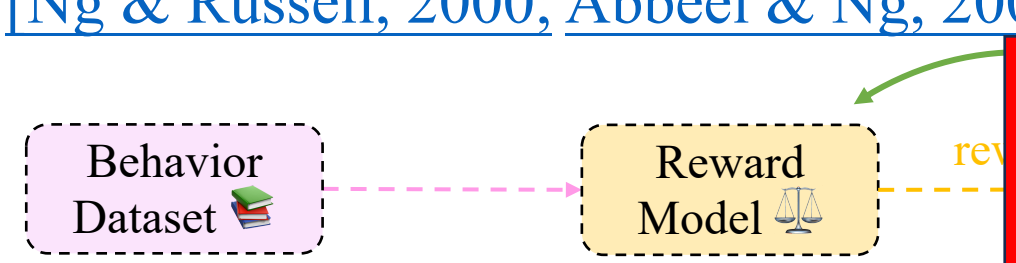

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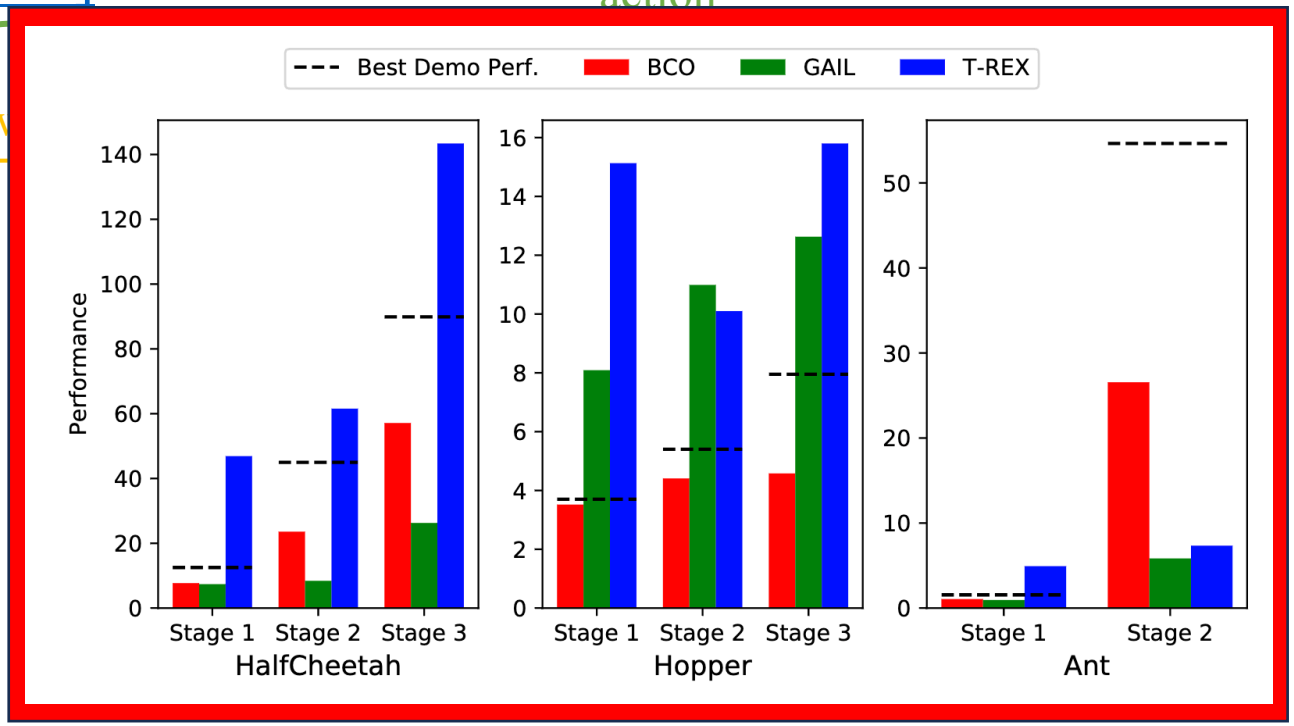
Can outperform demonstration



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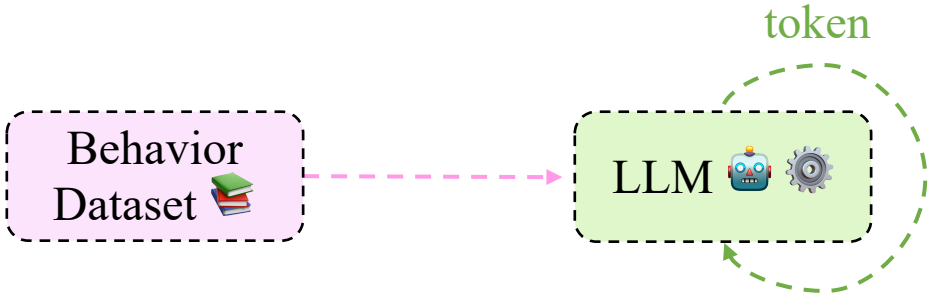
LLM Optimization via Imitation

- LLMs as language imitators



- Pre-train: large scale behavior clone
  [Obtain (strong) ability of understanding]

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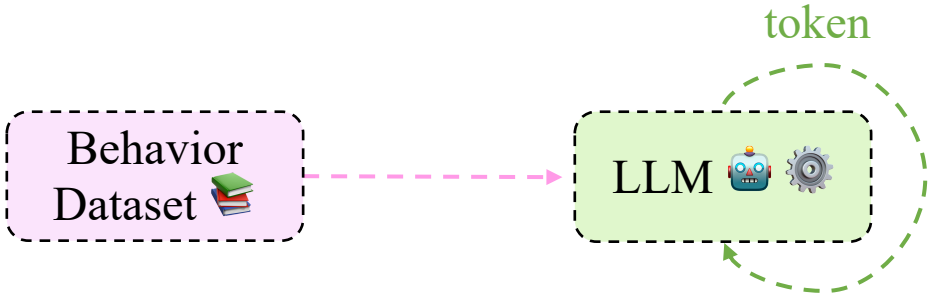

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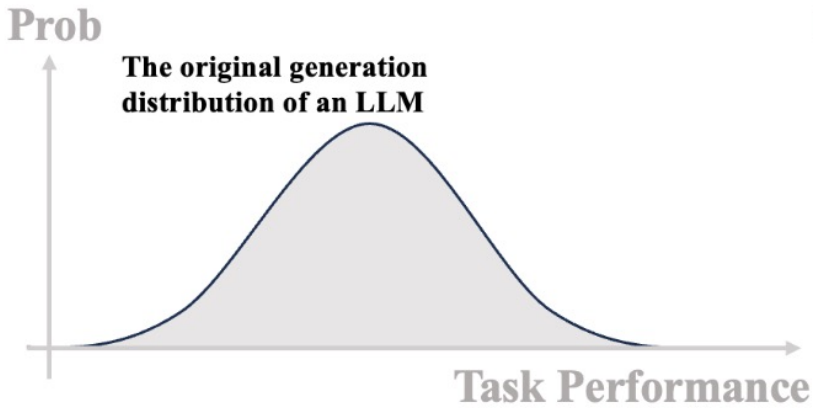

(1) LLM *Can* do Any Task as a *Universal Sampler*

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LLM Optimization via Imitation

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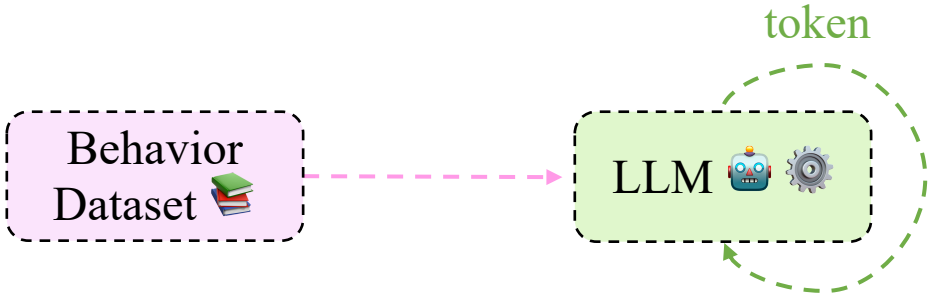

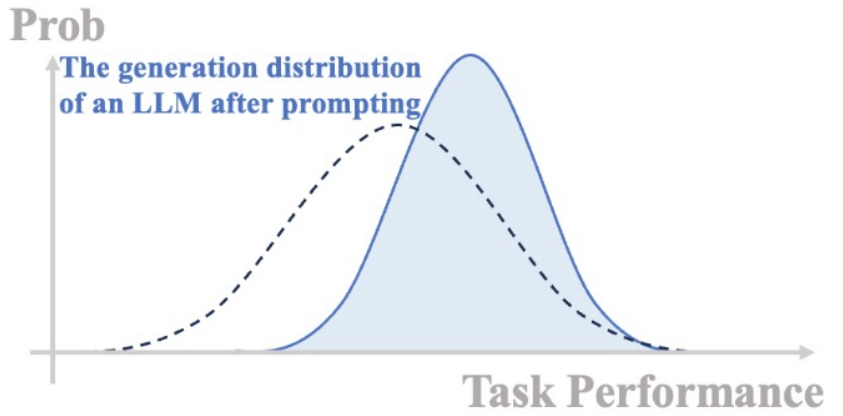

(2) Prompting *Can* Improve Performance by shifting the generation

- Pre-train: large scale behavior clone
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- Post-train/alignment: optimization on a specific task
  - Smart prompting strategy [Kojima et al., 2022]

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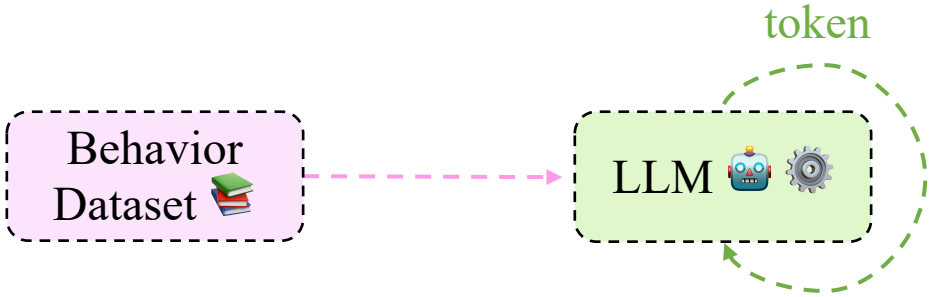

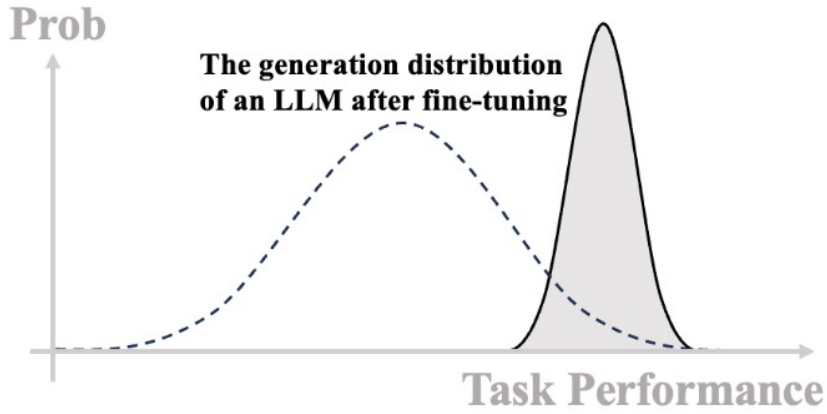

(3) Fine-Tuning *Can* Improve Performance by shifting the generation

- Pre-train: large scale behavior clone
  [Obtain (strong) ability of understanding]
- Post-train/alignment: optimization on a specific task
  - Smart prompting strategy [Kojima et al., 2022]
  - Supervised fine-tuning

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Why Do We Need Inverse RL?

- Preference feedback can be more scalable & practical

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Why Do We Need Inverse RL?

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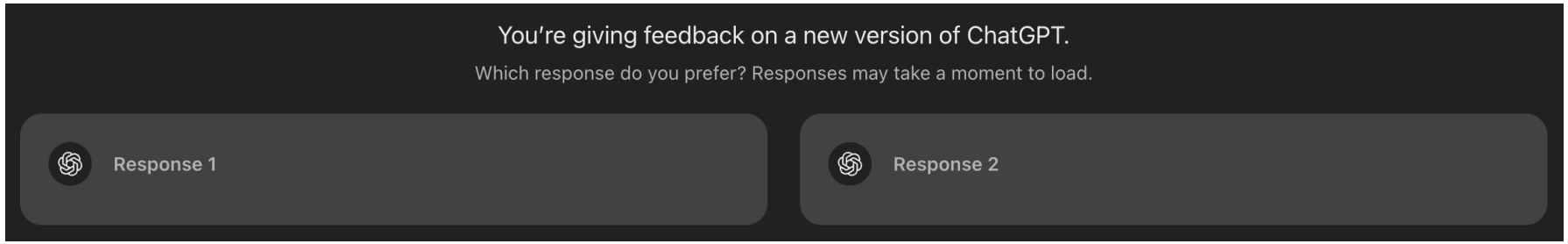
Preference Dataset 📚



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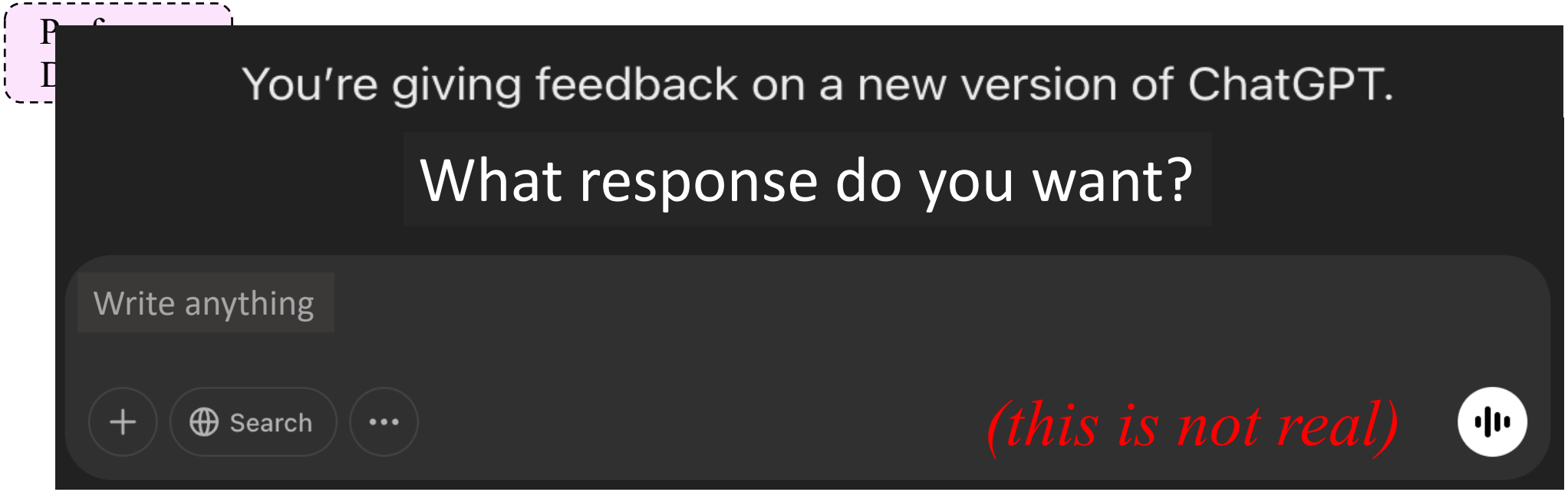

Why Do We Need Inverse RL?

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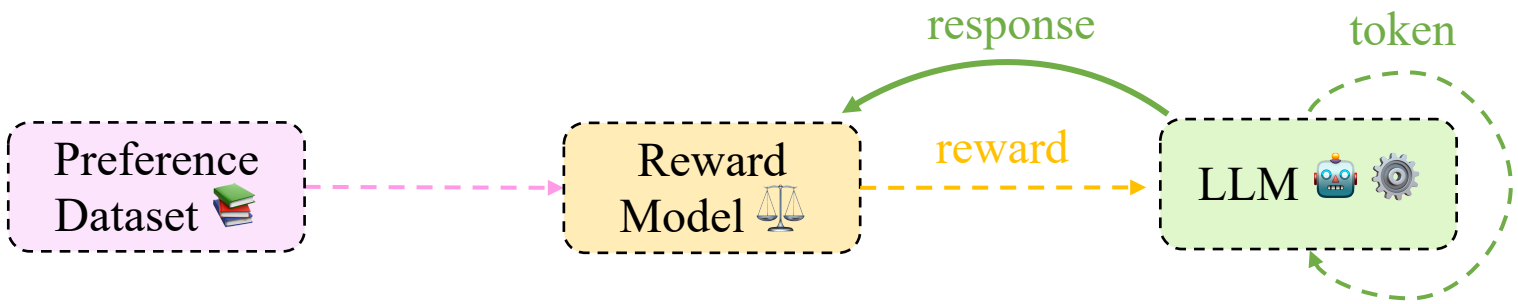

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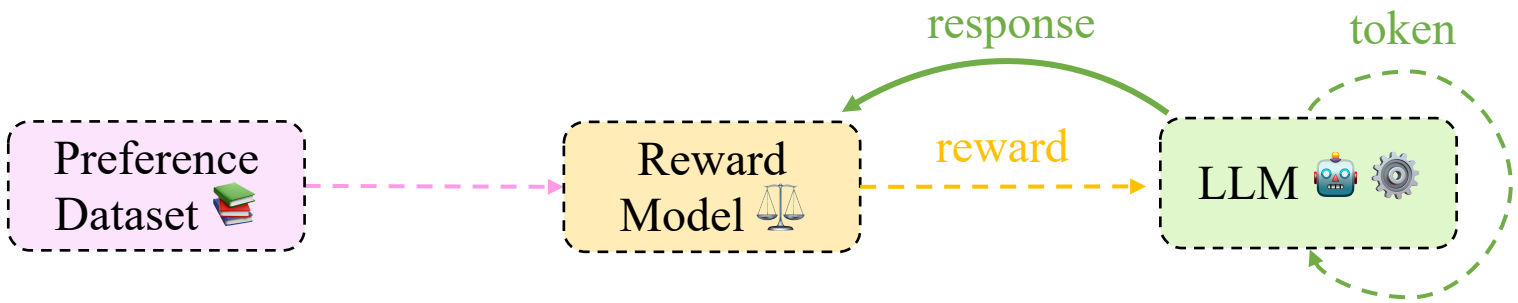
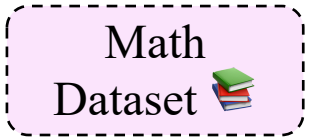


- Math: find a more generalizable reasoning path toward correct answers



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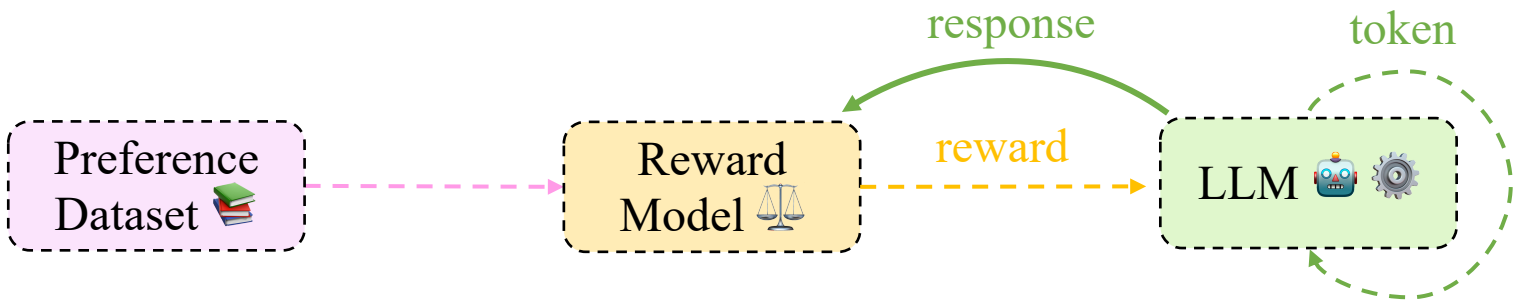

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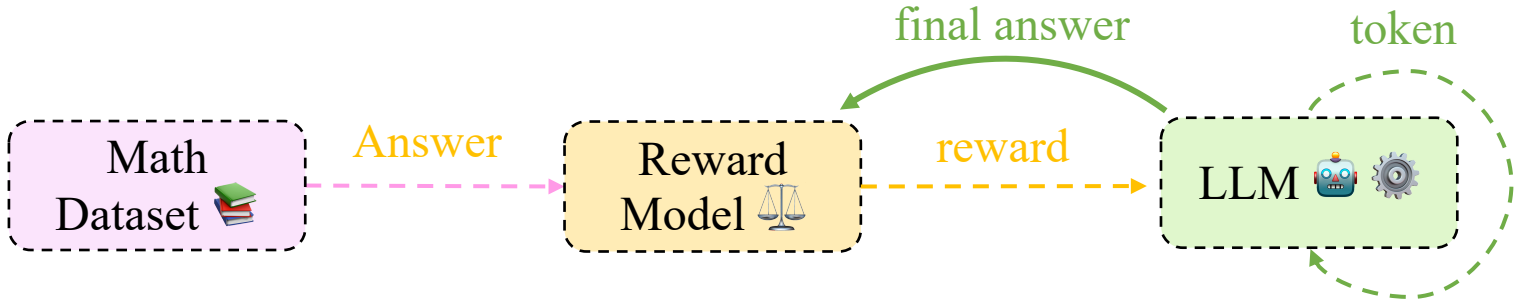

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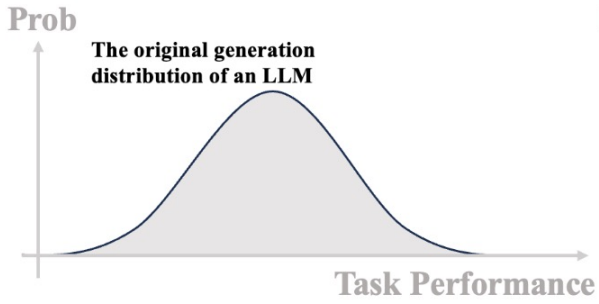
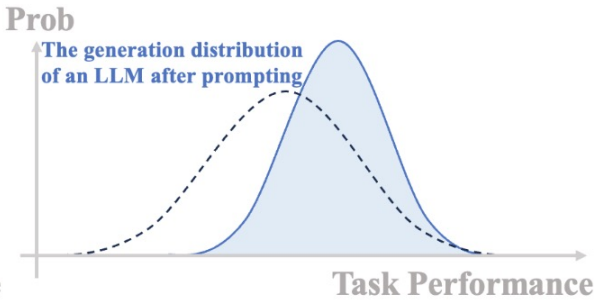
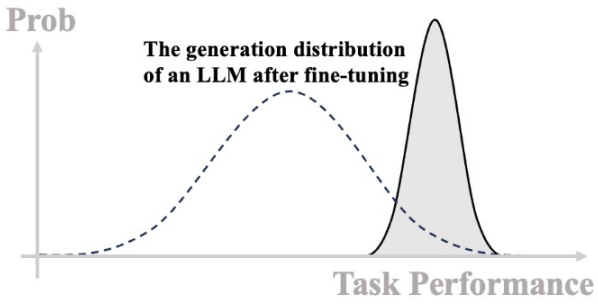
RMs Enable Test-Time Optimization [Sun et al., 2024]



(1) LLM *Can* do Any Task as a *Universal Sampler*



(2) Prompting *Can* Improve Performance by shifting the generation



(3) Fine-Tuning *Can* Improve Performance by shifting the generation

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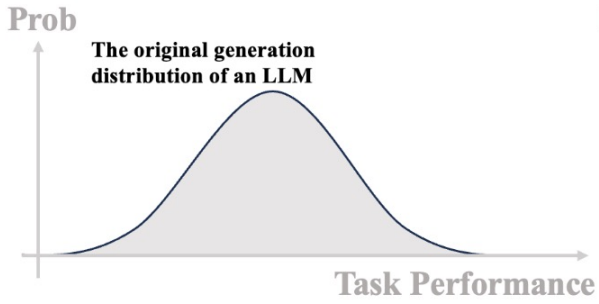

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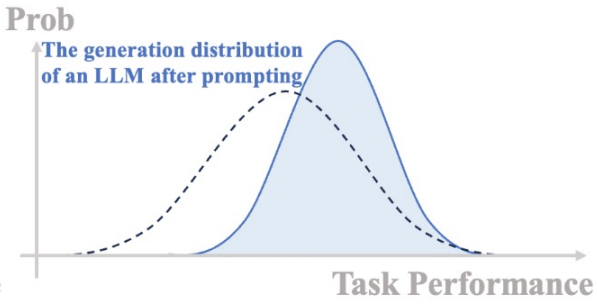

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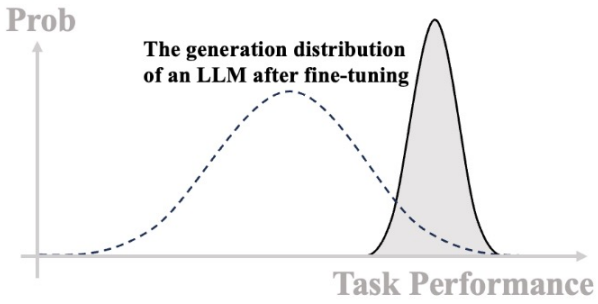

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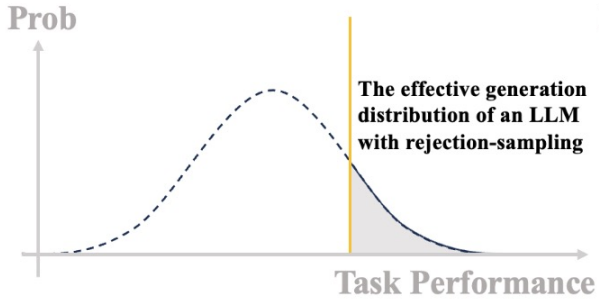

(4) Rejection-Sampling with *Reward Models* *Can* Improve Performance by filtering the generation

Reward Models
Enable Test-time Optimization

van_der_Schaar \ LAB

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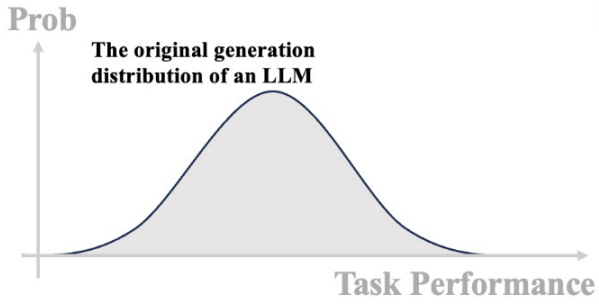

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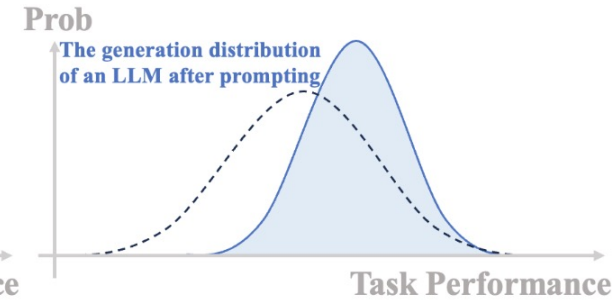

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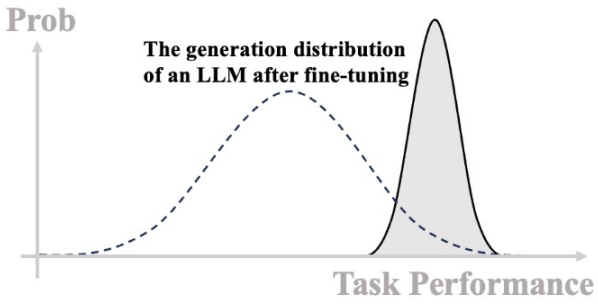

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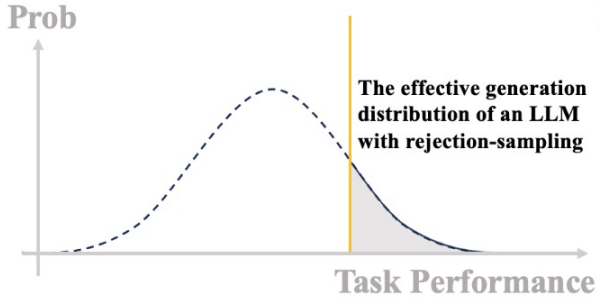
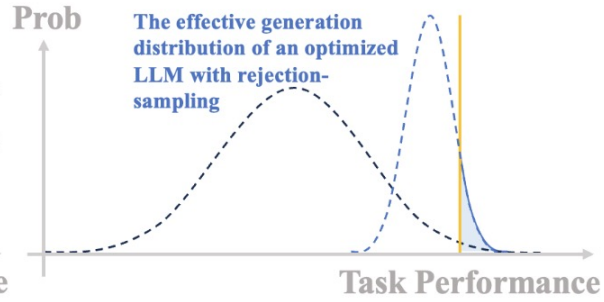
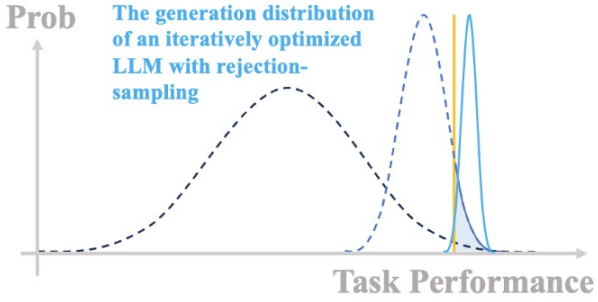


(4) Rejection-Sampling with *Reward Models* *Can* Improve Performance by filtering the generation



(5) On Hard Tasks, Reward Models are Crucial as they enable search and *Inference-Time-Optimization*



(6) Searching with Reward Models can generate datasets that enable *iterative fine-tuning*

Reward Models Enable Test-time Optimization

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Takeaways:

- 1. RL can be formally described as MDP
- 2. There is no silver bullet in RL
- 3. IL and Inverse RL as MDP\R: policy learning from behavior
- 4. LLM pre-train/ SFT are imitation learning
- 5. Reason use Inverse RL:
  - Scalable & Flexible
  - Generalizes better than SFT
  - Enables Test-Time Optimization

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Part 2:

Learning Reward Models from Data

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Learning Reward Models from Data

RMs from different data types

RM from Binary (e.g., Math Reasoning)

RM from Preference (e.g., Classical RLHF)

RM from Demonstration (e.g., Expert Data)

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RM from Binary Data: IRL for *Prompt Optimization*

Prompt-OIRL [Sun et al., 2024]

- Prompt engineering is useful, but empirical…

(User Directly Asks the Question)
a^4 = 1, what is a?

(GPT-4 gives the *correct* answer)
Given the equation $a^4 = 1$, we can find the possible values for a. (…*some intermediate steps*…) So, a could be 1, -1, i, or $-i$.

(User Uses Multi Agent Debate Prompting)
a^4 = 1, what is a? Two experts are debating on the answer:

(GPT-4 gives a *wrong* answer)
If $a^4 = 1$, then there are multiple possible values for a. (…*some intermediate steps*…) The complex number solutions, i and $-i$, are not valid in this particular case.

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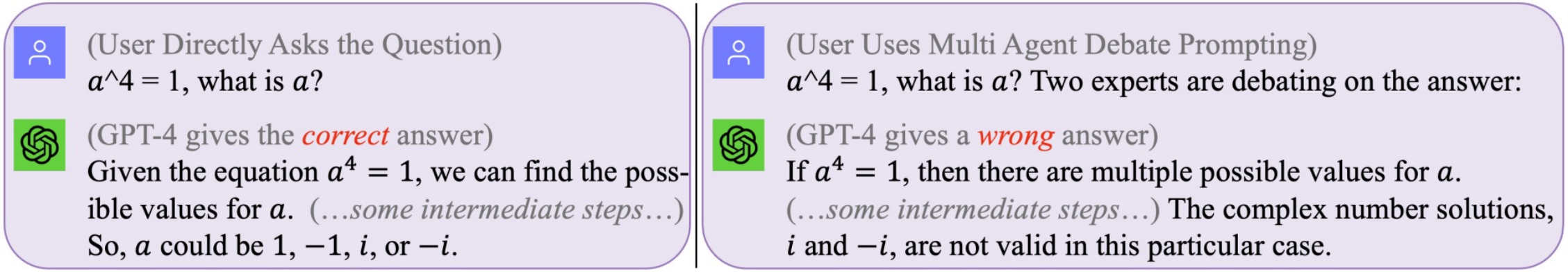

- Automatic prompt engineering using RL?

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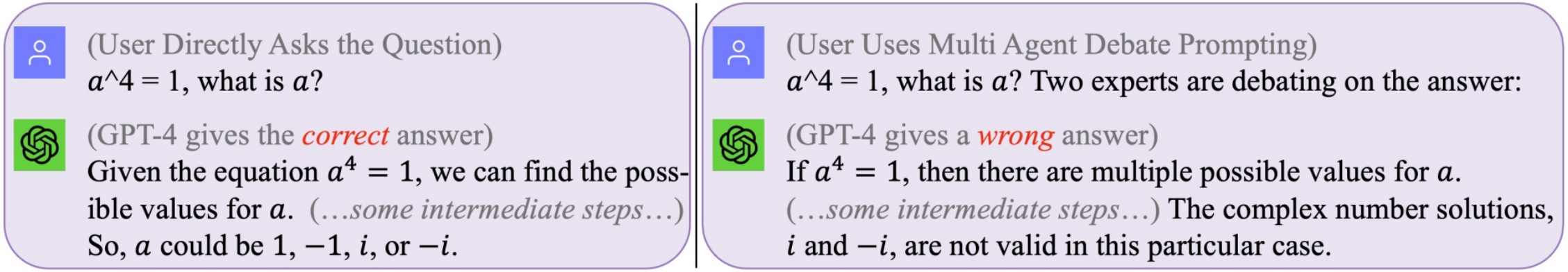

- Automatic prompt engineering using RL?
  - Huge vocabulary space
  - Expensive
  - Prompt-Dependent

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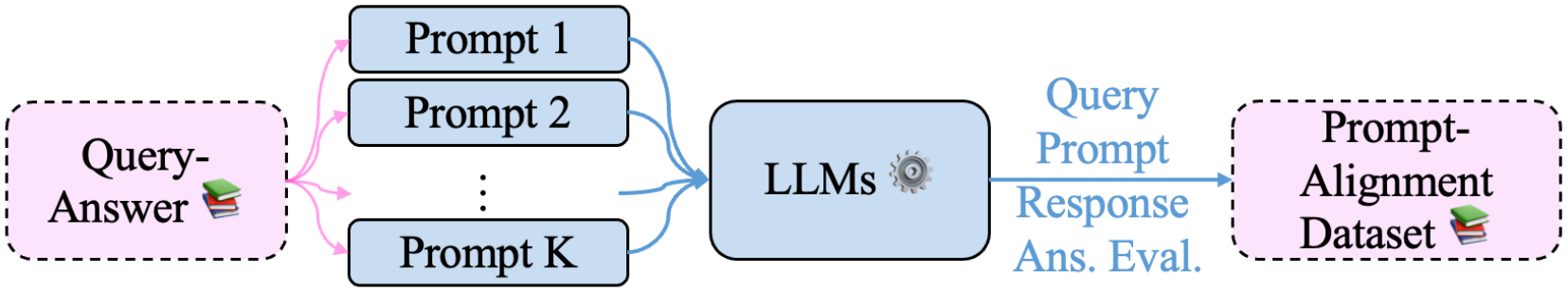
RM from Binary Data: IRL for *Prompt Optimization*

Prompt-OIRL [Sun et al., 2024]

- Learning from demonstrative behaviors can be more efficient!

- Prompt Optimization as Inverse RL: learning from expert prompts



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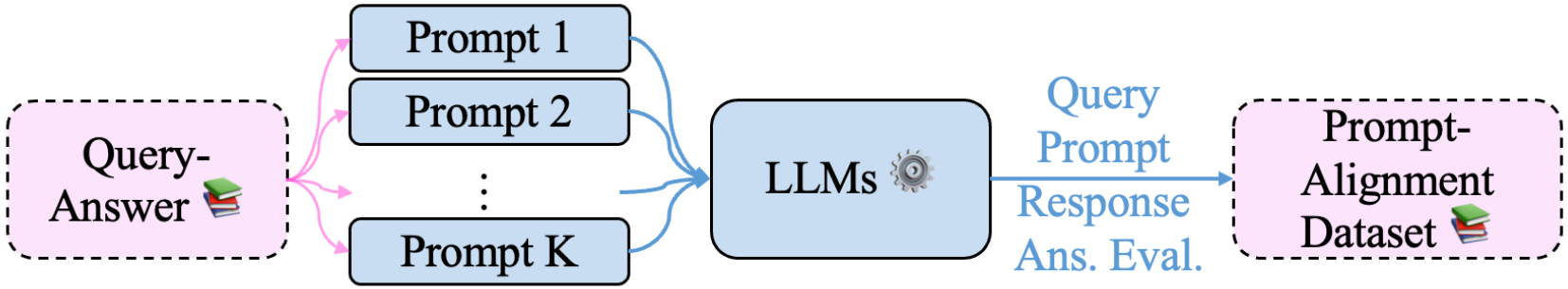
RM from Binary Data: IRL for *Prompt Optimization*

- Prompt-alignment dataset: [Query, Prompt, Response, Correctness]



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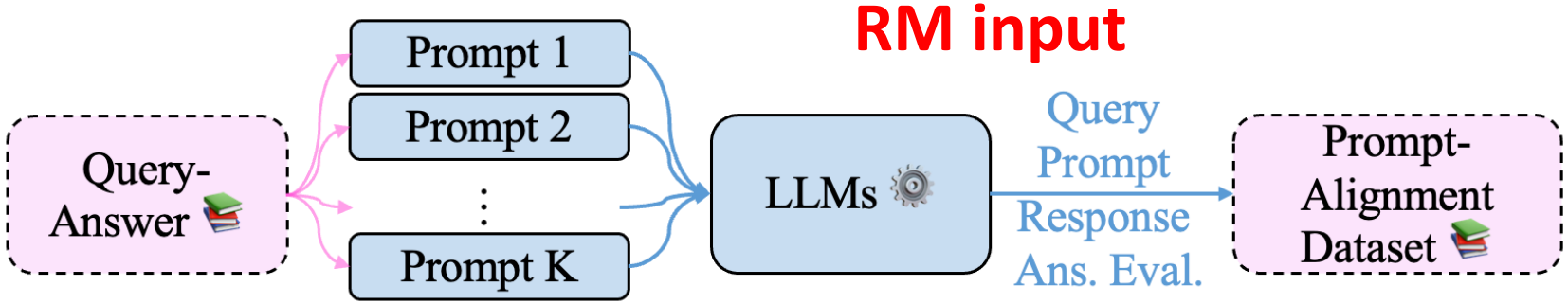
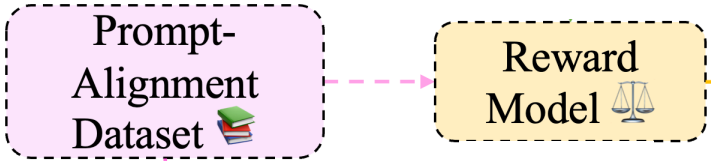
RM from Binary Data: IRL for *Prompt Optimization*

- Prompt-alignment dataset: [**Query, Prompt**, Response, **Correctness**]



- Inverse RL:
  - (training) Reward Model



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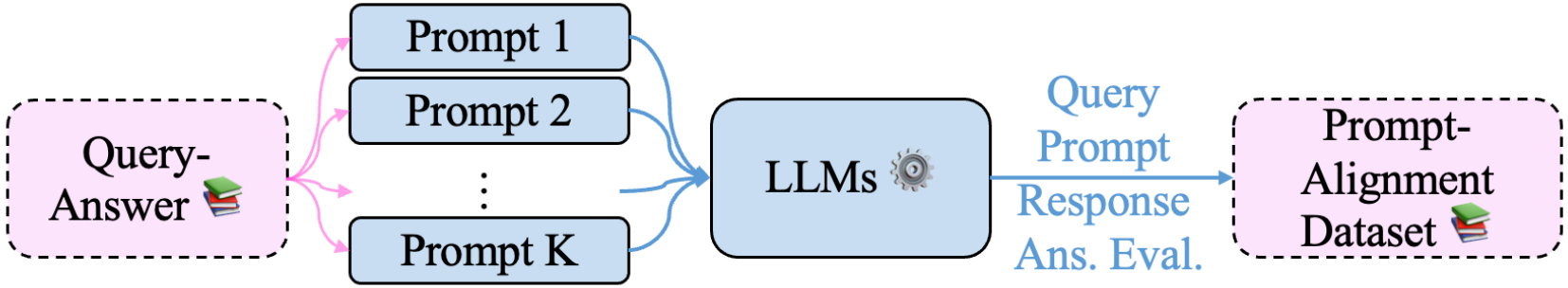
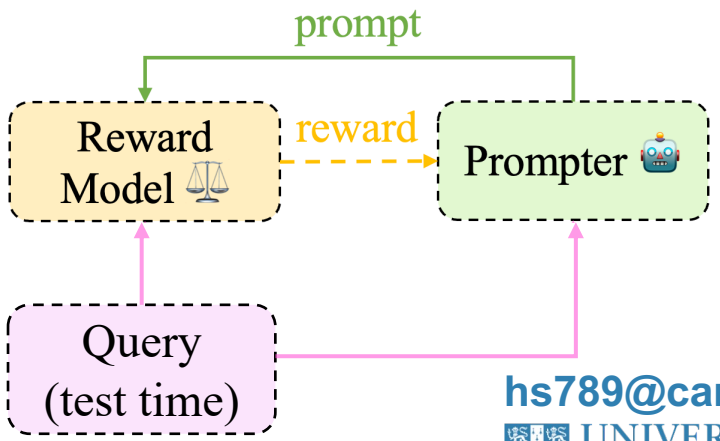


- Inverse RL:
  - (training) Reward Model
  - (test-time) Prompt Optimization
    select the *best* prompt for each query using RM



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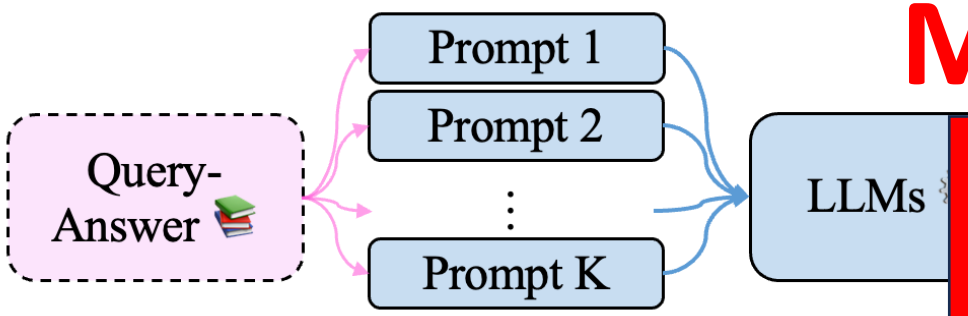
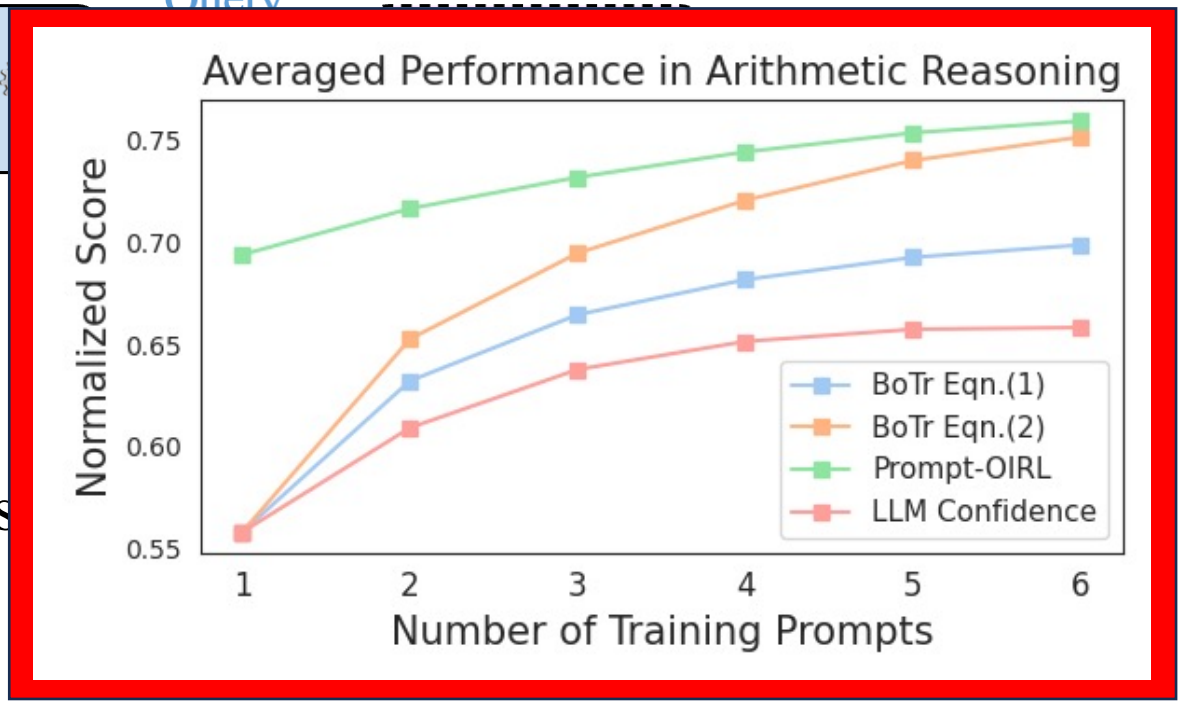


Math Reasoning Ability



- Inverse RL:
  - (training) Reward Model
  - (test-time) Prompt Optimization
    select the *best* prompt for each query us

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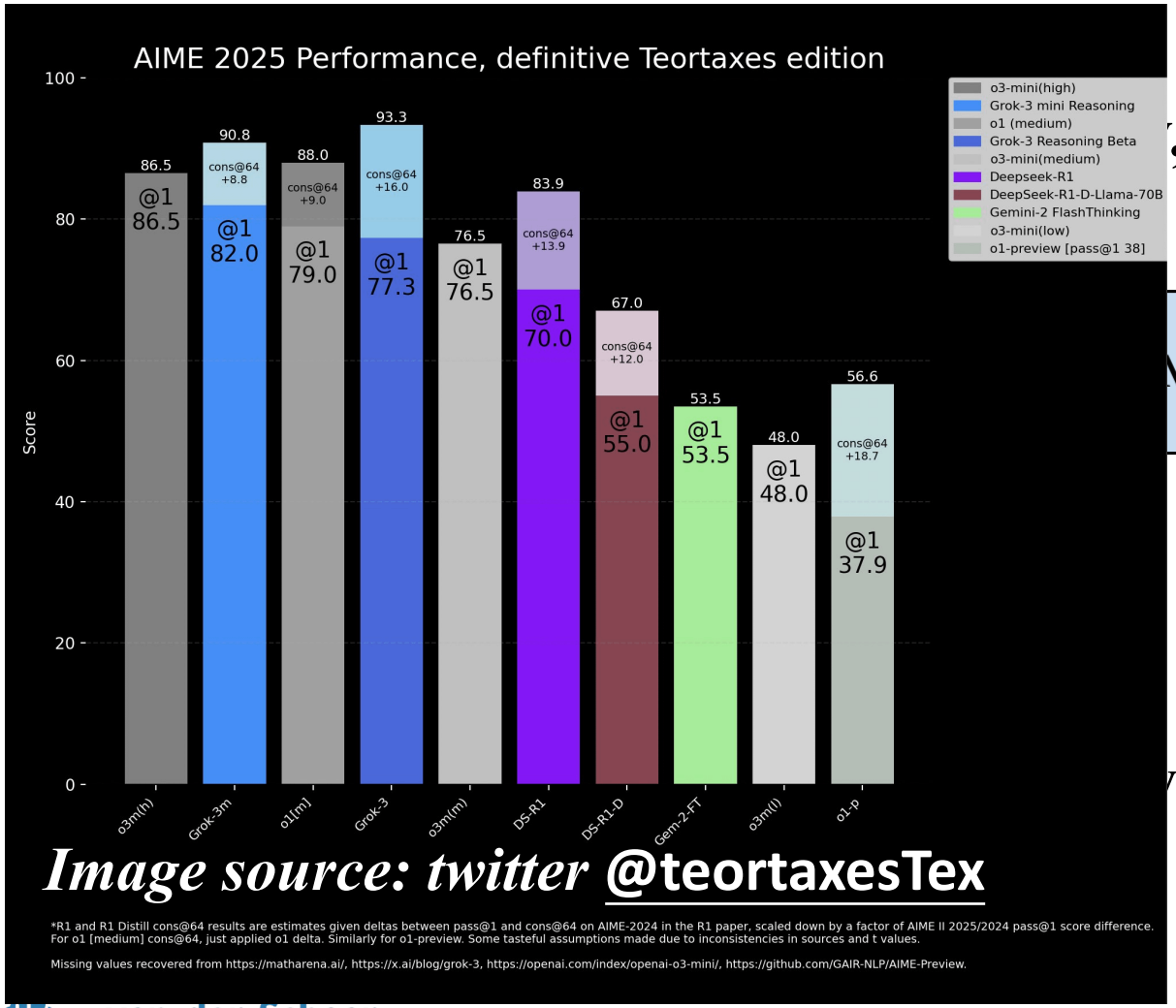
No need for 64 forward passes!

Pick the best using RM and do one single pass ☺

RM from Binary Data: IRL for *Prompt Optimization*



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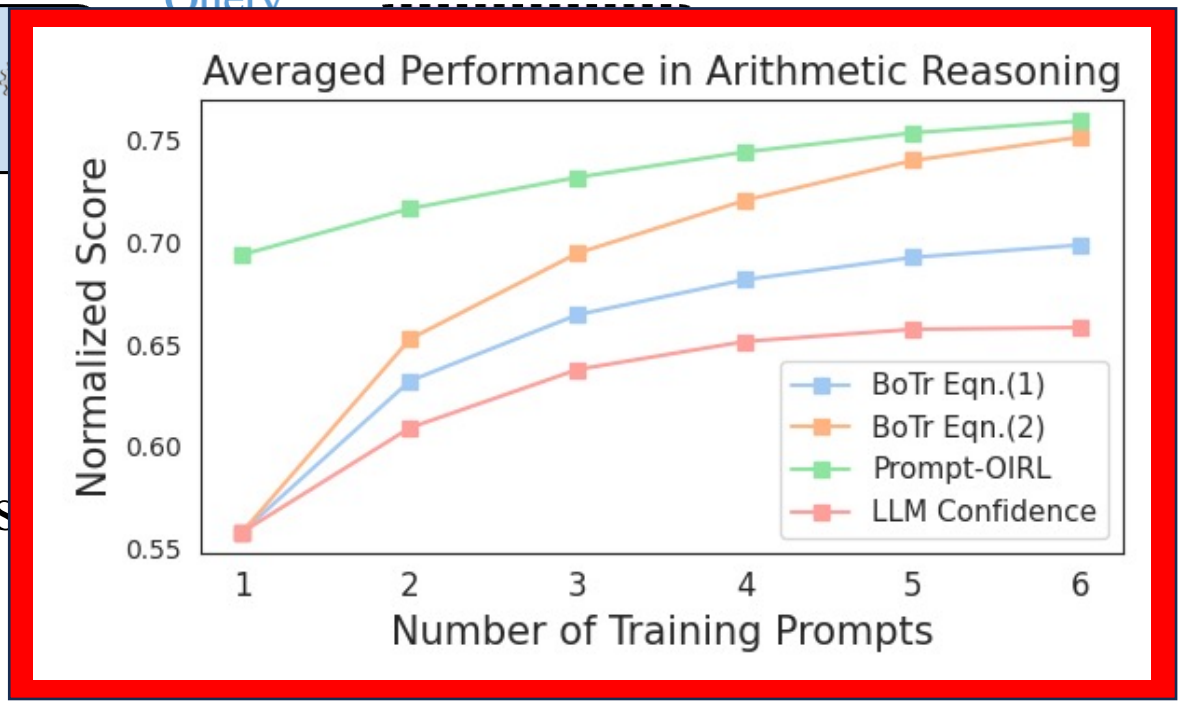
Math Reasoning Ability



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sites.google.com/view/irl-llm

Learning Reward Models from Data

RMs from different data types

RM from Binary (e.g., Math Reasoning)

RM from Preference (e.g., Classical RLHF)

RM from Demonstration (e.g., Expert Data)

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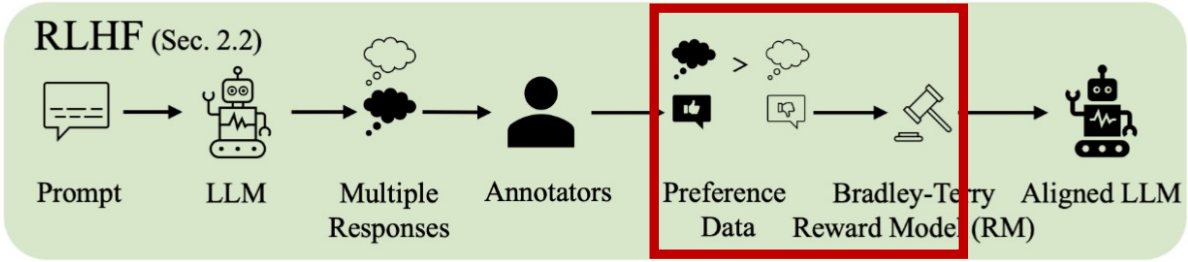
Preference-Reward Model Foundation Paper [Sun et al., 2025]

RM from Preference: Back to Ranking Theory

- How to build reward model?
  - RLHF: “use the Bradley-Terry Model”
  - But why?



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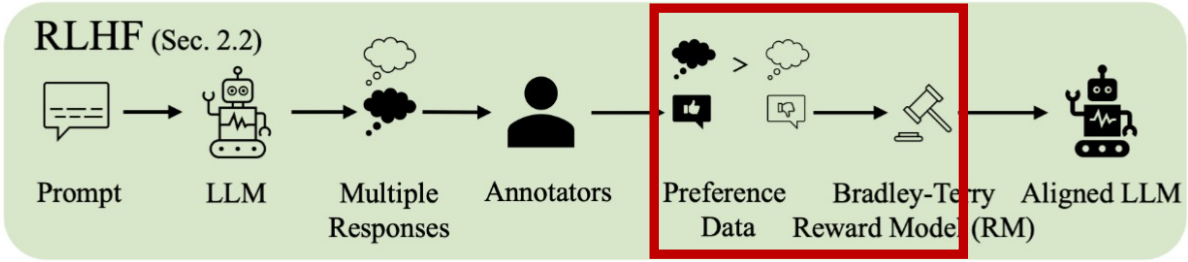

- What is the Bradley Terry Model?
  - Player i, with ability score r_i
  - Player j, with ability score r_j
  - In a game between player i and j,

$$P(i \text{ wins } j) = \frac{r_i}{r_i + r_j}$$

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RM from Preference: Back to Ranking Theory

- Classical Applications of the Bradley-Terry Models --- Parameter Estimation
  - In Chess/StarCraft/DOTA II: we estimate player scores using match history/outcomes
  - In LLM arena, we have 150 models, 2M competitions, each LLM plays ~10,000 games

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Rank* (UB)	Rank (StyleCtrl)	Model	Arena Score	95% CI	Votes
1	1	Gemini-2.0-Flash-Thinking-Exp-01-21	1384	+6/-9	10022
1	1	Gemini-2.0-Pro-Exp-02-05	1379	+7/-6	7853
3	1	ChatGPT-4o-latest (2024-11-20)	1365	+4/-3	38148
3	1	DeepSeek-R1	1361	+8/-7	4193
3	7	Gemini-2.0-Flash-001	1357	+8/-7	5576
4	1	o1-2024-12-17	1352	+6/-6	12021
7	5	o1-preview	1335	+4/-3	33174
7	7	Qwen2.5-Max	1332	+12/-11	3394
8	9	DeepSeek-V3	1316	+5/-5	16583
9	9	Gemini-2.0-Flash-Lite-Preview	1306	+9/-8	5083
9	12	GLM-4-Plus-0111	1305	+11/-10	2791
9	13	Step-2-16K-Exp	1304	+8/-9	5128
10	13	o1-mini	1305	+3/-4	52726
10	9	Gemini-1.5-Pro-002	1302	+3/-4	49653

Image source: lmsys-llm-arena, screenshot date: Feb-5-2025

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We need a **large number of matches/games** for a consistent estimation.
e.g., consider sorting: we need $\boldsymbol{N \log N}$

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- In RLHF,
  - we have m prompts, 2m responses --- 2m players
  - Each pair only "compete" once --- $m \ll 2m\log(2m)$ comparisons
  - + we need predictions, how is this possible?

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RM from Preference: Back to Ranking Theory

- Why does BT model work?

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RM from Preference: Back to Ranking Theory

- Why does BT model work?
  - An analogy:

    knowing the results of 5 groups of 1 on 1 running matches between 10 people.

    predict who is the best runner in **another** 100 people.

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    predict who is the best runner in **another** 100 people.

  - It's impossible, unless we have a stopwatch!

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RM from Preference: Back to Ranking Theory

- Why does BT model work?
  - We are working on the *embedding space*
  - RMs in the embedding space generalize well
  - Theoretical justification is in the paper

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  - BT model: precisely predicting win rates
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  - BT model: precisely predicting win rates
  - Is it necessary in RLHF?

    NO, we only need *order consistency*

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RM from Preference: Order Consistency

- In test-time optimization, we use RM to pick the best of possible choices.
- e.g.,

Q-A Pairs	Q + Answer 1	Q + Answer 2	Q + Answer 3	Q + Answer 4
True Reward	9.8	9.0	7.0	6.0
Reward Model 1	1.0	0.9	0.8	0.7
Reward Model 2	100	99	80	50
Reward Model 3	9.0	9.8	7.0	6.0

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- RM 1 = RM 2 > RM 3

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- Spearman Ranking Correlation: **Classification Models!**

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RM from Preference: Classification Models

- Classification models are…
  - Flexible

	Input	Output	Model
Bradley Terry Model	A Pair	Score difference	Neural Networks
Classification Model	1 response	Score	Any ML Models

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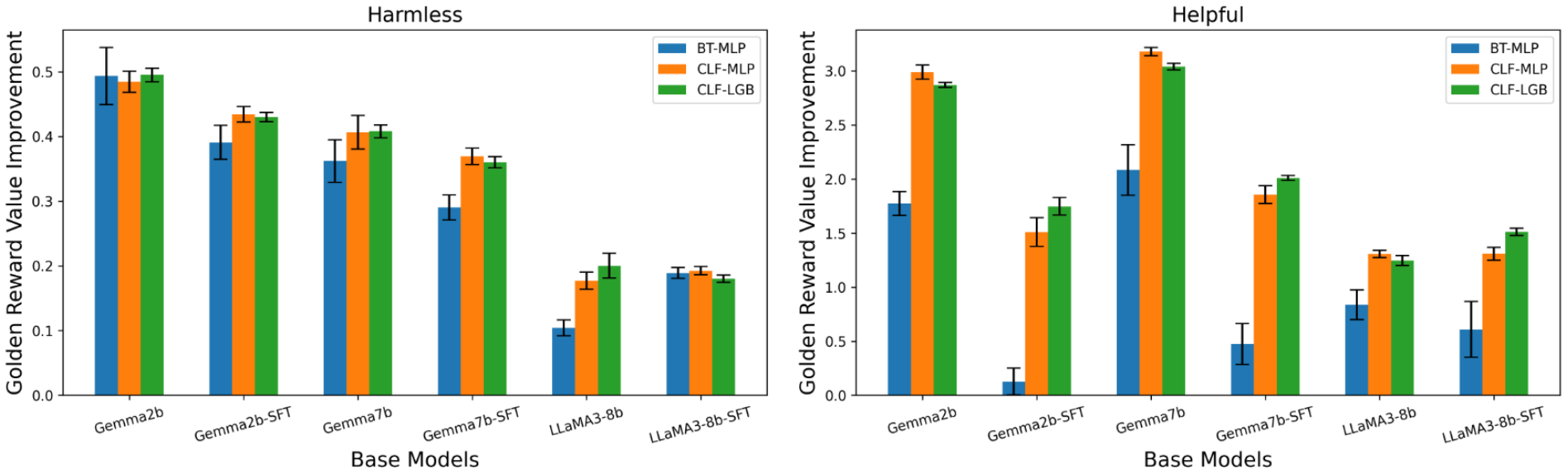
RM from Preference: Classification Models

- Classification models are…
  - Flexible
  - Better than BT models (when *labels are noisy*)



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RM from Preference: Classification Models

- Classification models are…
  - Flexible
  - Better than BT models (when *labels are noisy*)
  - Robust to annotation noises

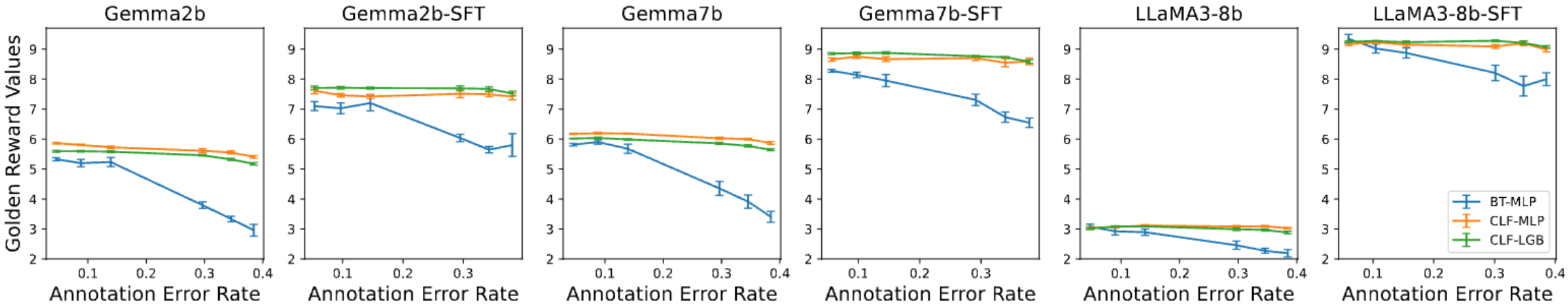

Figure 2: *Changing the annotation quality. Dataset: Harmless, Helpful.*

RM from Preference: Classification Models

- Classification models are…
  - Flexible
  - Better than BT models (when *labels are noisy*)
  - Robust to annotation noises and data scarcity

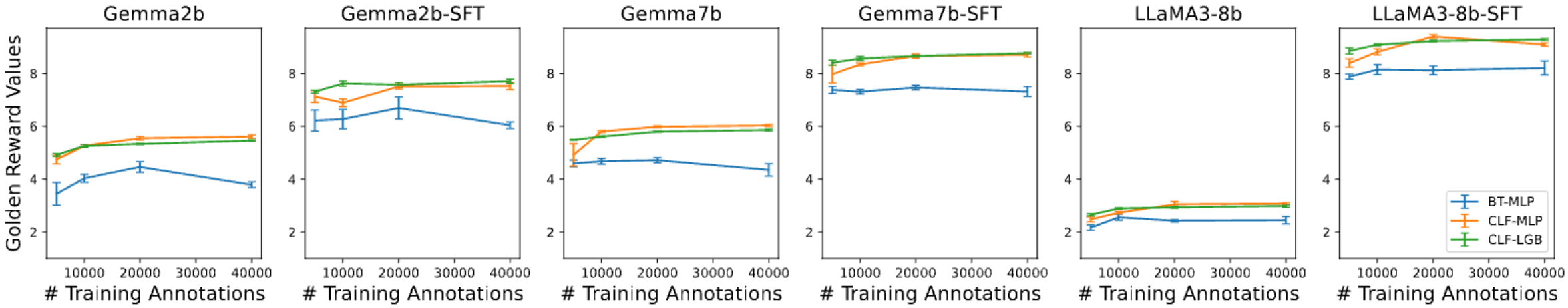

Figure 3: *Changing the annotation quantity. Dataset: Harmless, Helpful.*

RM from Preference: Cross-Prompt Comparisons

- Local Tournaments – Global Tournaments?

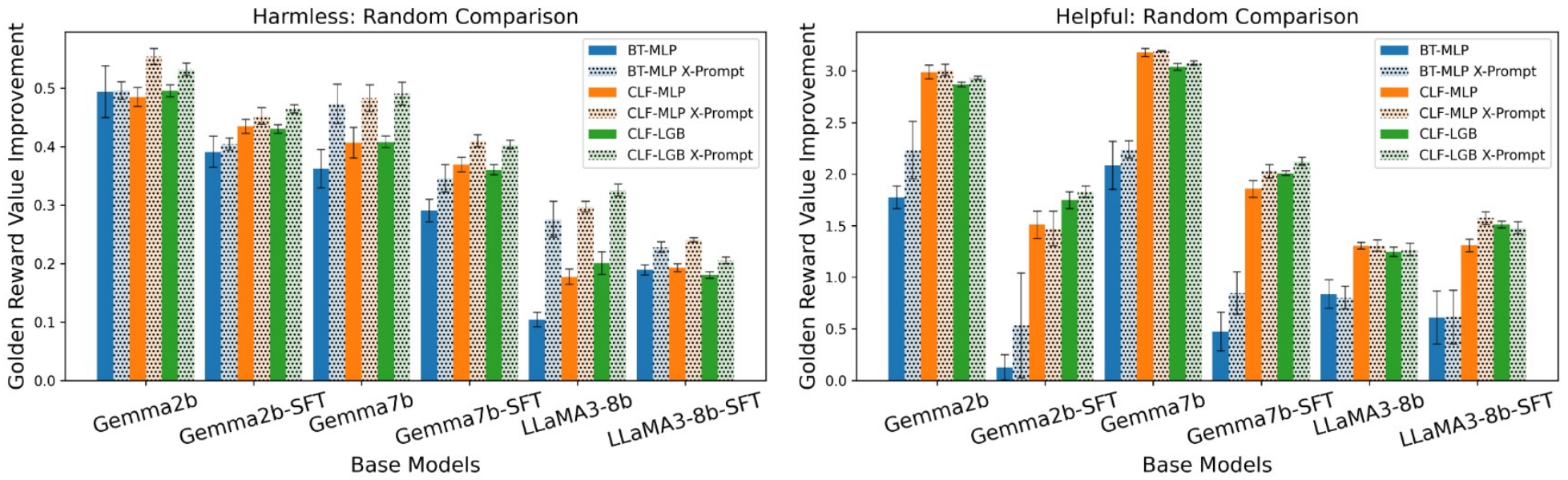

Figure 4: *Results comparing cross-prompt comparison based annotations.* Preference annotations on cross-prompt comparisons outperform same-prompt comparisons.

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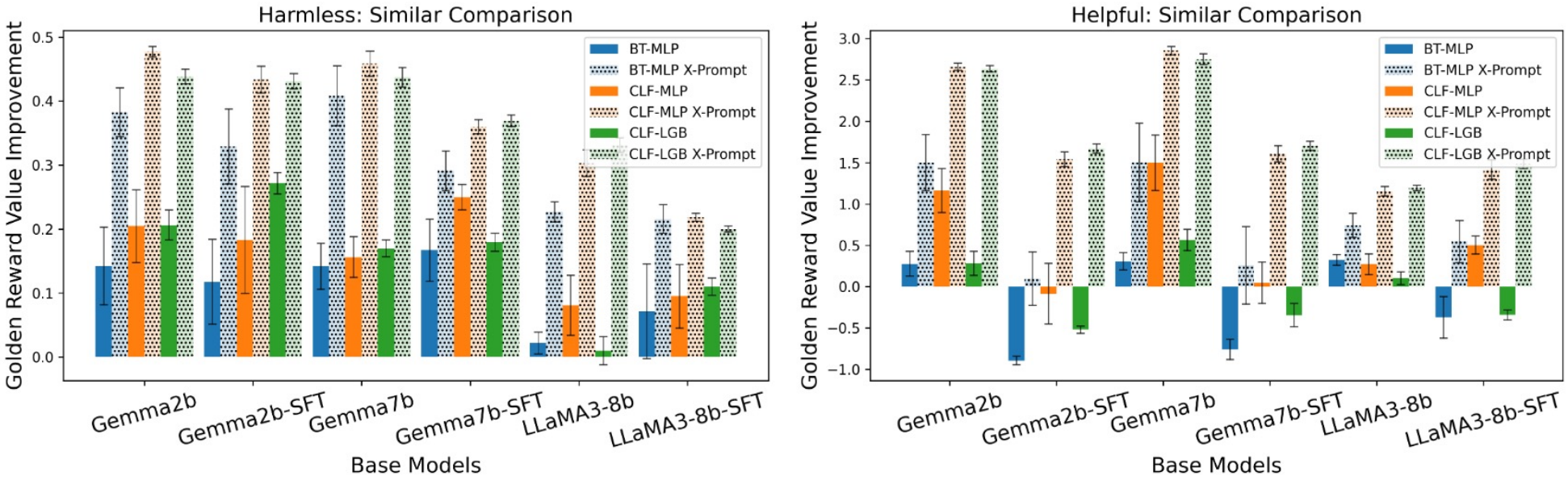
RM from Preference: Cross-Prompt Comparisons

- When and Why? Generation Diversity Matters

  Low diversity case: clear improvement



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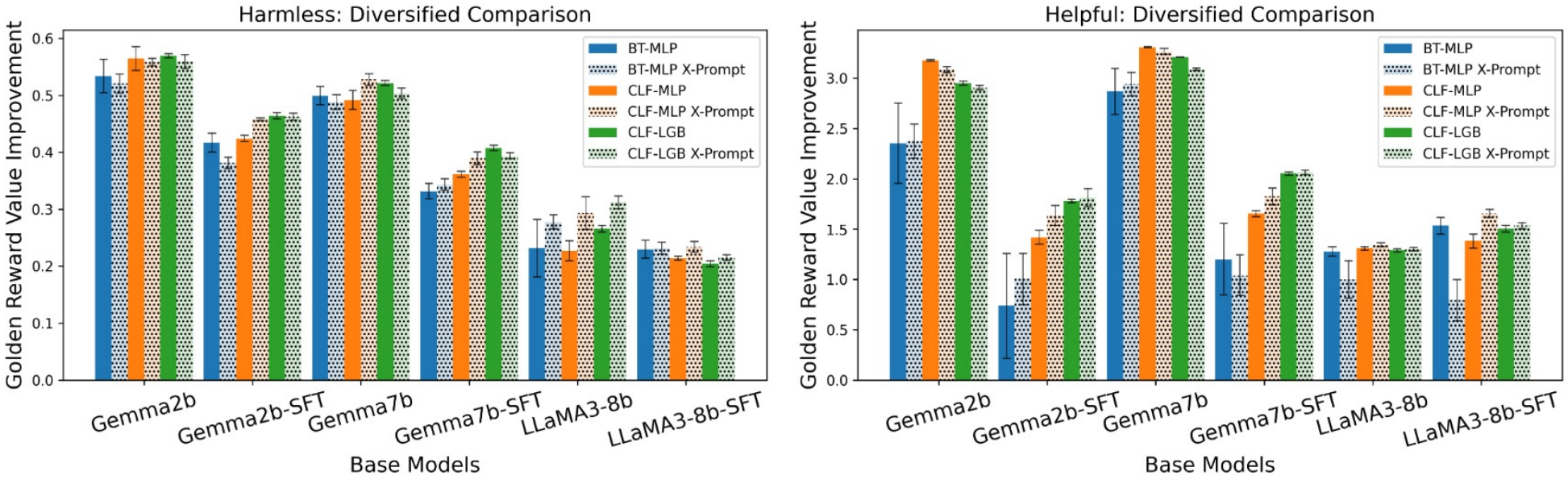
RM from Preference: Cross-Prompt Comparisons

- When and Why? Generation Diversity Matters

  High diversity case: no improvement



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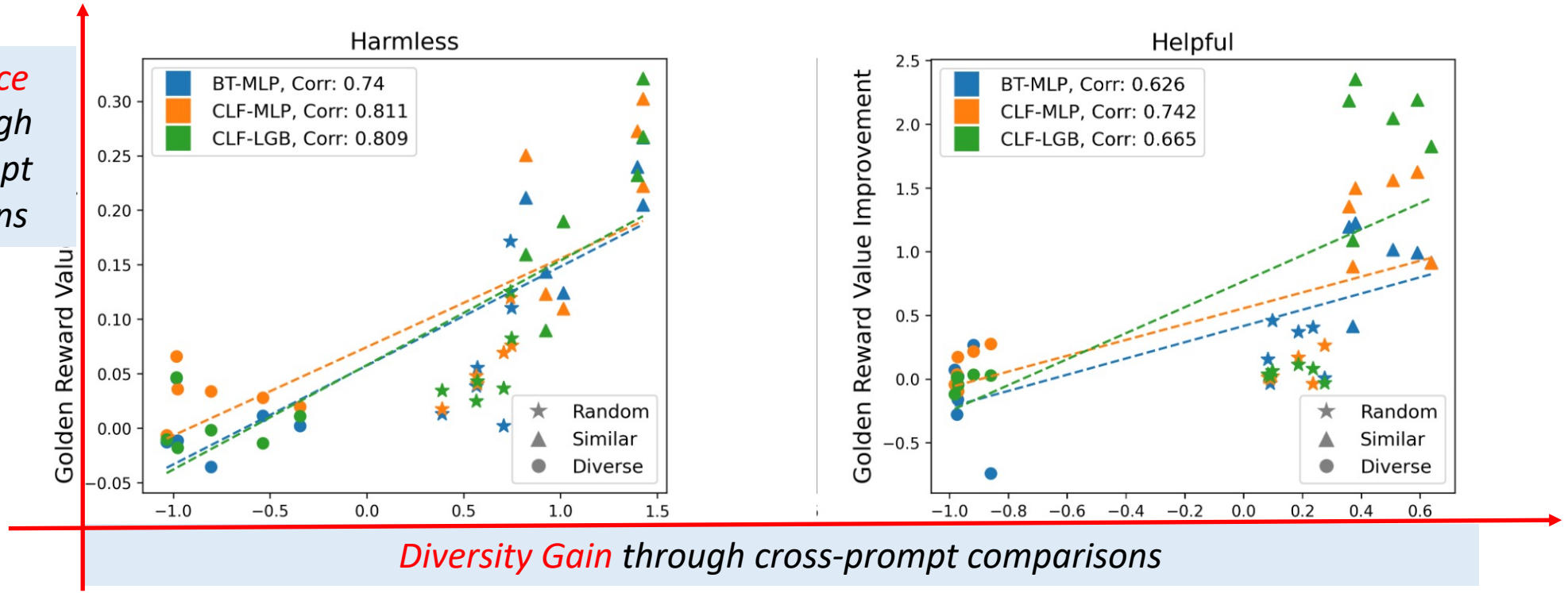
RM from Preference: Cross-Prompt Comparisons

- When and Why? *Comparison* Diversity Matters

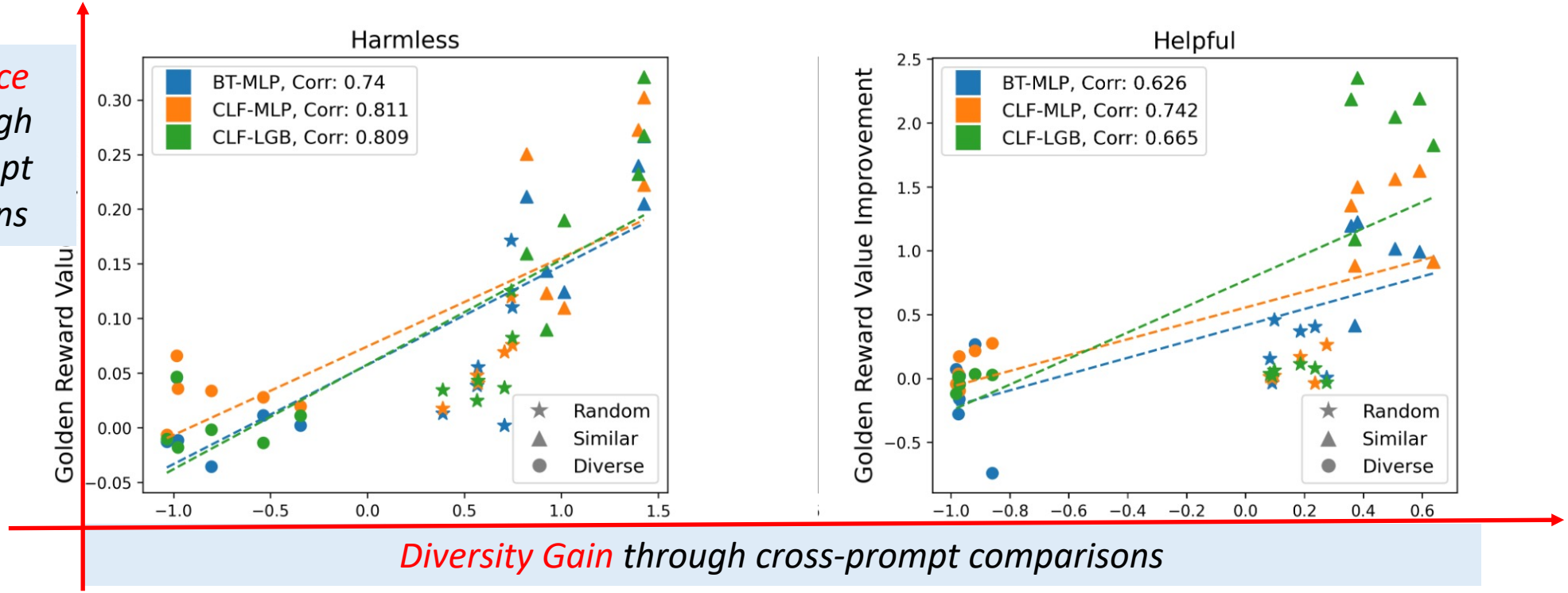
Performance Gain through cross-prompt comparisons



RM from Preference: Cross-Prompt Comparisons

- When and Why? *Comparison* Diversity Matters
  Proof in the paper: Cross-prompt comparisons always improves diversity

Performance Gain through cross-prompt comparisons



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RM from Preference: Takeaways

- Preference learning with less than $N \log N$ comparisons relies on the embeddings.
- Bradley-Terry models are good, but not necessary.
- Order consistency is the objective of RM.
- Classification methods work well.
- Use cross-prompt comparisons for diverse comparisons.

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Learning Reward Models from Data

RMs from different data types

RM from Binary (e.g., Math Reasoning)

RM from Preference (e.g., Classical RLHF)

RM from Demonstration (e.g., Expert Data)

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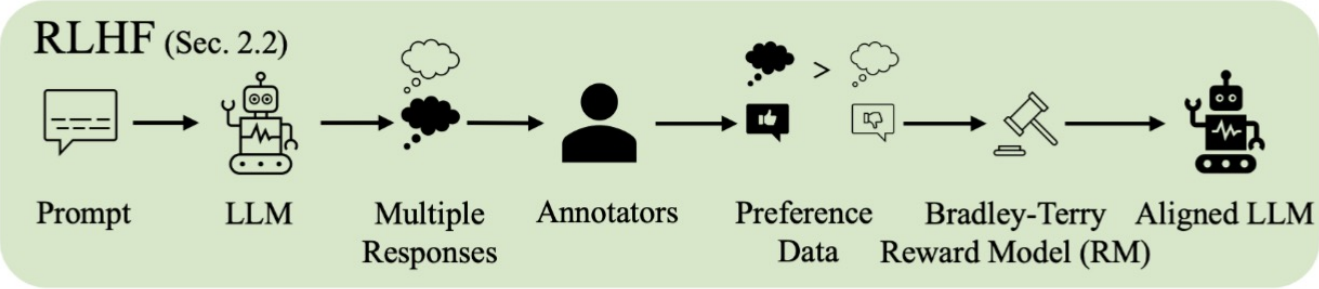
RM from Demonstration: Inverse RL for Alignment

- Common practice of alignment: RLHF



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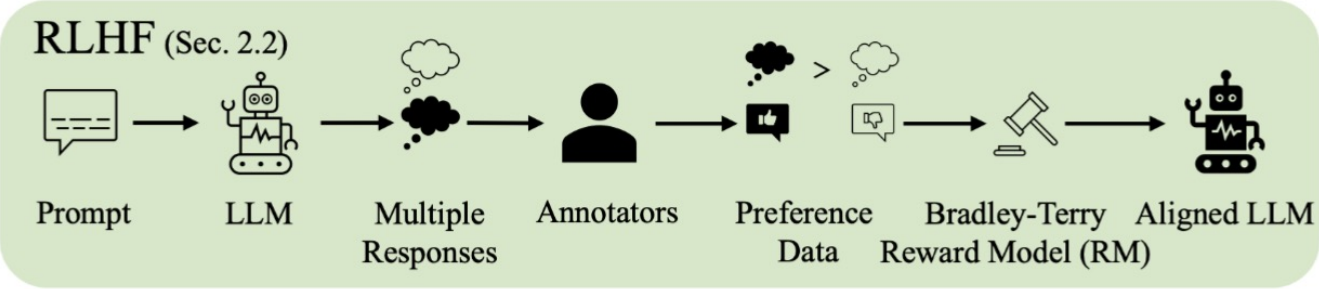

- Why do we need to align LLMs from demonstrations?

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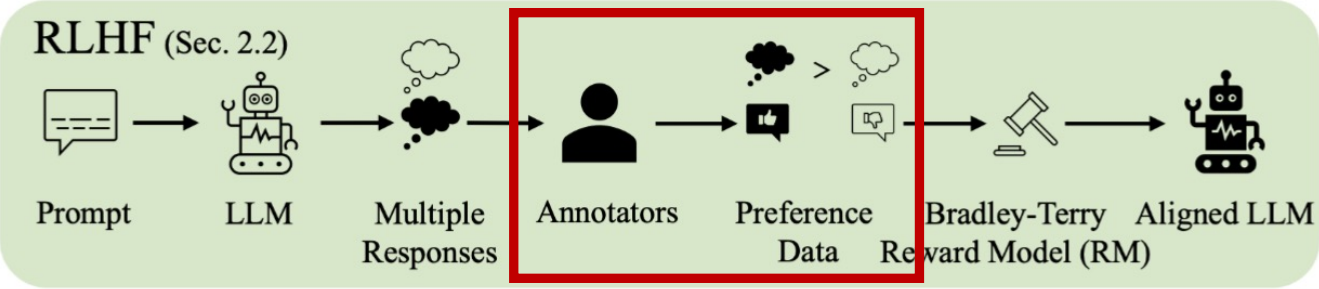

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  - 1. Preference-based alignment is expensive

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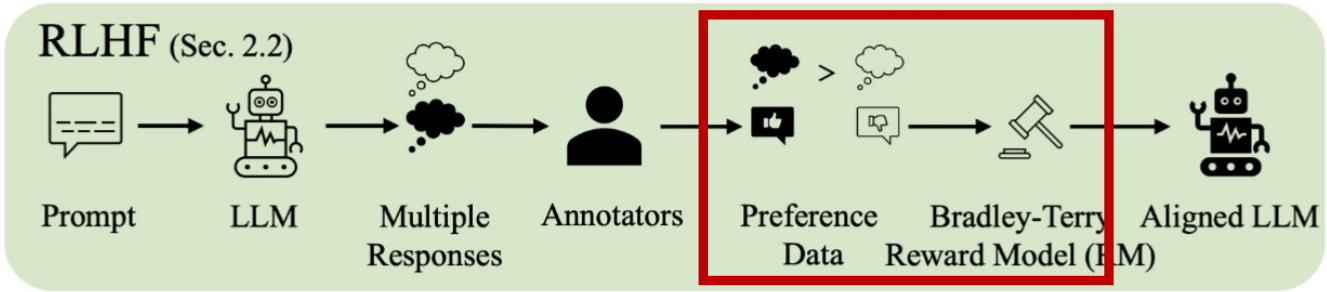

- Why do we need to align LLMs from demonstrations?
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  - 2. Assumptions such as Bradley-Terry models are needed

RM from Demonstration: Inverse RL for Alignment

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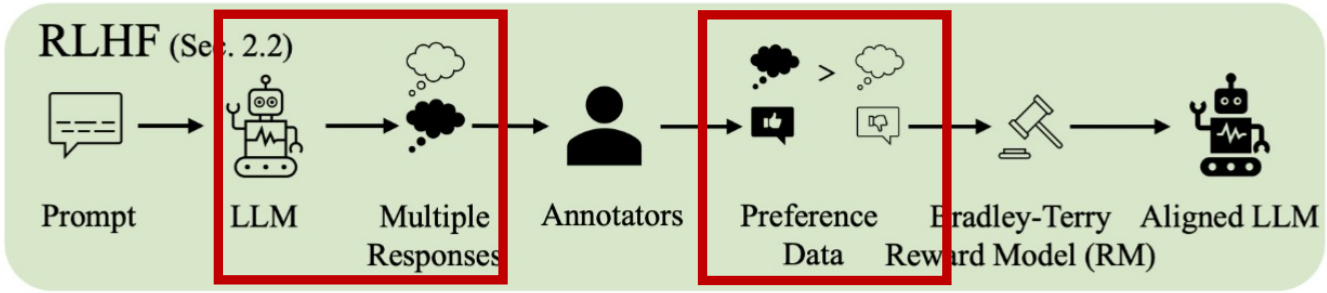

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  - 3. Noisy preference annotations

RM from Demonstration: Inverse RL for Alignment

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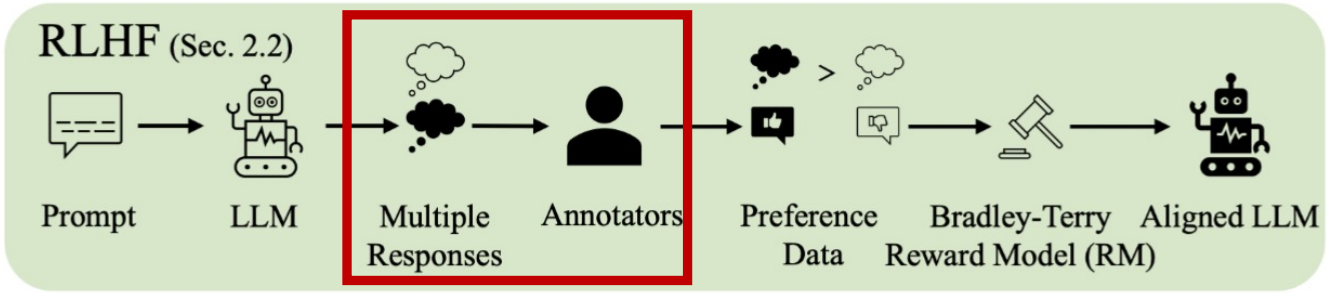

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  - 4. Privacy concerns

RM from Demonstration: Inverse RL for Alignment

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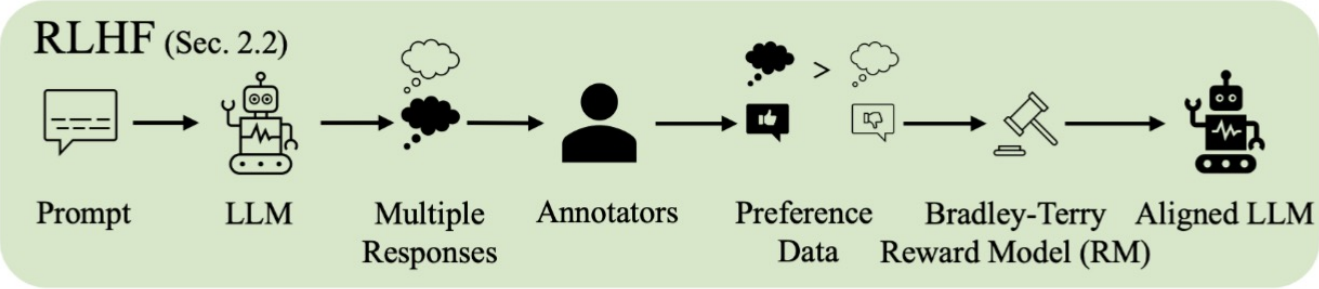

- In applications, we have *high-quality* demonstration data
  - Personalized emails/articles [Shaikh et al., 2024]
  - Medical prescriptions

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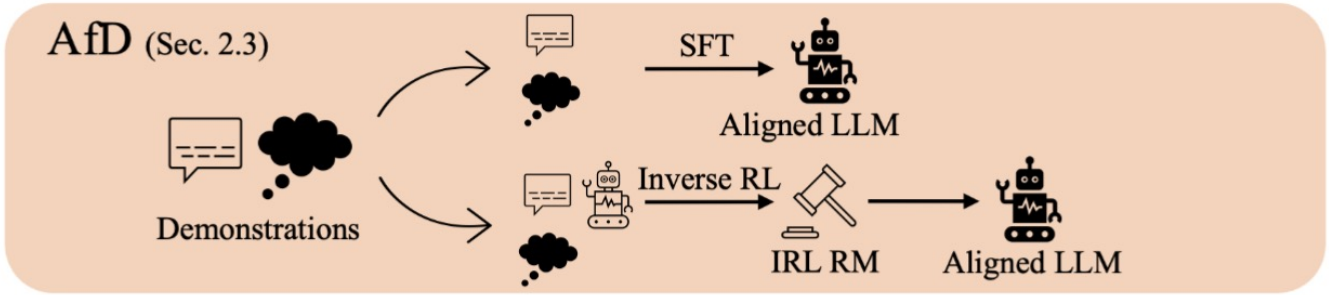
RM from Demonstration: Inverse RL for Alignment

- Alignment from Demonstrations?



- Vanilla setup in Inverse RL!
  - SFT: Behavior cloning
  - Inverse RL [Sun & van der Schaar, 2024] [Wulfmeier et al., 2024]
  - Imitation Learning [Chen et al., 2024] [Xiao et al., 2024]

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RM from Demonstration: Inverse RL for Alignment

- In SPIN [Chen et al., 2024]:

  Lemma 1: Method A can align LLMs using preference data

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RM from Demonstration: Inverse RL for Alignment

- In SPIN [Chen et al., 2024]:

  Lemma 1: Method A can align LLMs using preference data

  Create dataset:

Preferred	---	Demonstration
Dis-preferred	---	Current LLM generated

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RM from Demonstration: Inverse RL for Alignment

- In SPIN [Chen et al., 2024]:

  Lemma 1: Method A can align LLMs using preference data

  Create dataset:

Preferred	---	Demonstration
Dis-preferred	---	Current LLM generated

  Apply *Lemma 1*

  Method A can align LLMs using demonstration data

- The objective is to match performance of demonstrations

*Method A in SPIN is DPO [Rafailov et al., 2023]

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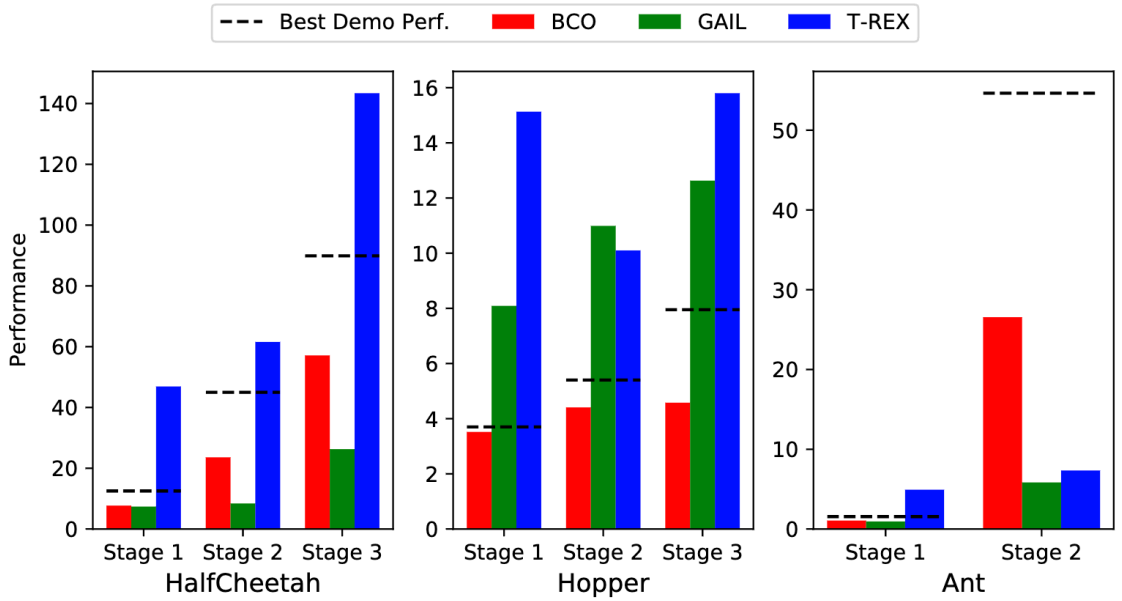
RM from Demonstration: Inverse RL for Alignment

- Can we do better with explicit reward modeling?
  [Brown et al., 2019]: extrapolation improves performance



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RM from Demonstration: Inverse RL for Alignment

- Can we do better with explicit reward modeling?
  [Brown et al., 2019]: extrapolation improves performance

- In [Sun & van der Schaar, 2024] Discriminator as Reward Model:

Create dataset:

Positive	---	Demonstration
Negative	---	Current LLM generated

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RM from Demonstration: Inverse RL for Alignment

- Can we do better with explicit reward modeling?
  [Brown et al., 2019]: extrapolation improves performance

- In [Sun & van der Schaar, 2024] Discriminator as Reward Model:

  Create dataset:

  Positive --- ~~Demonstration~~ (*need a fix!*)

  Negative --- Current LLM generated

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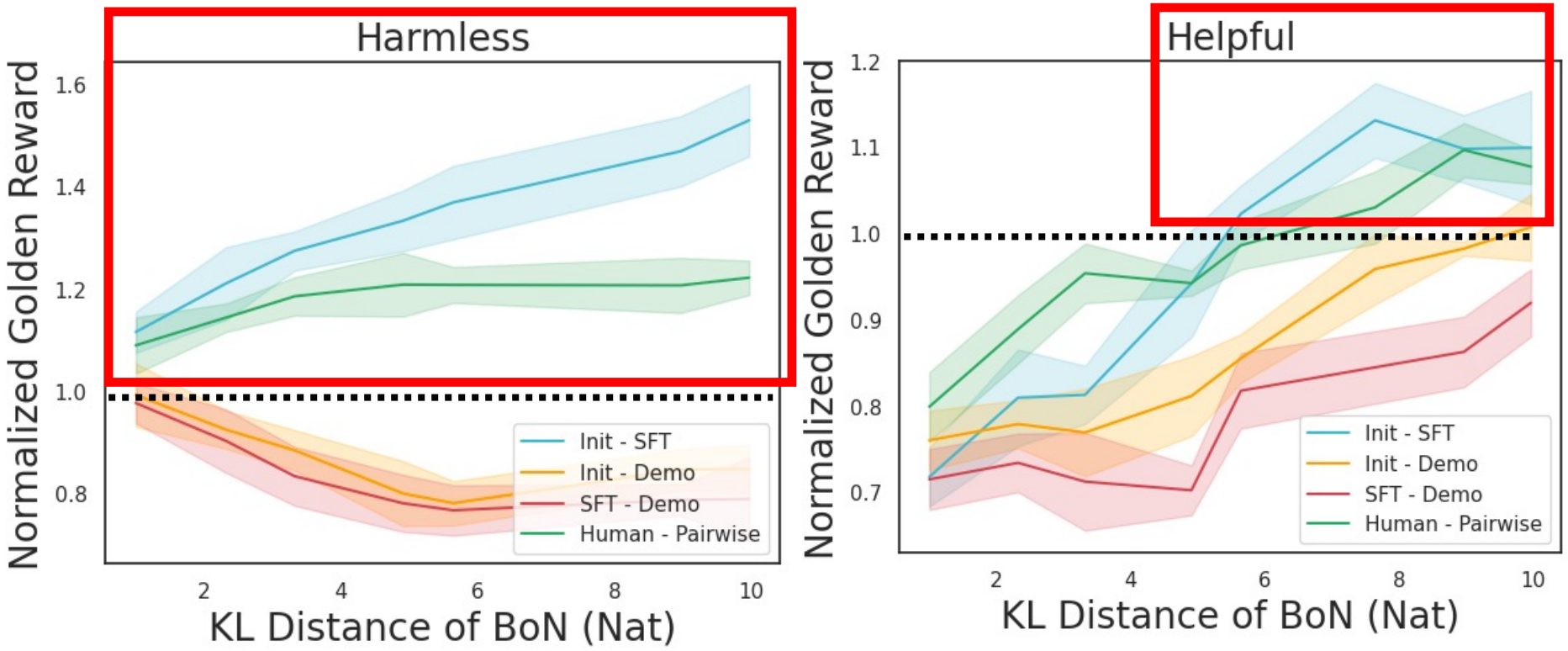
RM from Demonstration: Inverse RL for Alignment

Super-demonstration performance achieved inside the red boxes.

Dotted lines: Demonstration quality



- Super-demonstration performance! (after solving some reward hacking)

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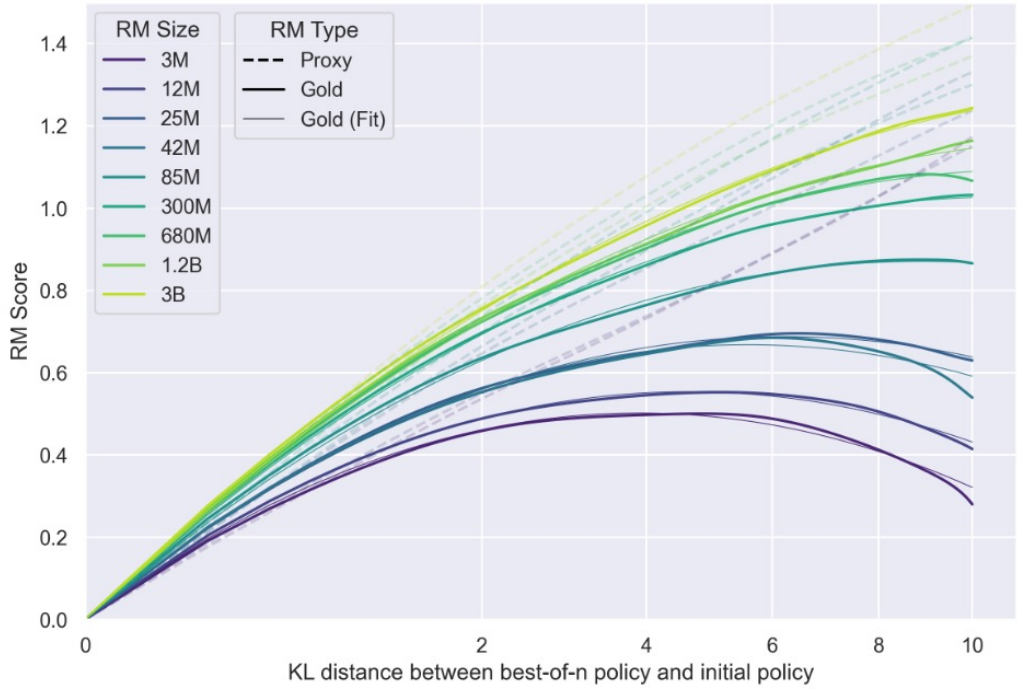
Challenges and Opportunities

- Reward Model overoptimization [Gao et al., 2022]



(a) BoN

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Challenges and Opportunities

- Reward Model overoptimization [Gao et al., 2022]
  - RM ensemble [Coste et al., 2024] [Ahmed et al., 2024] [Zhang et al., 2024]

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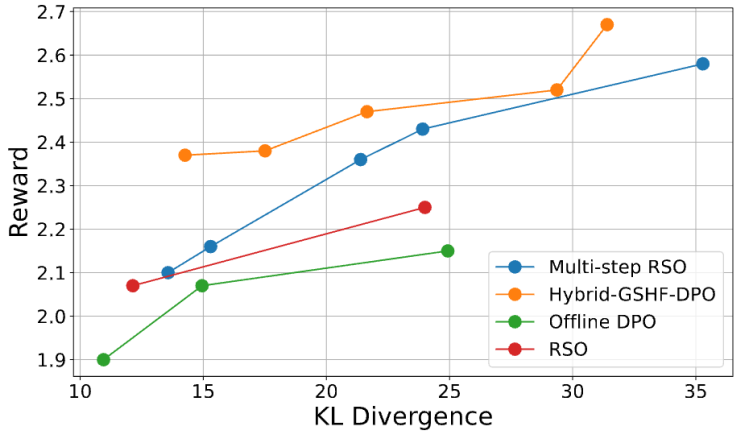

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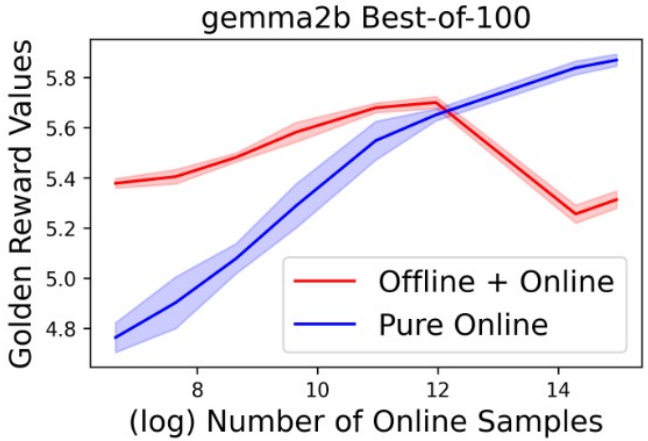

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- How to effectively collect preference data?
  - Max-Margin/Entropy [Muldrew et al., 2024]
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Challenges and Opportunities

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- Other data type?
  - Critique data [Zhang et al., 2025] [Ankner et al., 2024] [Wu et al., 2024]

Challenges and Opportunities

The Challenge of *Generalization*

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  - RM ensemble [Coste et al., 2024] [Ahmed et al., 2024] [Zhang et al., 2024]
- On-policy/Off-policy annotations
  - Iterative online annotation improves efficiency [Xiong et al. 2024]
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- Other data type?
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Part 4:

Insights from the Sparse-Reward RL Literature

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What are Unique with LLMs?

Task	Action Space	State Space	Reward Signal	Method	Transition
Atari	Disc. ~ 1e1	Image	Dense (mostly)	DQN	Unknown
Atari-Explore	Disc. ~ 1e1	Image	Sparse	Curiosity-Driven	Unknown
Go	Disc. ~ 1e2	Disc. ~1e100	Sparse	MCTS, Self-Play	Known
Dota2	Disc. ~ 1e6	Partial Observable	Dense & Sparse	(MA)PPO	Unknown
StarCraft	Disc. ~ 1e26	Partial Observable	Dense & Sparse	BC, AC, League	Unknown
Multi-Goal	Cont. Dim~1e2	Cont. Dim~1e2	Sparse	Hindsight Exp. Replay	Unknown
Reasoning	**Disc. ~ 1e6**	**Vocab.^Token_n**	**Sparse**	GRPO	**Known**
Alignment	**Disc. ~ 1e6**	**Vocab.^Token_n**	**Noisy Preference**	PPO, DPO, REINFORCE	**Known**

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Transferrable Insights?

Task	Action Space	State Space	Reward Signal	Method	Transition
Atari	Disc. ~ 1e1	Image	Dense (mostly)	DQN	Unknown
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Dota2	Disc. ~ 1e6	Partial Observable	Dense & Sparse	(MA)PPO	Unknown
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Reasoning	**Disc. ~ 1e6**	**Vocab.^Token_n**	**Sparse**	GRPO	**Known**
Alignment	**Disc. ~ 1e6**	**Vocab.^Token_n**	**Noisy Preference**	PPO, DPO, REINFORCE	**Known**

Learning from Failure?

Reward Shaping?

Self-Play?

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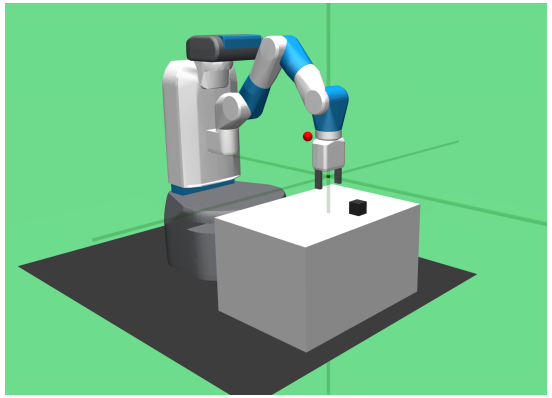
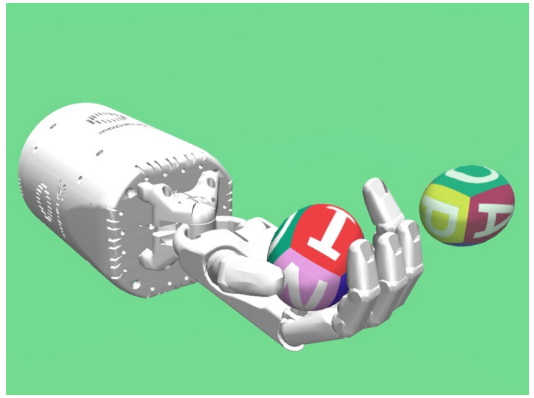
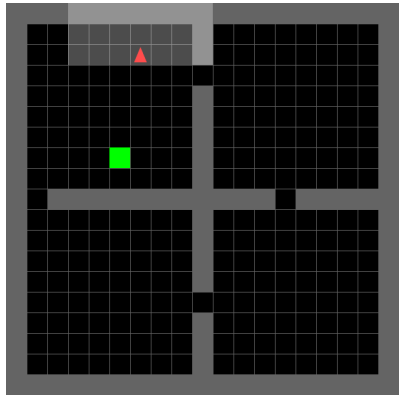
Hindsight Methods [Andrychowicz et al., 2017]

- Multi-Goal task
- Failing in achieve a certain goal = successfully achieving another goal







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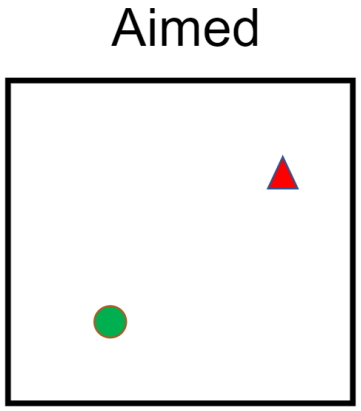
Hindsight Methods [Andrychowicz et al., 2017]

- How?

- Key insight explained in a simplified supervised learning setup:

learn how to reach goal g : $\pi(\cdot\,|s_0, g)$



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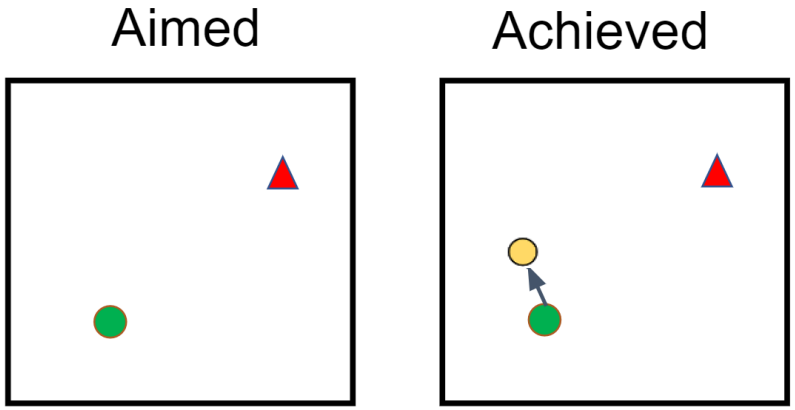

$a_1,$

$s_1,$

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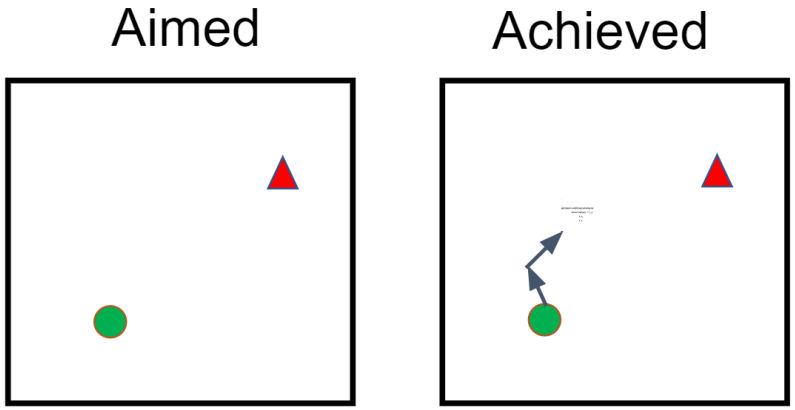

$a_1, a_2,$

$s_1, s_2,$

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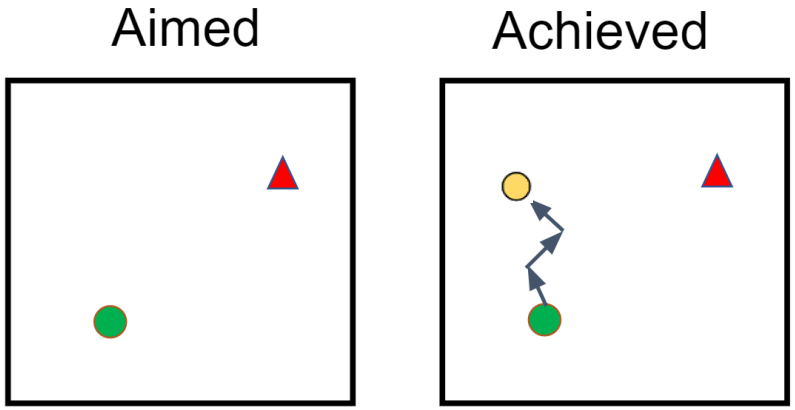

a_1, a_2, a_3

s_1, s_2, s_3

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Hindsight Methods [Andrychowicz et al., 2017]

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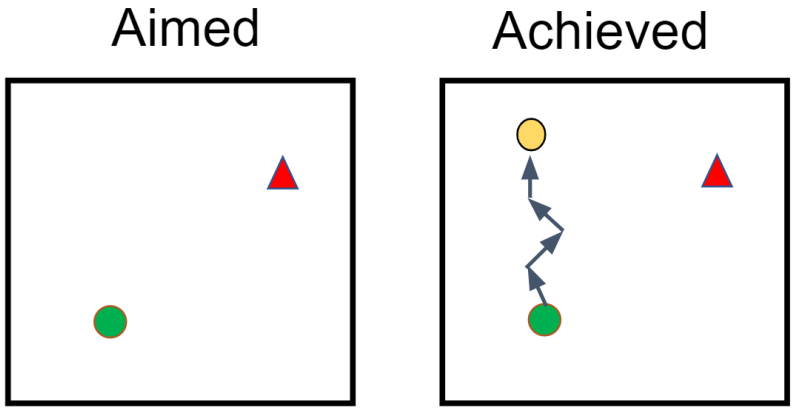

a_1, a_2, a_3, a_4

s_1, s_2, s_3, s_4

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Hindsight Methods [Andrychowicz et al., 2017]

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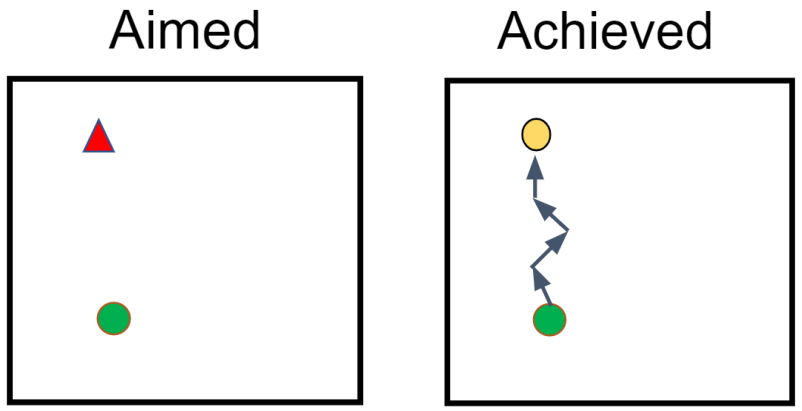

a_1, a_2, a_3, a_4

s_1, s_2, s_3, s_4

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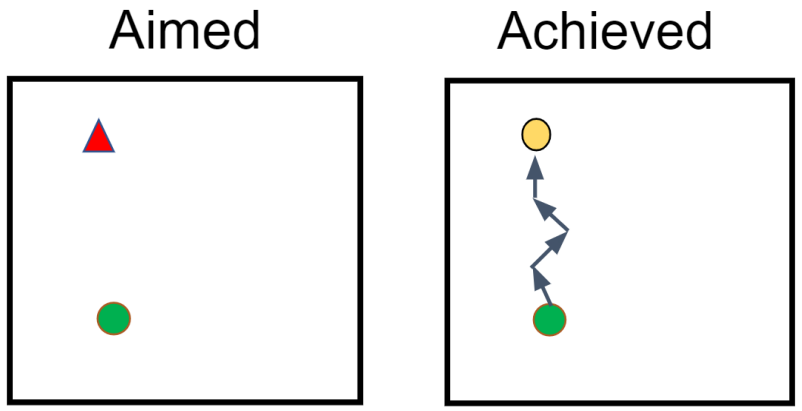
Hindsight Methods [Andrychowicz et al., 2017]

- How?

- Key insight explained in a simplified supervised learning setup:

learn how to reach goal g : $\pi(\cdot\,|s_0, g)$



a_1, a_2, a_3, a_4

s_1, s_2, s_3, s_4

$a_1 \leftarrow \pi(\cdot\,|s_0, g)$

$a_2 \leftarrow \pi(\cdot\,|s_1, g)$

$a_3 \leftarrow \pi(\cdot\,|s_2, g)$

$a_4 \leftarrow \pi(\cdot\,|s_3, g)$

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Hindsight Methods [Andrychowicz et al., 2017]

- How?

- Key insight explained in a simplified supervised learning setup:
  Hindsight Self-Imitate Learning [Sun et al., 2019]

- **Multi-goal** tasks in LLM alignment?

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- How?

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- **Multi-goal** tasks in LLM alignment?
  LLM Web Agent [He et al., 2024]
  more to explore!

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Reward Shaping (and Credit Assignment)

- Given *delayed* reward, assign credit to each action?

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Reward Shaping (and Credit Assignment)

- Given *delayed* reward, assign credit to each action?
  - Credit Assignment Problem [Sutton, 1984] Recent Survey [Pignatelli et al., 2024]
  - Return Decomposition [Arjona-Medina et al., 2019][Ren et al., 2022]

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  - Return Decomposition [Arjona-Medina et al., 2019][Ren et al., 2022]
- In LLM alignment:
  - Free-of-anno.: Token-level dense reward using attention [Chan et al., 2024]
  - Free-of-anno.: PRMs from Monte-Carlo Tree Search [Wang et al. 2023]
  - Anno.: Process-supervised Reward Models (PRMs) [Lightman et al., 2023]

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  - Anno.: Process-supervised Reward Models (PRMs) [Lightman et al., 2023]
- Conservative reward shaping keeps the optimal policy [Ng et al., 1999]
- Reward shaping can change learning behavior before optimal [Sun et al., 2022]

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Best Reward: Dense or Sparse?

- Learning from sparse reward is challenging --- hard exploration
- Is learning from dense reward always better?

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Best Reward: Dense or Sparse?

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  - 1. DeepSeek-R1 [DeepSeek-AI, 2025]

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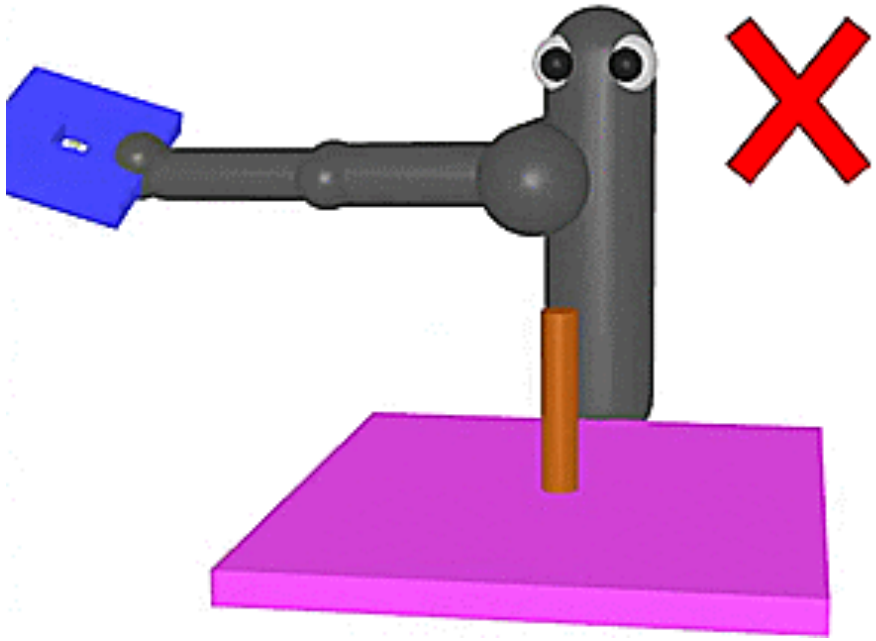

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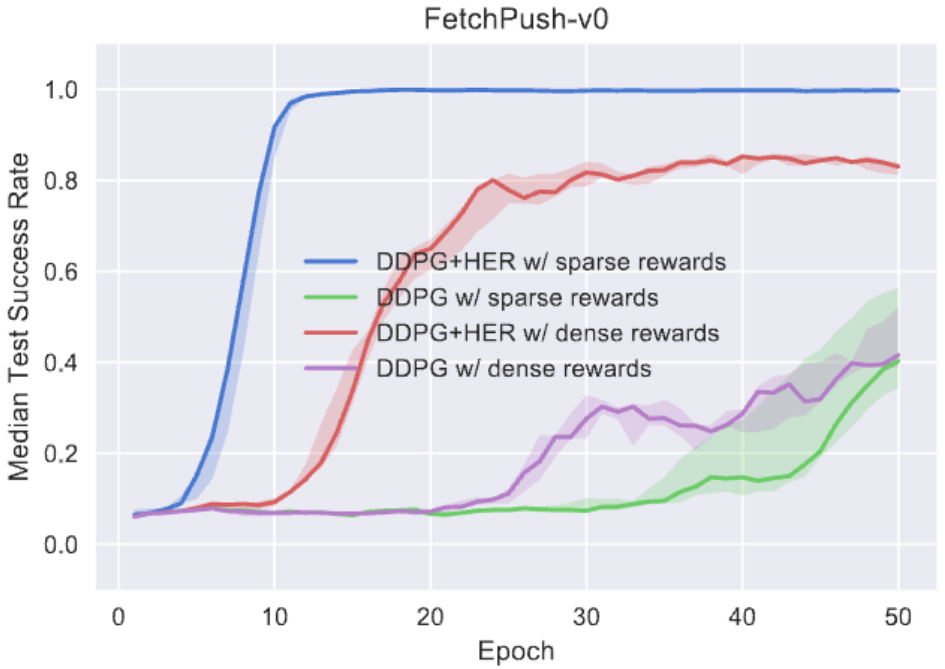
  - 3. In multi-goal tasks [Plappert et al., 2018]



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  - 4. Reward hacking [Skalse et al., 2022]

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- Do we need dense reward?
  - Warm-start from demo [Nair et al., 2017]

Best Reward: Dense or Sparse?

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  - 4. Reward hacking [Skalse et al., 2022]
- Do we need dense reward?
  - No --- Warm-start from demo [Nair et al., 2017]
  - Yes --- AlphaGo

Self-Play

- What can we learn from the success of AlphaGo (Zero)?

Self-Play

- What can we learn from the success of AlphaGo (Zero)?
- Why AlphaGo?

Task	Action Space	State Space	Reward Signal	Method	Transition
Go	Disc. ~ 1e2	Disc. ~1e100	Sparse	MCTS, Self-Play	Known
Reasoning	**Disc. ~ 1e6**	**Vocab.^Token_n**	**Sparse**	GRPO	**Known**
Alignment	**Disc. ~ 1e6**	**Vocab.^Token_n**	**Noisy Preference**	PPO, DPO, REINFORCE	**Known**

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- Self-Play are also widely used in LLM alignment / reasoning

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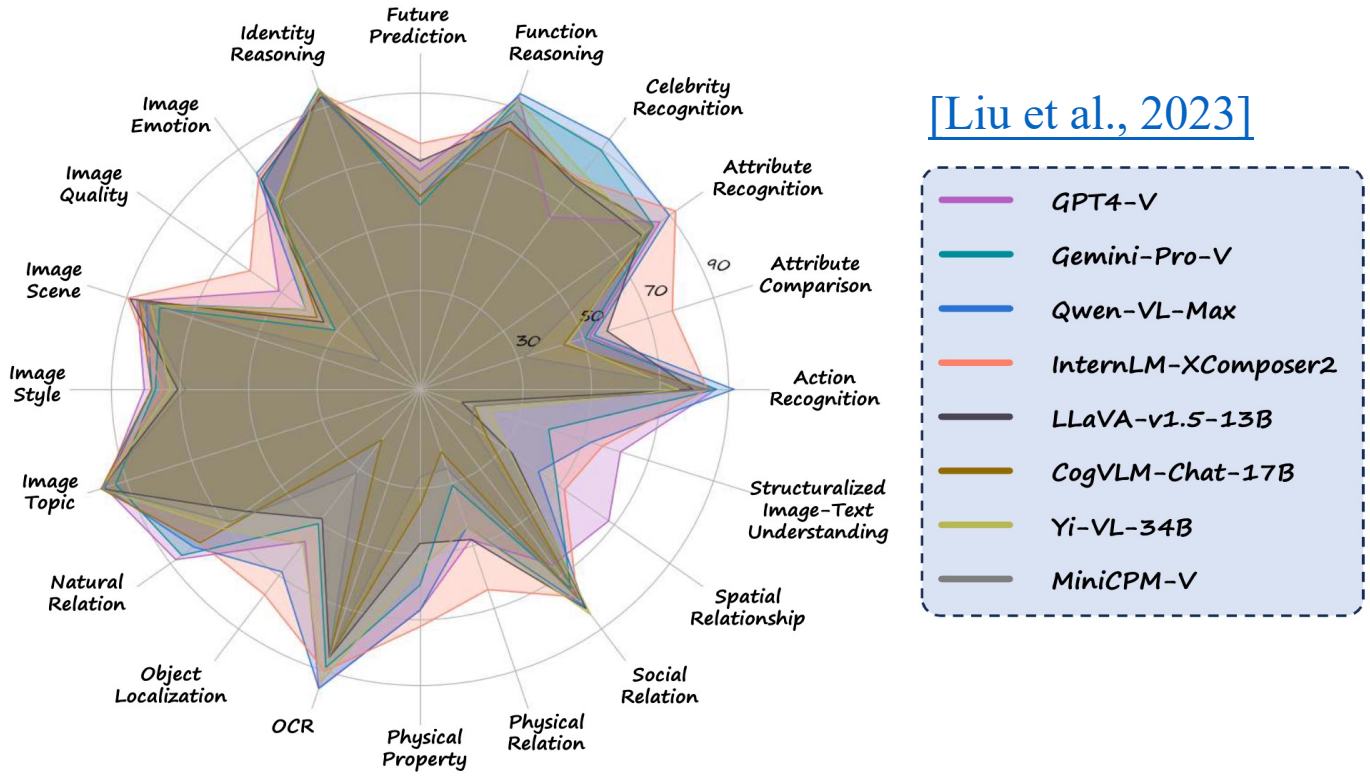
Self-Play

- Self-Play in LLMs: self-critique/-correction/-evaluation
  - LLMs are good at *some* aspects than *others*
  - Improvement is not guaranteed / bounded



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Self-Play

- Self-Play in LLMs: self-critique/-correction/-evaluation
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- Self-Play in Go(Shogi/Chess)/StarCraft:
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  - Winning the old policy is improvement (by definition)

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- Real Self-Play in games?
  - [Cheng et al., 2024] [Hu et al., 2024] [Duan et al., 2025]

Takeaways

- In Multi-Goal tasks, Hindsight methods have great potential
- 3 methods for dense reward:
  - Free using attention weights (stability)
  - Free using MCTS (not as good as using sparse reward)
  - Extra annotation (?)
- Dense reward not designed properly may lead to suboptimal
- In AlphaGo, searching is needed to achieve super-human performance
- Self-Play can be powerful

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Future of IRL x LLMs

The AlphaGo moment of LLMs will come ☺

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Thank you!

sites.google.com/view/irl-llm

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