Lecture 5

CME 295: Transformers & Large Language Models


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Stanford University

ICME

Recap of last episodes...

Initialized model

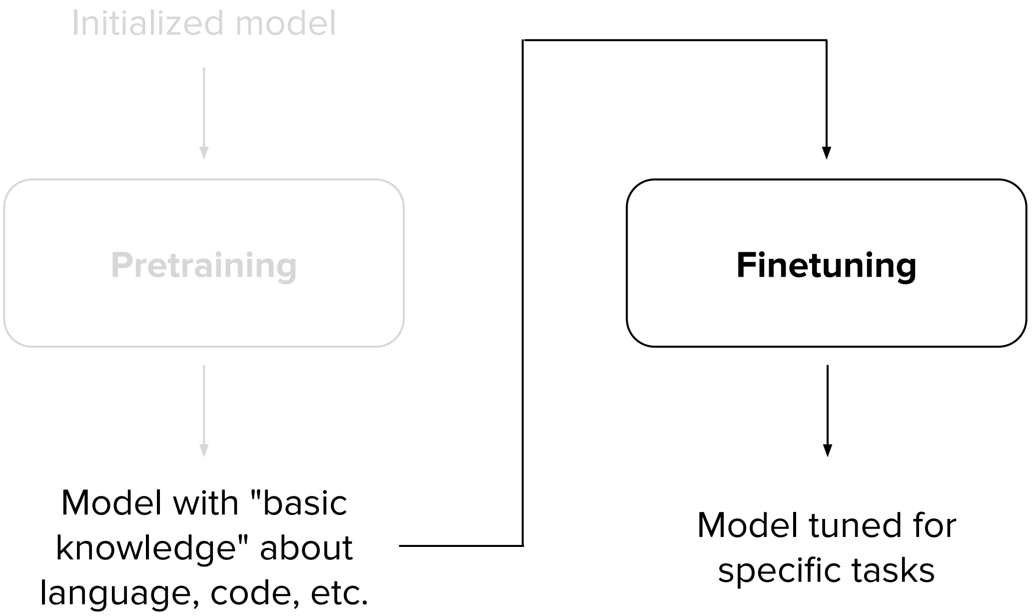
↓

Pretraining

↓

Model with "basic knowledge" about language, code, etc.

Recap of last episodes...



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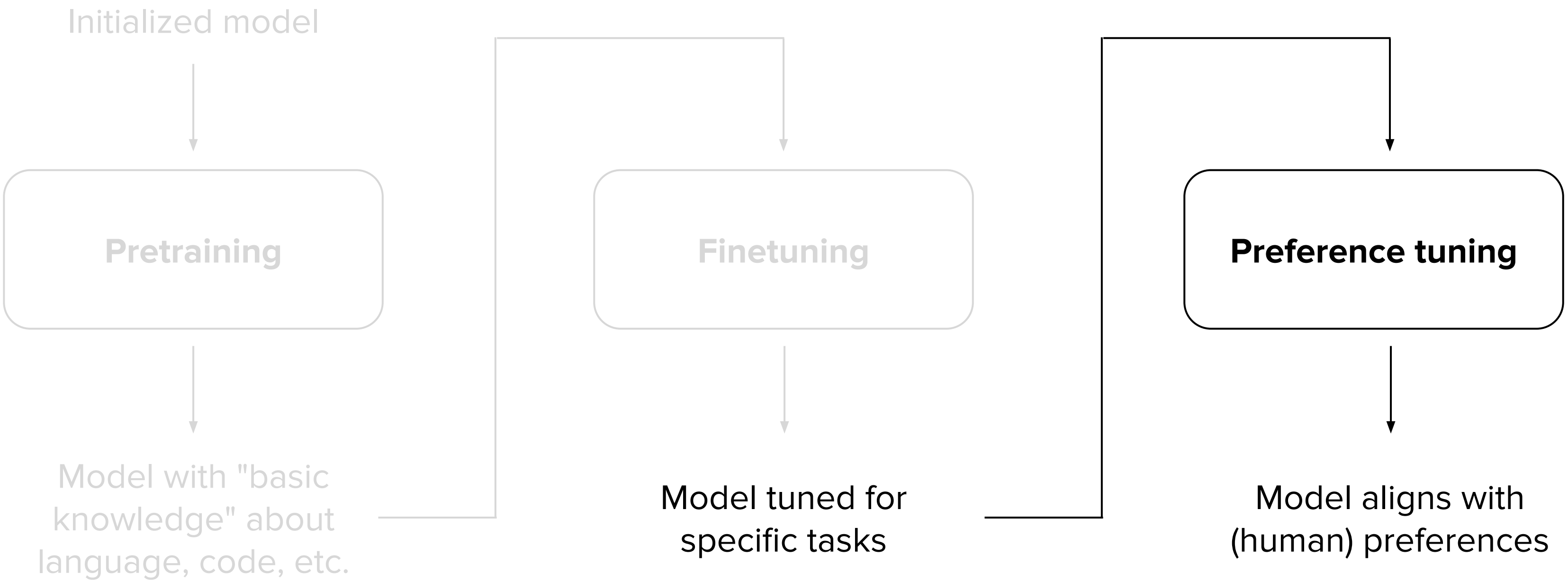
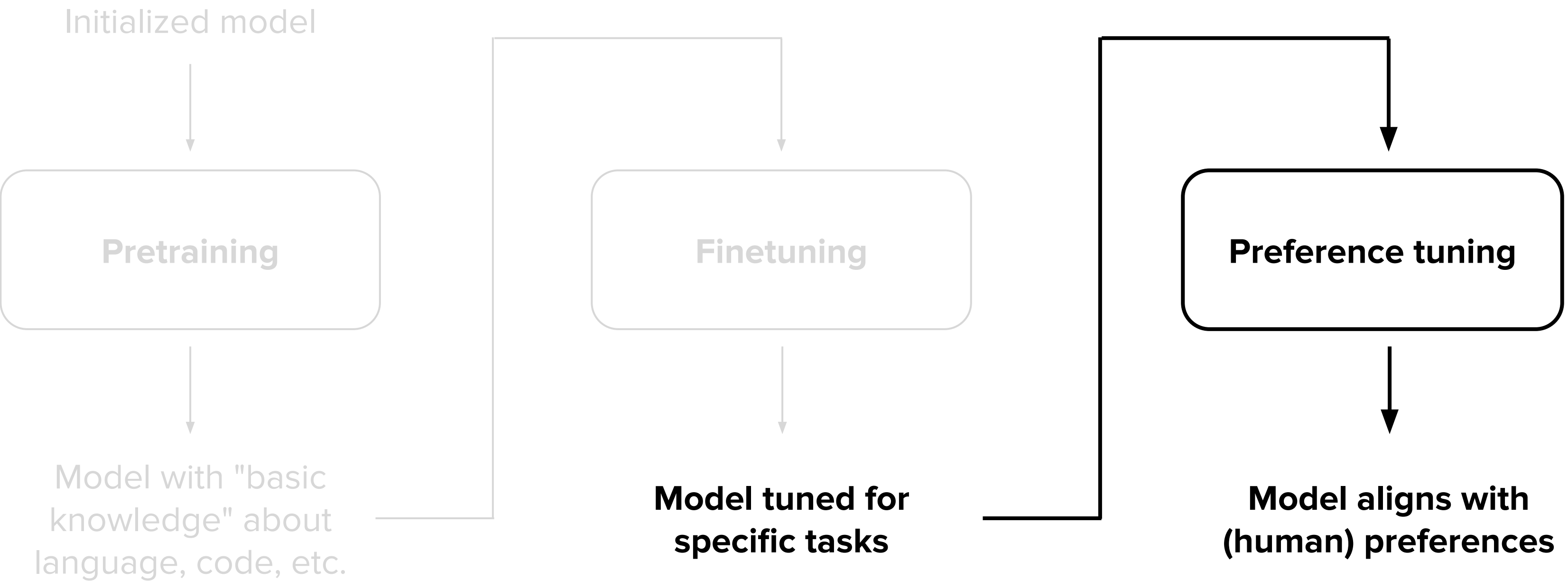


Today's focus



Transformers & Large Language Models

Preference tuning

Data collection

RLHF

DPO

Preference tuning

Context. Model may misbehave. Need to inject negative signals.

```
Suggest a new activity I
could do with my teddy bear.
```

$\longrightarrow$ $\boxed{LLM_{SFT}}$ $\longrightarrow$

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I'd suggest you do not
spend much time with your
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Of course! Teddy bears not only make awesome
companions for a delightful sleep, but can
also be great buddies for fun activities. How
about you both watch a movie together?
```

✓

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Why preference tuning?

- **Easier** to **compare** (e.g. A better than B) than **generate** (e.g. generate A from scratch)

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- **Not scalable**: data quality is very important and hard to get

Why preference tuning?

- **Easier** to **compare** (e.g. A better than B) than **generate** (e.g. generate A from scratch)
- **Distribution** is very important for SFT: easy to "mess up"
- **Not scalable**: data quality is very important and hard to get

However, "model misbehaving" can also be a good wake-up call to check **SFT data quality**

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Preference data

Observation = (prompt x, response $\widehat{y}$)

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Pointwise

Obs 1	0.4
Obs 2	0.9
Obs 3	0.1
Obs 4	0.2

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Pairwise

Obs 1	<	Obs 2
Obs 1	>	Obs 3
Obs 1	>	Obs 4
Obs 2	>	Obs 3

Preference data

Observation = (prompt x, response $\widehat{y}$)

Pointwise		Pairwise			Listwise	
Obs 1	0.4	Obs 1	$<$	Obs 2	Obs 2	1
Obs 2	0.9	Obs 1	$>$	Obs 3	Obs 1	2
Obs 3	0.1	Obs 1	$>$	Obs 4	Obs 4	3
Obs 4	0.2	Obs 2	$>$	Obs 3	Obs 3	4

Preference data

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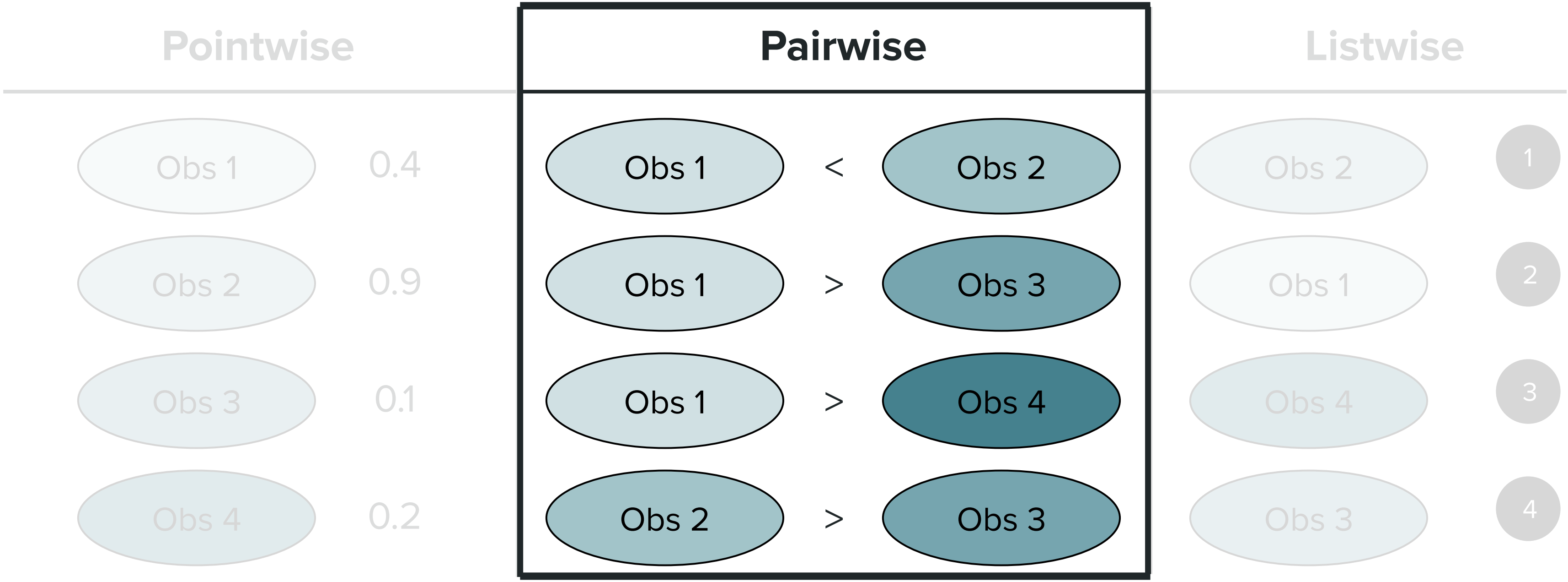

Recipe to get (pairwise) preference data

1. **Generate** pair of responses $(\widehat{y}_1, \widehat{y}_2)$ for the same prompt x
   - Input x via logs / reference distribution
   - Output $\widehat{y}$ via SFT model with $T > 0$ / synthetic / rewrites

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2. **Label** $(x, \widehat{y}_1)$ and $(x, \widehat{y}_2)$
   - Human rating
   - Proxies (e.g. LLM-as-a-judge, BLEU, ROUGE, etc.)
   - Variants: binary scale (better or worse) vs "nuanced" scale

Transformers & Large Language Models

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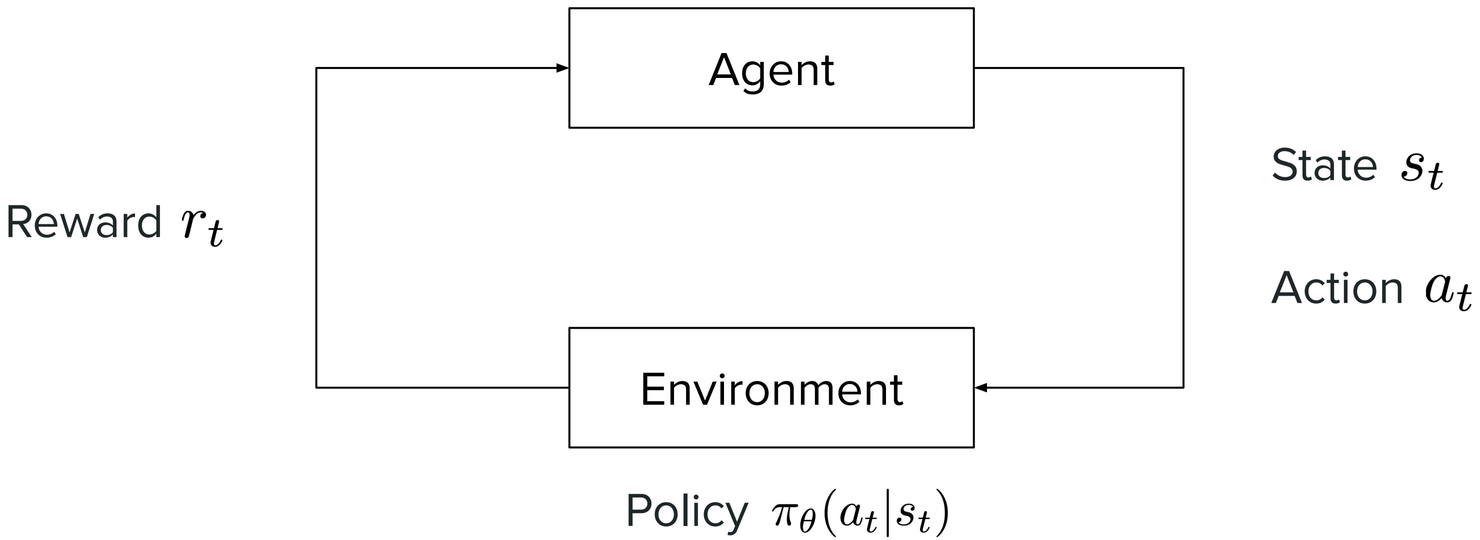
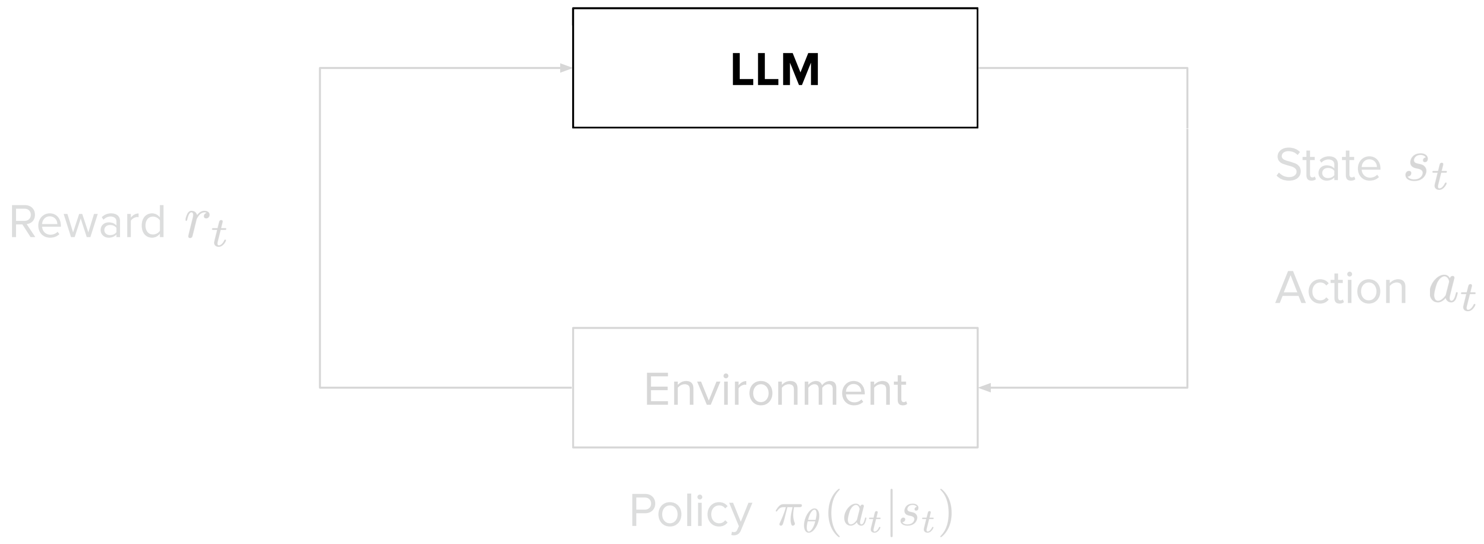
RL formulation



RL formulation for LLMs



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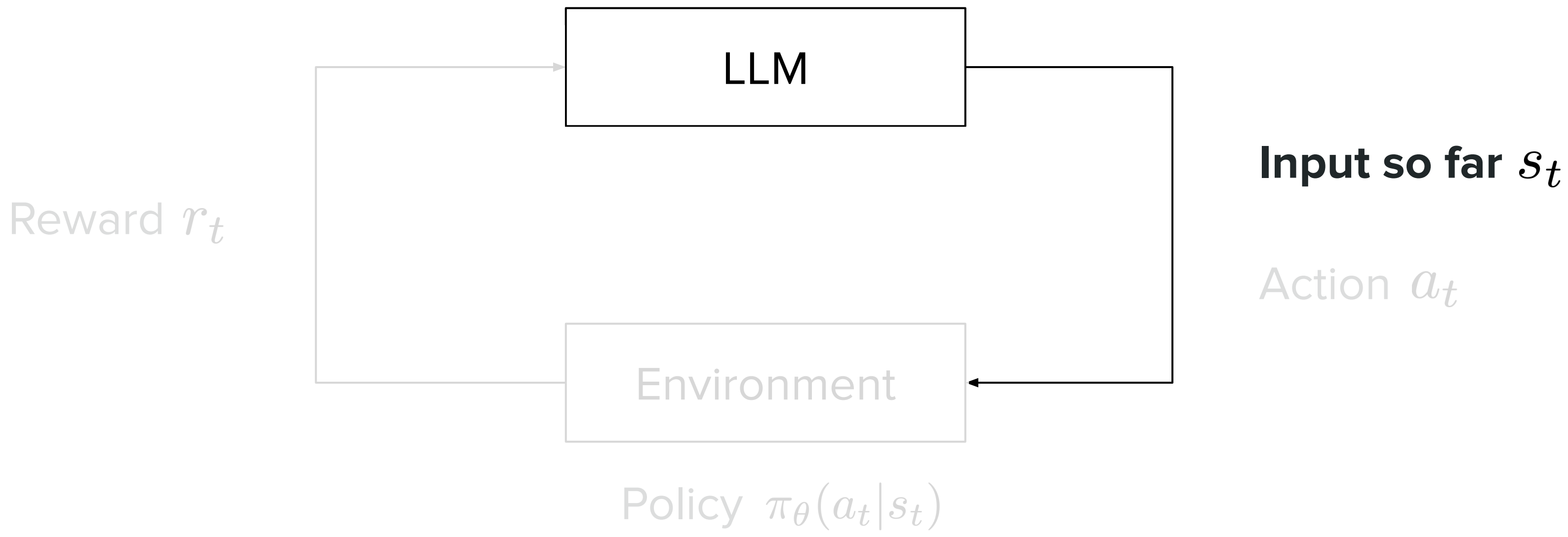

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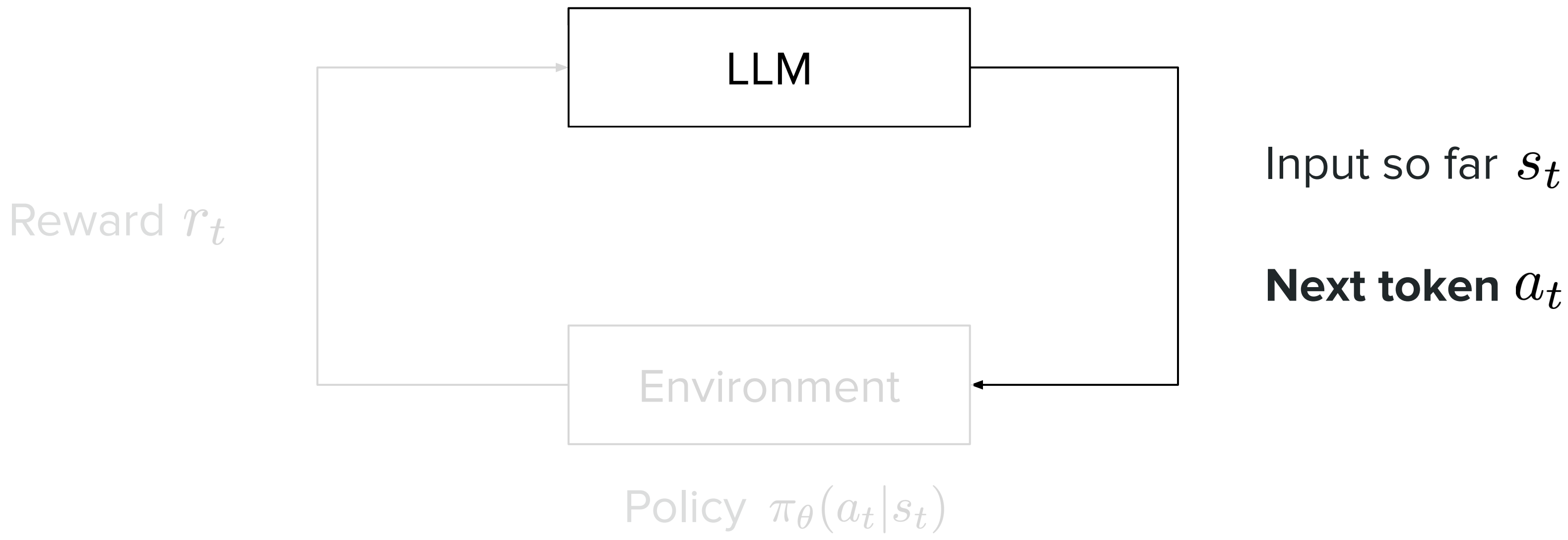

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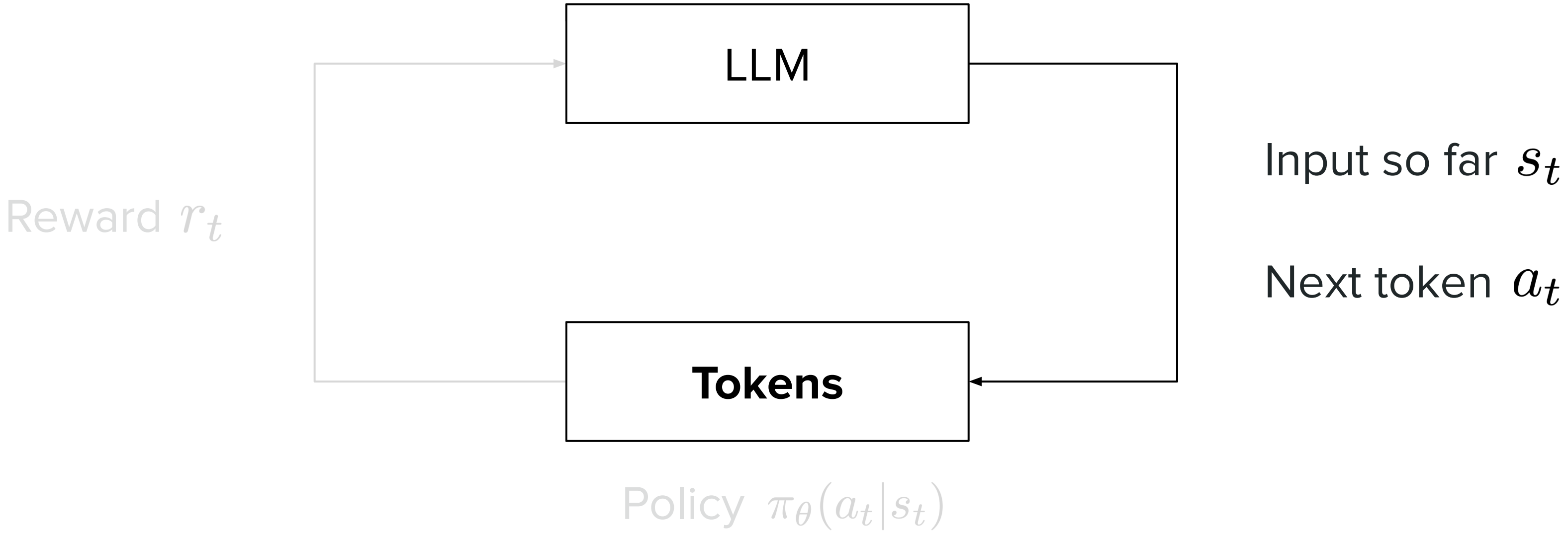

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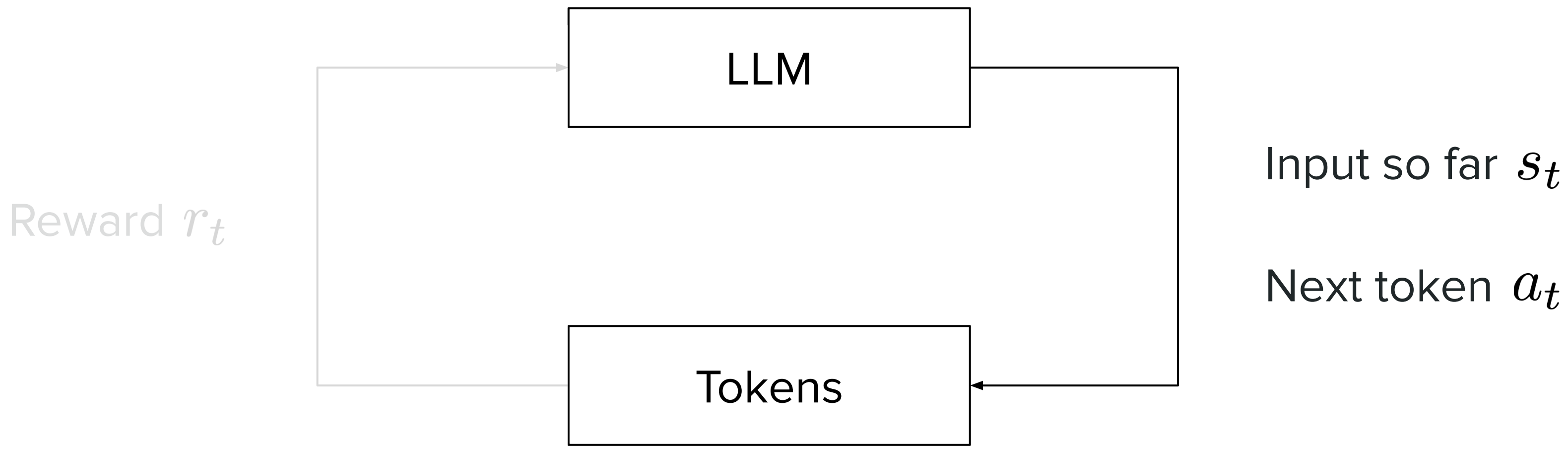
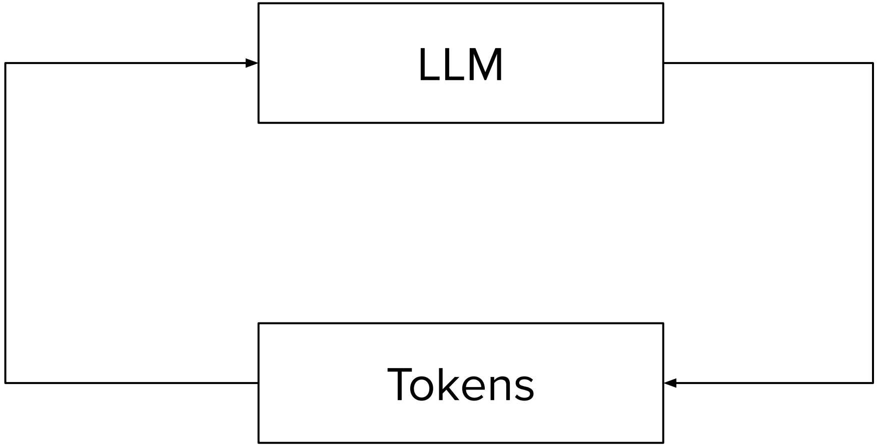


Probability of next token $\pi_\theta(a_t|s_t)$

RL formulation for LLMs



Human preference r_t

Input so far s_t

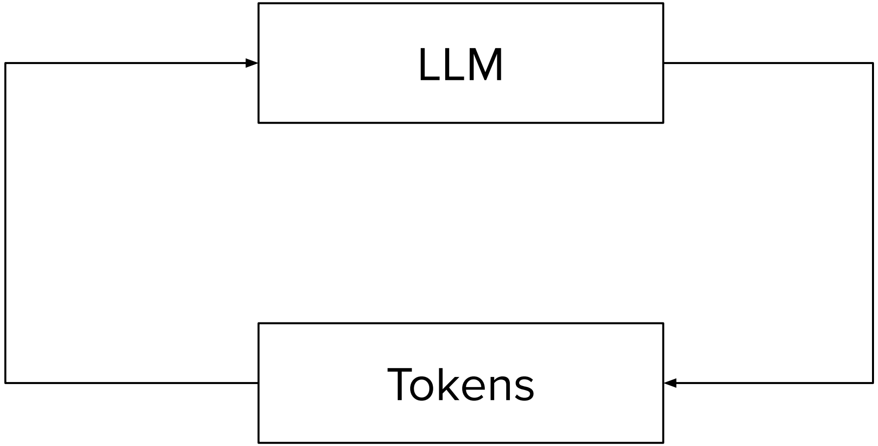
Next token a_t

Probability of next token $\pi_\theta(a_t|s_t)$

RL formulation for LLMs

Idea. Learn θ so that π_θ aligns with human preferences

Human preference r_t



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RLHF overview

RLHF = **R**einforcement **L**earning from **H**uman **F**eedback

"*Training language models to follow instructions with human feedback*", *Ouyang et al., 2022.*

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⚖️ **Step 1 – Reward modeling**: Distinguish good from bad!

- Input: (prompt x, response $\widehat{y}$)
- Output: quantitative score $r(x, \widehat{y})$

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RLHF overview

RLHF = **R**einforcement **L**earning from **H**uman **F**eedback

Step 1 – Reward modeling: Distinguish good from bad!

- Input: (prompt x, response $\widehat{y}$)
- Output: quantitative score $r(x, \widehat{y})$

Step 2 – Reinforcement learning: Align the model!

- Input: prompt x
- Output: response $\widehat{y}$

"*Training language models to follow instructions with human feedback*", *Ouyang et al., 2022.*

Step 1: Reward modeling

Idea. Know which answers are bad and which are good via **Reward Model**.

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`Suggest a new activity I could do with my teddy bear.` prompt

Of course! Teddy bears not only make awesome companions for a delightful sleep, but can also be great buddies for fun activities. How about you both watch a movie together? → RM →

I'd suggest you do not spend much time with your teddy bear at all. → RM →

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Step 1: Reward modeling

Bradley-Terry formulation. Probability that y_i better than y_j is **defined** as:

$$\boxed{p(y_i > y_j) = \frac{e^{r_i}}{e^{r_i} + e^{r_j}} = \sigma(r_i - r_j)}$$

where r_i, r_j rewards of y_i, y_j respectively

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"The rank analysis of incomplete block designs: I. the method of paired comparisons", *Bradley et al., 1952.*

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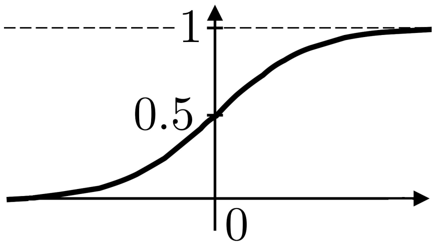

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

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Step 1: Reward modeling

Training. Learn r based on **pairwise** preference data

$$
\begin{tikzcd}
(x, \hat{y}_w) \arrow[r] & \boxed{\mathrm{RM}} \arrow[r] & r(x, \hat{y}_w) \arrow[d, leftrightarrow, "\mathscr{L}"] \\
(x, \hat{y}_l) \arrow[ru] & & r(x, \hat{y}_l)
\end{tikzcd}
$$

Figure from "Super Study Guide: Transformers and Large Language Models", Amidi et al., 2024.

Step 1: Reward modeling

Training. Learn r based on **pairwise** preference data

$$\begin{array}{ccccc} (x,\hat{y}_w) & \longrightarrow & & \longrightarrow & r(x,\hat{y}_w) \\ & & \boxed{\text{RM}} & & \updownarrow \mathscr{L} \\ (x,\hat{y}_l) & \longrightarrow & & \longrightarrow & r(x,\hat{y}_l) \end{array}$$

$$\boxed{\mathscr{L}(\theta) = -\mathbb{E}\Big[\log(\sigma(r(x,\widehat{y}_w) - r(x,\widehat{y}_l)))\Big]}$$

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Step 1: Reward modeling

Data.

- O(10,000) observations
- label = human rating (which is where the "HF" from RLHF comes from)

"*Training language models to follow instructions with human feedback*", *Ouyang et al., 2022.*

Step 1: Reward modeling

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Model.

- Pretrained LLM with classification head (instead of next token prediction)
- Encoder-only: BERT and the like via [CLS] projection

"RewardBench: Evaluating Reward Models for Language Modeling", Lambert et al., 2024.

Step 2: Reinforcement learning

Idea. Change weights of LLM to penalize bad answers and promote good answers via **Reinforcement Learning** using the **Reward Model**.

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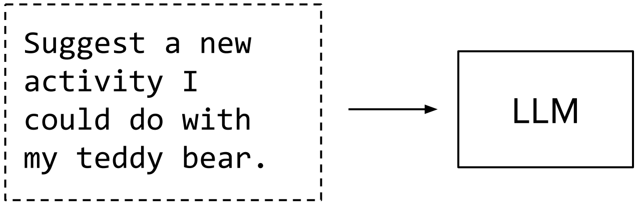

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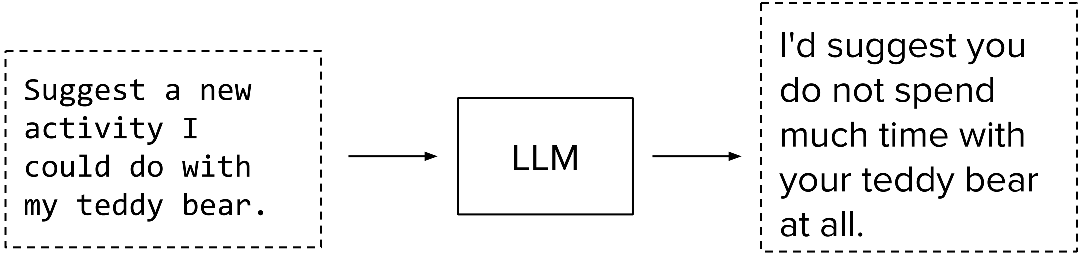

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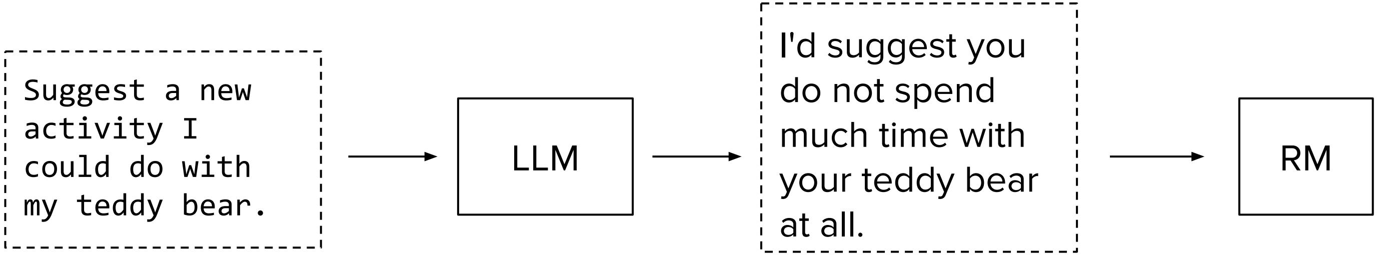

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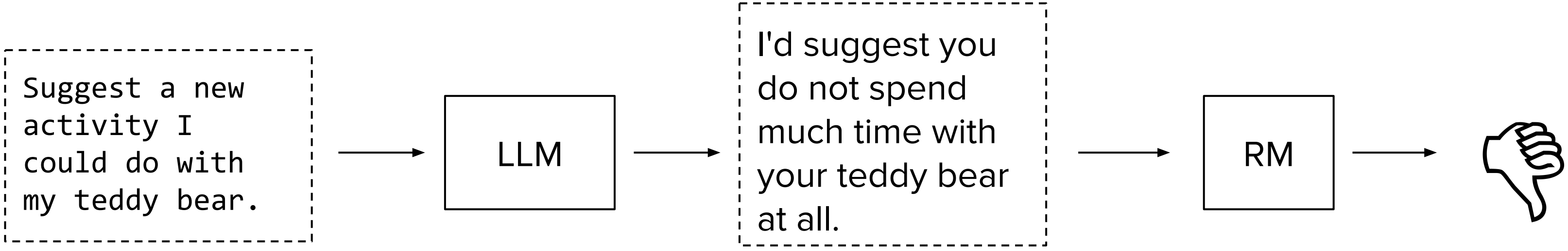

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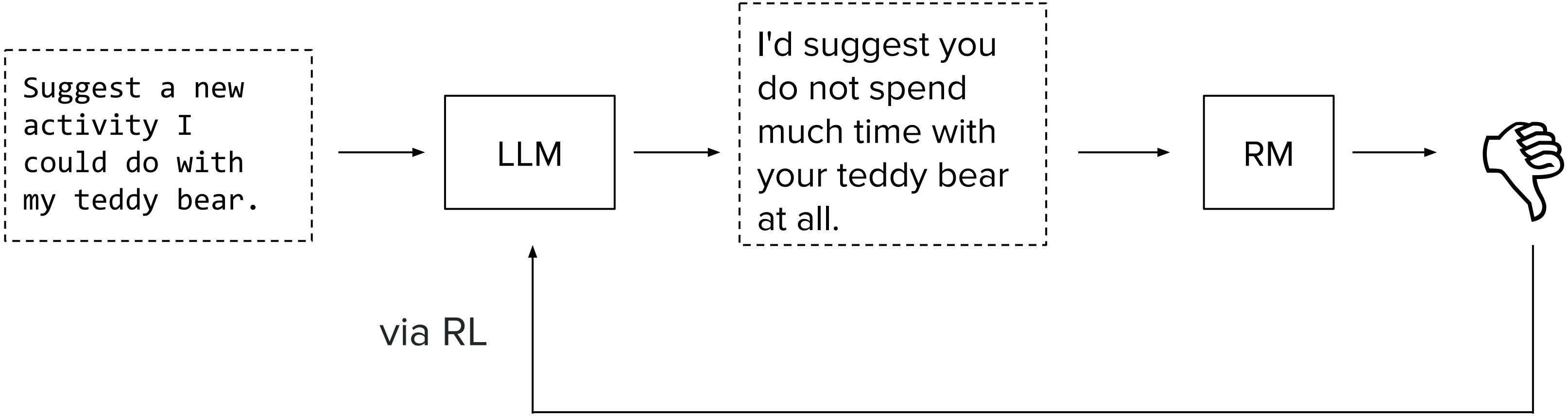

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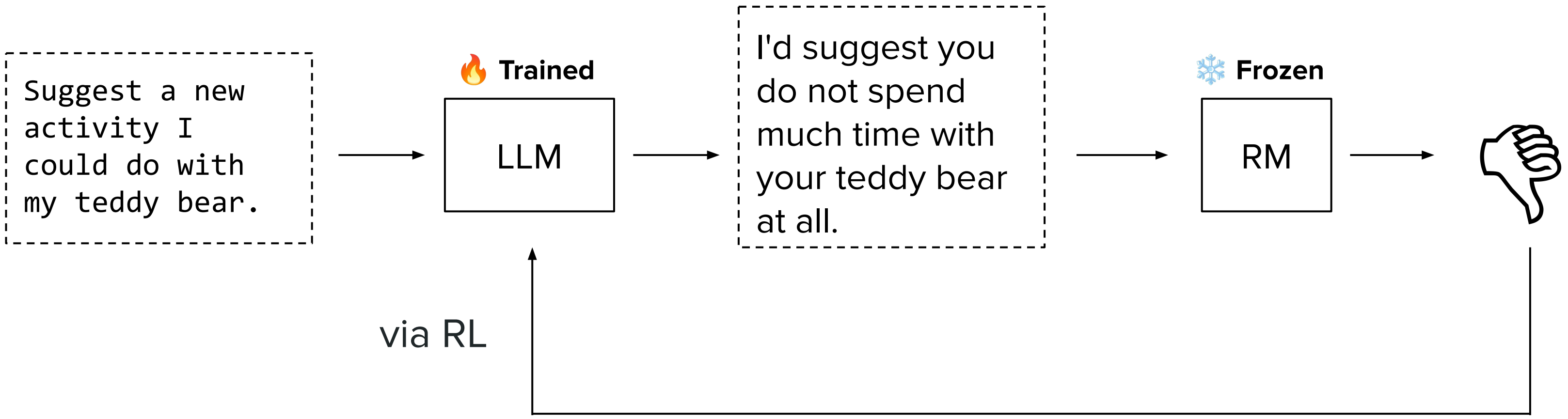

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Objective function optimizes for **higher rewards without going too far** from the **base model**

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- label = score given by reward model

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Model. Initialized at SFT model

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Training. Change weights of policy (LLM) via objective function:

$$\mathscr{L}(\theta) = \boxed{\text{Maximize rewards}} + \boxed{\text{Don't deviate too much from base model}}$$

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Avoid "**reward hacking**" + **training instability**

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Common RL algorithm: PPO

PPO = **P**roximal **P**olicy **O**ptimization

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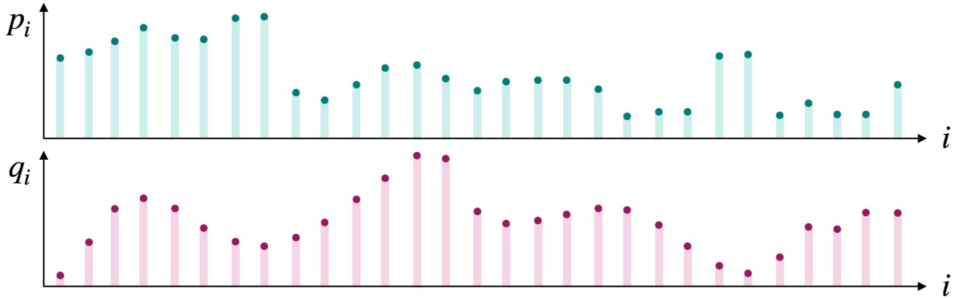

$$\boxed{\mathrm{KL}(P||Q) = \sum_{i=1}^{n} p_i \log\left(\frac{p_i}{q_i}\right)}$$

Figure from "Super Study Guide: Transformers and Large Language Models", Amidi et al., 2024.

PPO actually computes advantages (and not just rewards)

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Advantage ~ Reward - Baseline

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Value function.

- Token-level
- What would be the reward if follow the policy
- Trained jointly with policy
- Label = reward

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Advantage ~ Reward - Baseline ← Value function

Value function.

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GAE method

Suggested reading: "*High-Dimensional Continuous Control Using Generalized Advantage Estimation*", Schulman et al., 2015.

Variation 1: PPO-Clip

Idea. Clip ratio between new and old policy to prevent large updates

$$L^{CLIP}(\theta) = \hat{\mathbb{E}}_t\Big[\min(r_t(\theta)\hat{A}_t, \text{clip}(r_t(\theta), 1-\epsilon, 1+\epsilon)\hat{A}_t)\Big]$$

with $\quad r_t(\theta) = \frac{\pi_\theta(a_t \mid s_t)}{\pi_{\theta_{\text{old}}}(a_t \mid s_t)}$

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Terminology. Confusing since it is an objective function ("**maximize**") and NOT a loss.

"*Proximal Policy Optimization Algorithms*", *Schulman et al., 2017.*

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Terminology. Confusing since rewards noted "r".
Here we are talking about the ratio.

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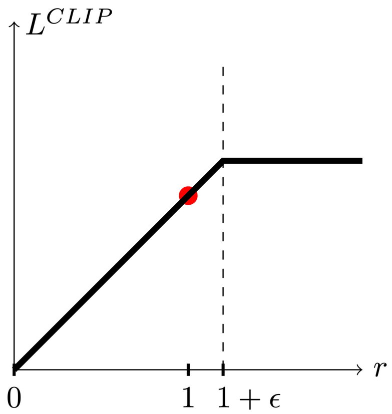
$A > 0$	$A < 0$
	

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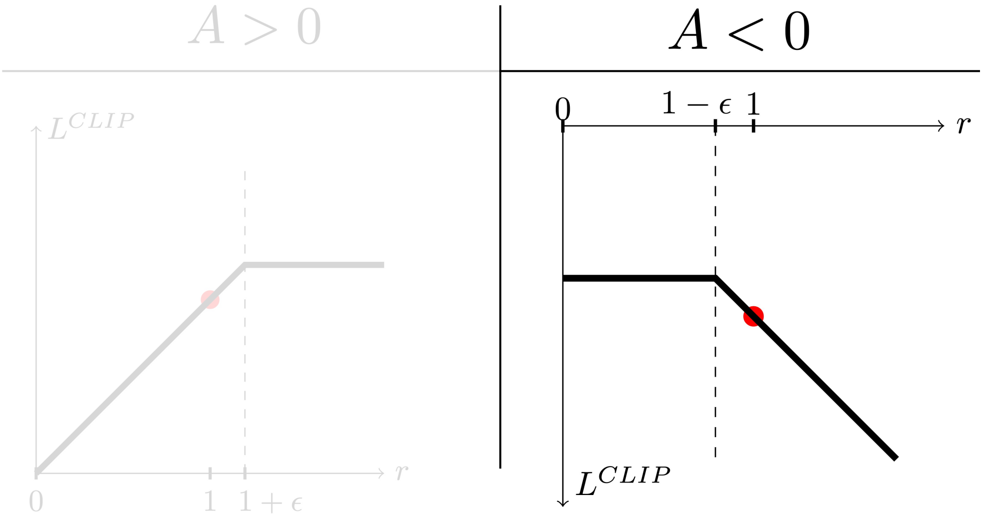

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Variation 2: PPO-KL Penalty

Idea. Penalize difference in policy distributions

$$L^{KLPEN}(\theta) = \hat{\mathbb{E}}_t \left[\frac{\pi_\theta(a_t \mid s_t)}{\pi_{\theta_{\text{old}}}(a_t \mid s_t)} \hat{A}_t - \beta \, \mathrm{KL}[\pi_{\theta_{\text{old}}}(\cdot \mid s_t), \pi_\theta(\cdot \mid s_t)] \right]$$

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Variation 2: PPO-KL Penalty

Idea. Penalize difference in policy distributions

$$L^{KLPEN}(\theta) = \hat{\mathbb{E}}_t\left[\frac{\pi_\theta(a_t \mid s_t)}{\pi_{\boxed{\theta_{\text{old}}}}(a_t \mid s_t)}\hat{A}_t - \beta\,\mathrm{KL}[\pi_{\boxed{\theta_{\text{old}}}}(\cdot \mid s_t), \pi_\theta(\cdot \mid s_t)]\right]$$

"*Proximal Policy Optimization Algorithms*", *Schulman et al., 2017.*

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Terminology.

- old = model from previous RL iteration
- ref = base model

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Nowadays, KL divergence is with respect to **ref** (base model)

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Alternatives of PPO

Limitations of PPO.

- Need 4 models (policy, value, reward model, base)
- Is it worth it?

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Variants.

- REINFORCE
- GRPO
- ... and many more!

"*DeepSeekMath: Pushing the Limits of Mathematical Reasoning in Open Language Models*", *Shao et al., 2024.*

Challenges with RL-based approach

- Requires training a reward model (**2-stage process**)

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Challenges with RL-based approach

- Requires training a reward model (**2-stage process**)
- Many hyperparameters to tune
- Training instability
- Metric to monitor training
- Need diversity in completions!
- Not abundantly clear why preference tuning absolutely needs RL

Workaround if we don't want to do RL

BoN = **B**est **of N**

Workaround if we don't want to do RL

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Idea. Skip the RL step and leverage the reward model scores

Workaround if we don't want to do RL

BoN = **B**est **of N**

Idea. Skip the RL step and leverage the reward model scores

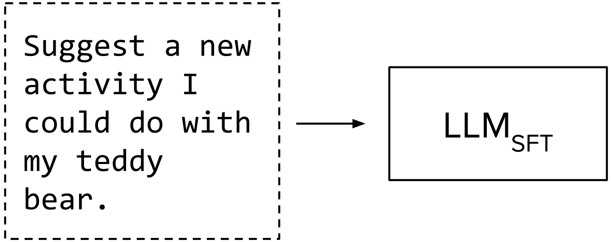
Strategy.

- Given a prompt, generate several outputs with SFT model
- Rank output with score given by reward model
- Take the best one

BoN in action

```
Suggest a new
activity I
could do with
my teddy
bear.
```

BoN in action



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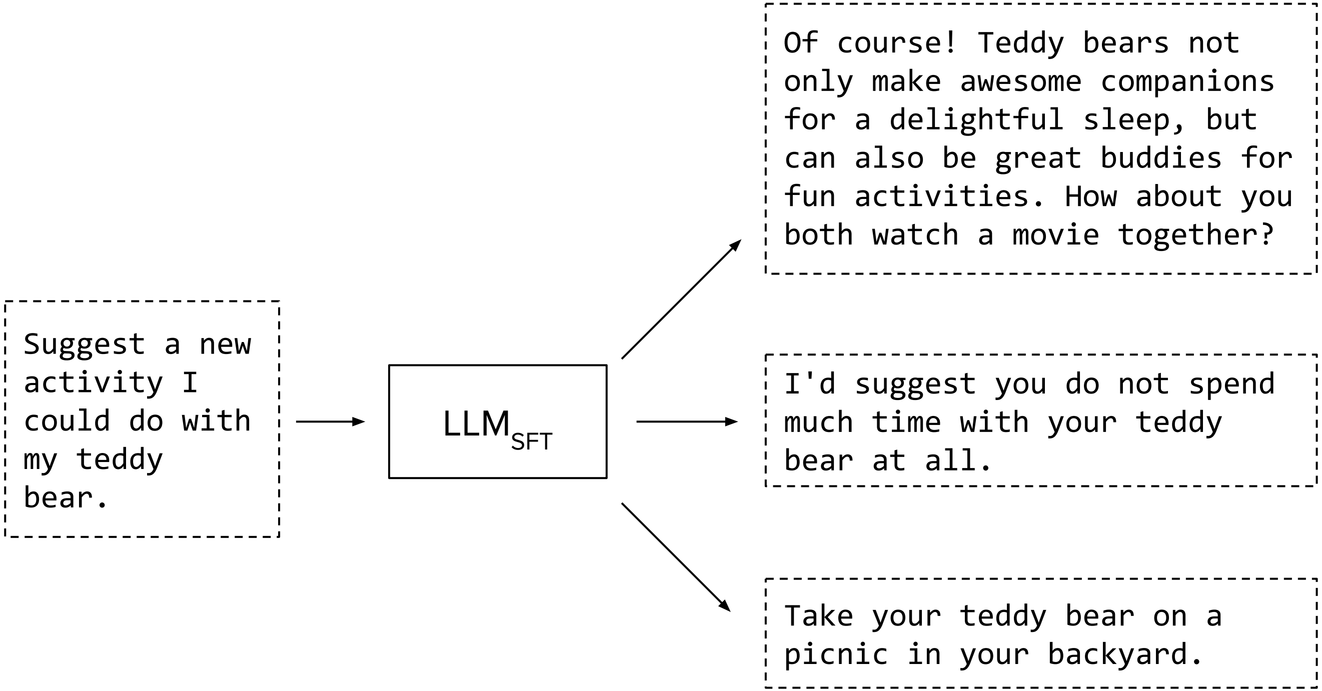

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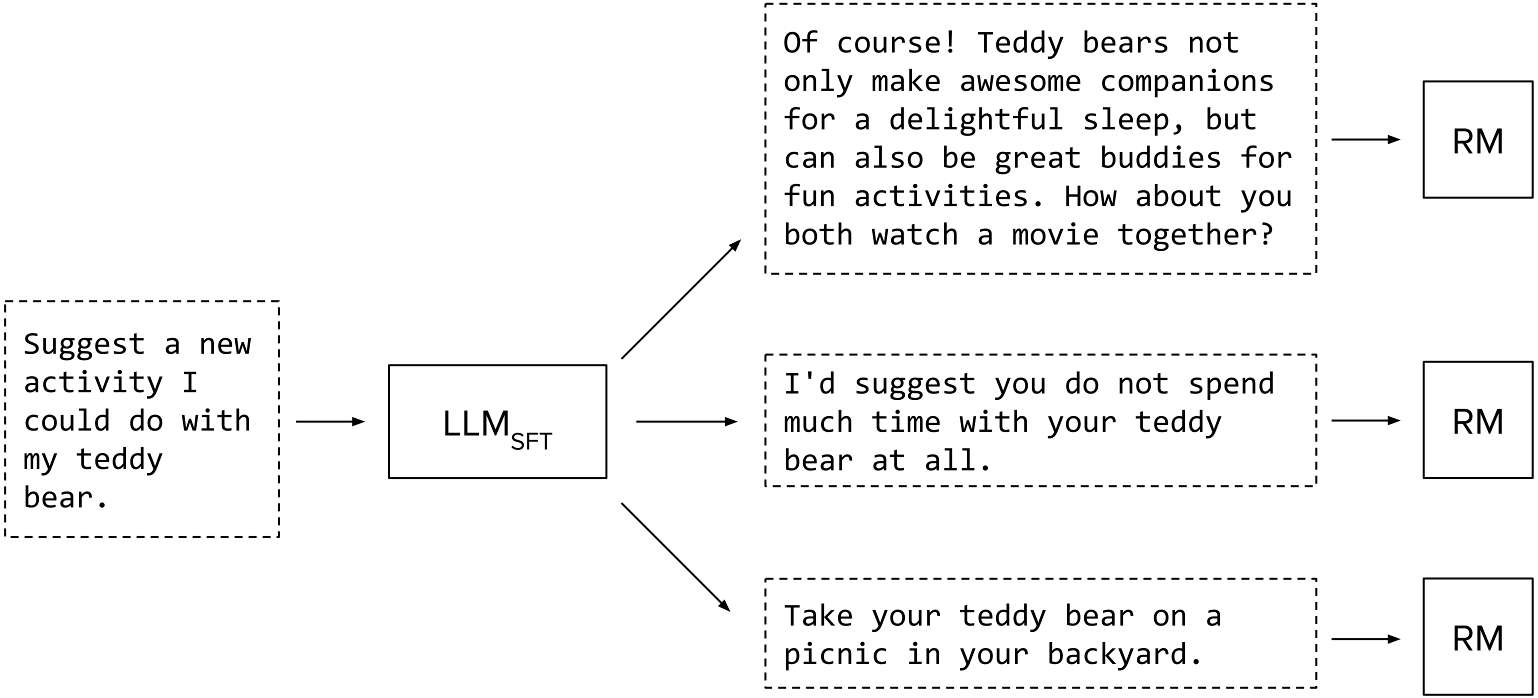

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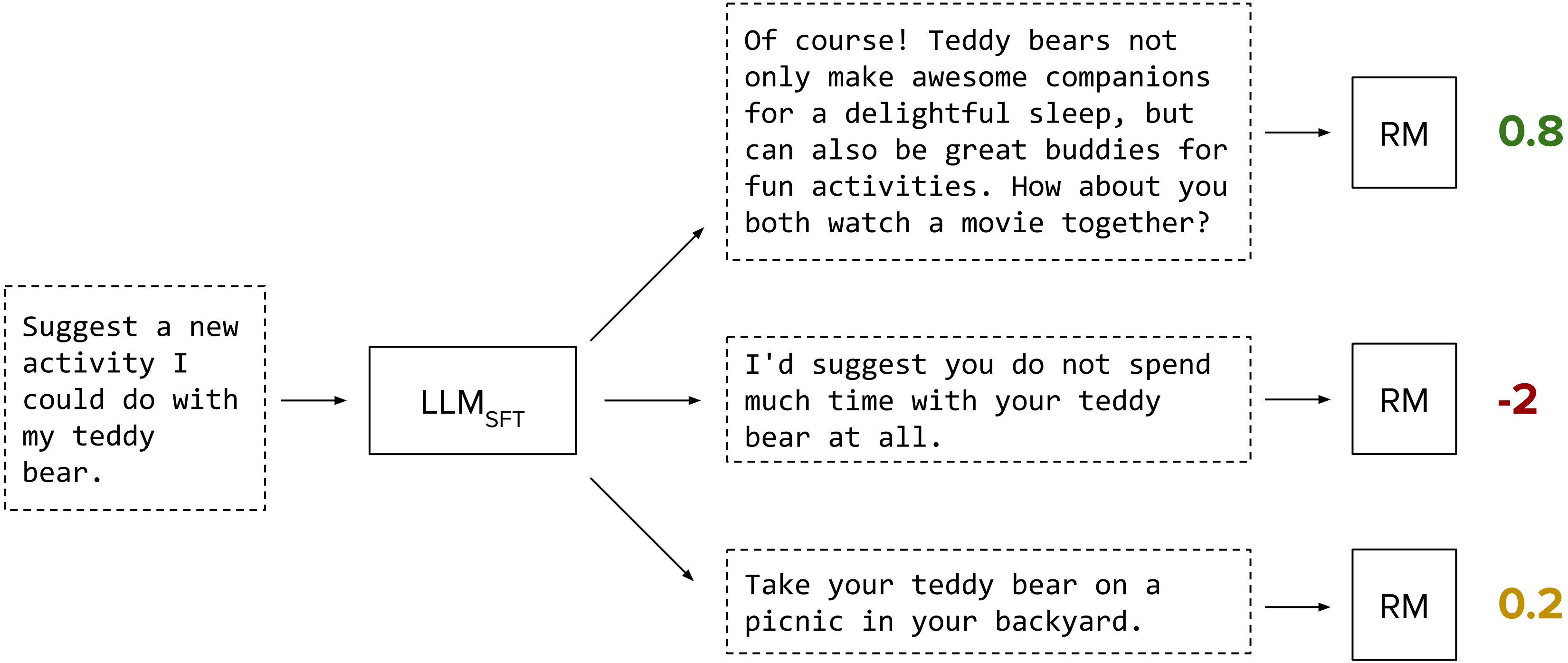

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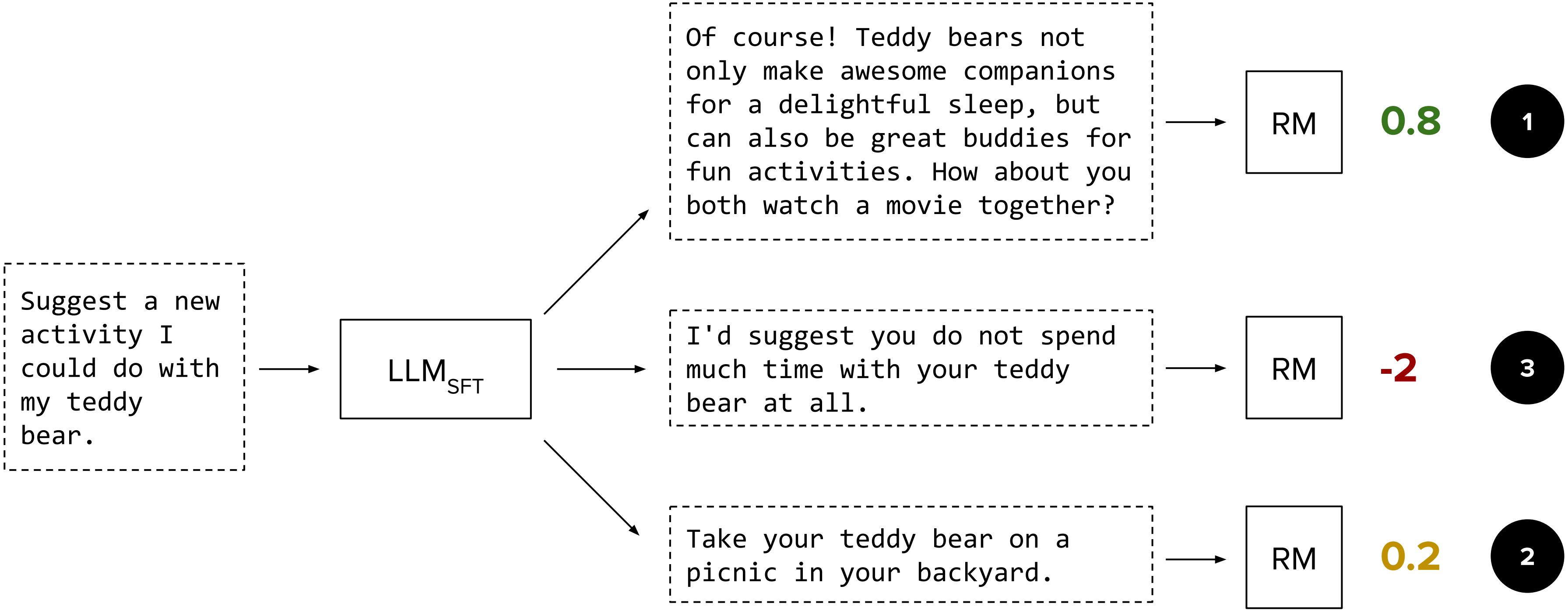

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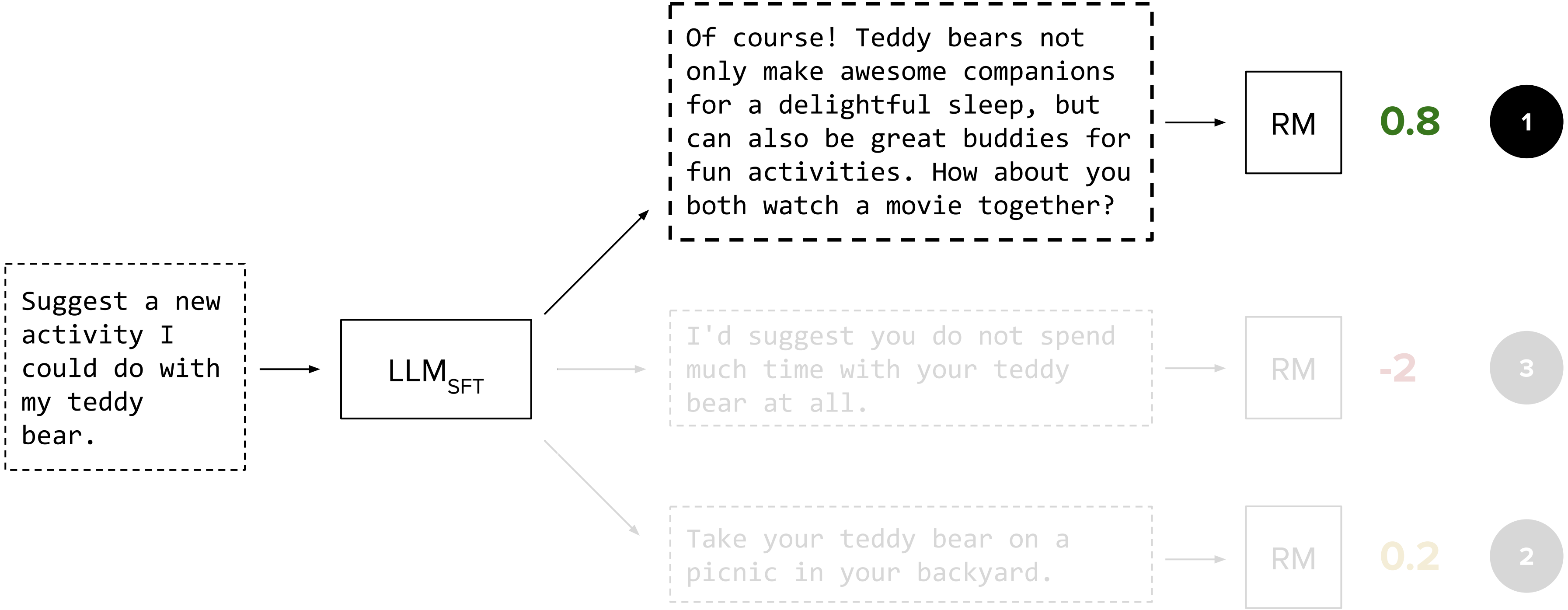

Transformers & Large Language Models

Preference tuning

Data collection

RLHF

DPO

Stanford University

ICME

Motivation

- Limitations using RL

$$L^{KLPEN}(\theta) = \hat{\mathbb{E}}_t\left[\frac{\overset{1}{\boxed{\pi_\theta(a_t \mid s_t)}}}{\underset{2}{\boxed{\pi_{\theta_{\text{old}}}(a_t \mid s_t)}}}\overset{3}{\underset{4}{\boxed{\hat{A}_t}}} - \beta\,\mathrm{KL}[\overset{2}{\boxed{\pi_{\theta_{\text{old}}}(\cdot \mid s_t)}}, \overset{1}{\boxed{\pi_\theta(\cdot \mid s_t)}}]\right]$$

Motivation

- Limitations using RL
- Best-of-N is costly at inference time

Motivation

- Limitations using RL
- Best-of-N is costly at inference time
- **Why don't we train in a supervised fashion?**

Supervised approach with DPO

DPO = **D**irect **P**reference **O**ptimization

Rewrite the **loss function** in a supervised way:

$$\boxed{\mathcal{L}_{\text{DPO}}(\pi_\theta; \pi_{\text{ref}}) = -\mathbb{E}_{(x, y_w, y_l) \sim \mathcal{D}} \left[\log \sigma \left(\beta \log \frac{\pi_\theta(y_w \mid x)}{\pi_{\text{ref}}(y_w \mid x)} - \beta \log \frac{\pi_\theta(y_l \mid x)}{\pi_{\text{ref}}(y_l \mid x)} \right) \right]}$$

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No r(x, y)!

- No need to train a separate reward model

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- No need to train a separate reward model
- Operates directly on preference data

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- No need to train a separate reward model

$$r_\theta(x, y) = \beta \frac{\pi_\theta(y|x)}{\pi_{\text{ref}}(y|x)}$$

- Operates directly on preference data
- Similar to the Bradley-Terry formulation with a special kind of reward!

Supervised approach with DPO

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$$\mathcal{L}_{\text{DPO}}(\pi_\theta; \pi_{\text{ref}}) = -\mathbb{E}_{(x, y_w, y_l) \sim \mathcal{D}} \left[\log \sigma \left(r_\theta(x, y_w) - r_\theta(x, y_l) \right) \right]$$

"*Direct Preference Optimization: Your Language Model is Secretly a Reward Model*", *Rafailov et al., 2023.*

Where does the DPO formulation come from?

1 **Start from PPO objective**

$$\max_{\pi_\theta} \mathbb{E}_{x\sim\mathcal{D}, y\sim\pi_\theta(y|x)}\big[r_\phi(x,y)\big] - \beta\mathbb{D}_{\mathrm{KL}}\big[\pi_\theta(y \mid x) \mid\mid \pi_{\mathrm{ref}}(y \mid x)\big]$$

Where does the DPO formulation come from?

1 Start from PPO objective

2 **Derive optimal policy**

$$\pi^*(y \mid x) = \frac{1}{Z(x)} \pi_{\text{ref}}(y \mid x) \exp\left(\frac{1}{\beta} r^*(x, y)\right)$$

"*Direct Preference Optimization: Your Language Model is Secretly a Reward Model*", *Rafailov et al., 2023.*

Where does the DPO formulation come from?

1 Start from PPO objective

2 Derive optimal policy

3 **Identify a "reward" term**

$$r^*(x, y) = \beta \log \frac{\pi^*(y \mid x)}{\pi_{\text{ref}}(y \mid x)} + \beta \log Z(x)$$

"Direct Preference Optimization: Your Language Model is Secretly a Reward Model", Rafailov et al., 2023.

Where does the DPO formulation come from?

1. Start from PPO objective
2. Derive optimal policy
3. Identify a "reward" term
4. **Write Bradley-Terry formulation for this "reward"**

$$p^*(y_w \succ y_\ell \mid x) = \frac{1}{1 + \exp\left(\beta \log \frac{\pi^*(y_\ell|x)}{\pi_{\text{ref}}(y_\ell|x)} - \beta \log \frac{\pi^*(y_w|x)}{\pi_{\text{ref}}(y_w|x)}\right)}$$

"*Direct Preference Optimization: Your Language Model is Secretly a Reward Model*", *Rafailov et al., 2023.*

Where does the DPO formulation come from?

1. Start from PPO objective
2. Derive optimal policy
3. Identify a "reward" term
4. Write Bradley-Terry formulation for this "reward"
5. **"Infer" DPO loss function**

$$\mathcal{L}_{\text{DPO}}(\pi_\theta; \pi_{\text{ref}}) = -\mathbb{E}_{(x, y_w, y_l) \sim \mathcal{D}} \left[\log \sigma \left(\beta \log \frac{\pi_\theta(y_w \mid x)}{\pi_{\text{ref}}(y_w \mid x)} - \beta \log \frac{\pi_\theta(y_l \mid x)}{\pi_{\text{ref}}(y_l \mid x)} \right) \right]$$

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Use PPO-based RLHF or DPO?

Ease of implementation.

RLHF	DPO
• Multi-stage training • Needs extra models: reward model, value model, base model	• Supervised learning • Base model is the only extra model needed

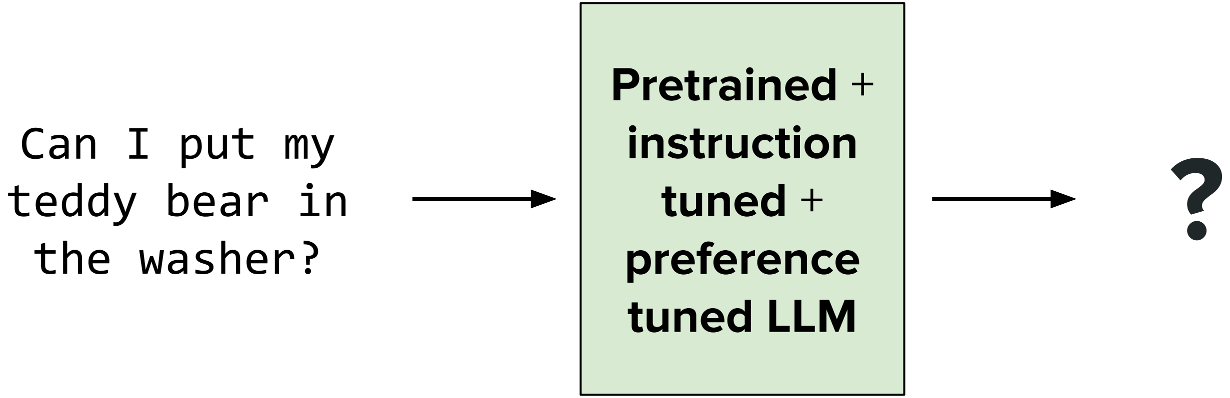
Performance. No common absolute consensus. Varies from task to task and sensitive to implementation.

"Is DPO Superior to PPO for LLM Alignment? A Comprehensive Study", Xu et al., 2024.

Behavior

Can I put my teddy bear in the washer? → **Pretrained** + **instruction tuned LLM** → No, it might get damaged. Try hand washing instead.

Behavior



Can I put my teddy bear in the washer?
Pretrained + instruction tuned + preference tuned LLM
?

Behavior

Can I put my teddy bear in the washer?

→

Pretrained + **instruction tuned** + **preference tuned LLM**

→

It's better not to. Your teddy could get hurt! A gentle hand wash is safer.

Thank you for your attention!