Lecture 5

CME 295: Transformers & Large Language Models

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ICME

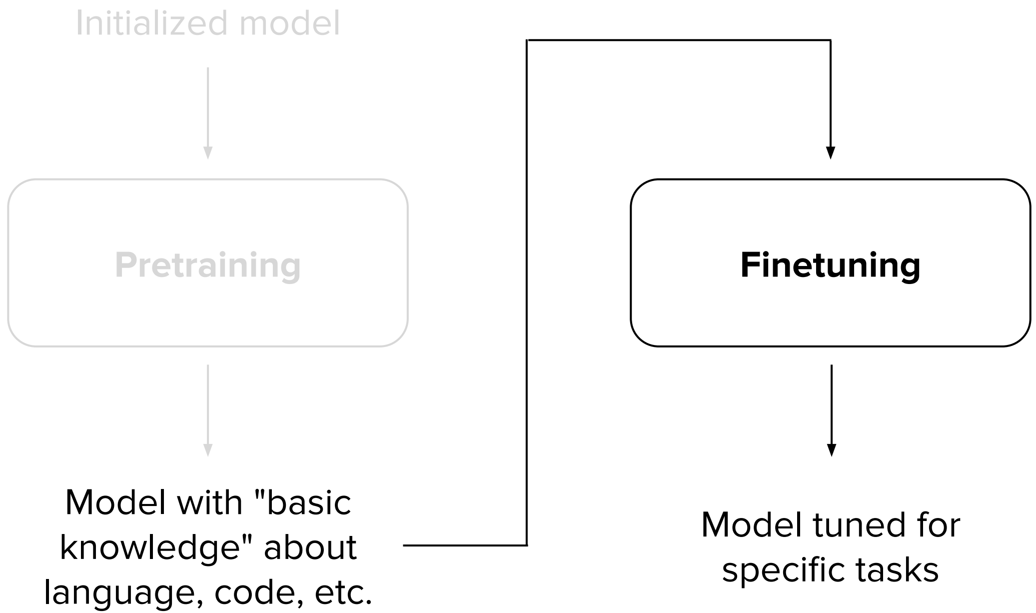
Recap of last episodes...

Initialized model

Pretraining

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

Recap of last episodes...



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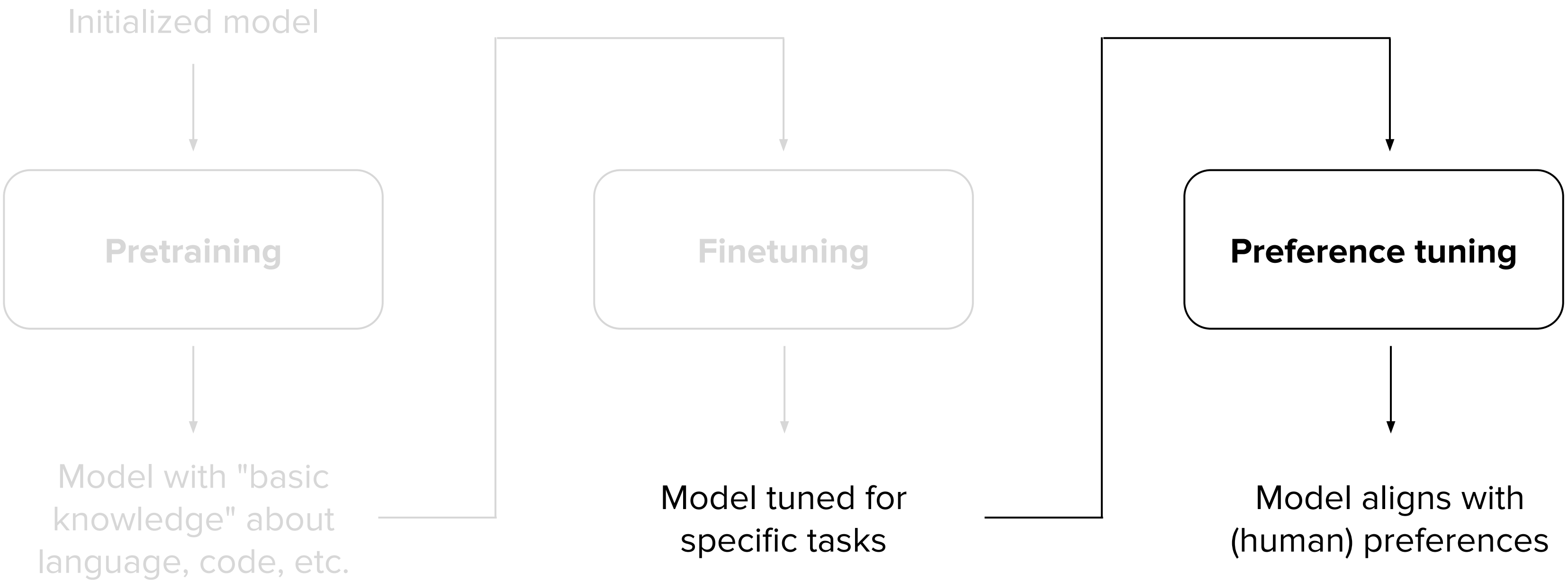
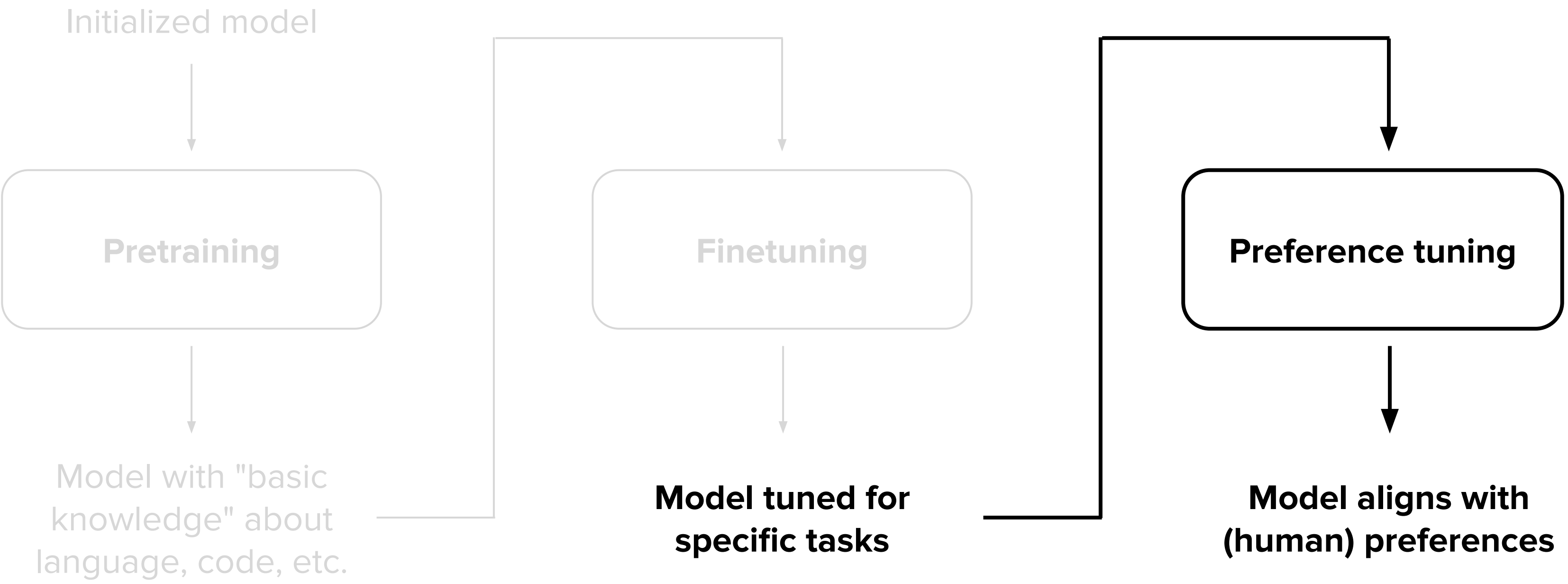


Today's focus



Transformers & Large Language Models

Preference tuning

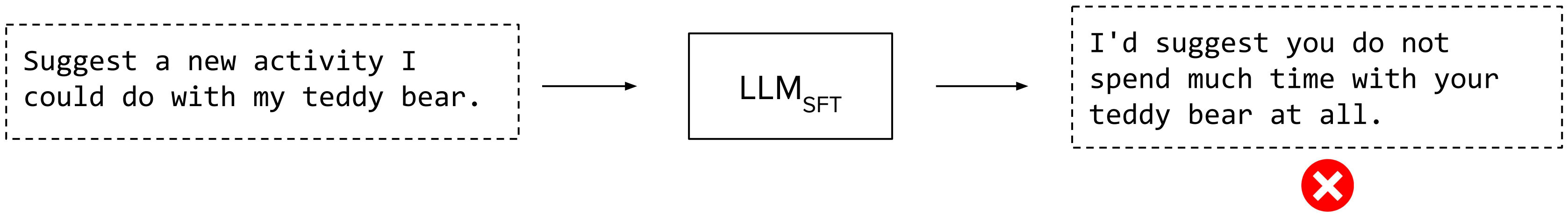
Data collection

RLHF

DPO

Preference tuning

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



Preference tuning

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

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

→ LLM_{SFT} →

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

❌

Idea. Collect preference pairs and train the model on it.

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Preference tuning

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Suggest a new activity I could do with my teddy bear. → LLM_{SFT} → I'd suggest you do not spend much time with your teddy bear at all.

Idea. Collect preference pairs and train the model on it.

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

allows to inject negative signal.
what not to predict

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

task can be similar to what LoRA is
used for but objective function is difl

Transformers & Large Language Models

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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
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Pairwise

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

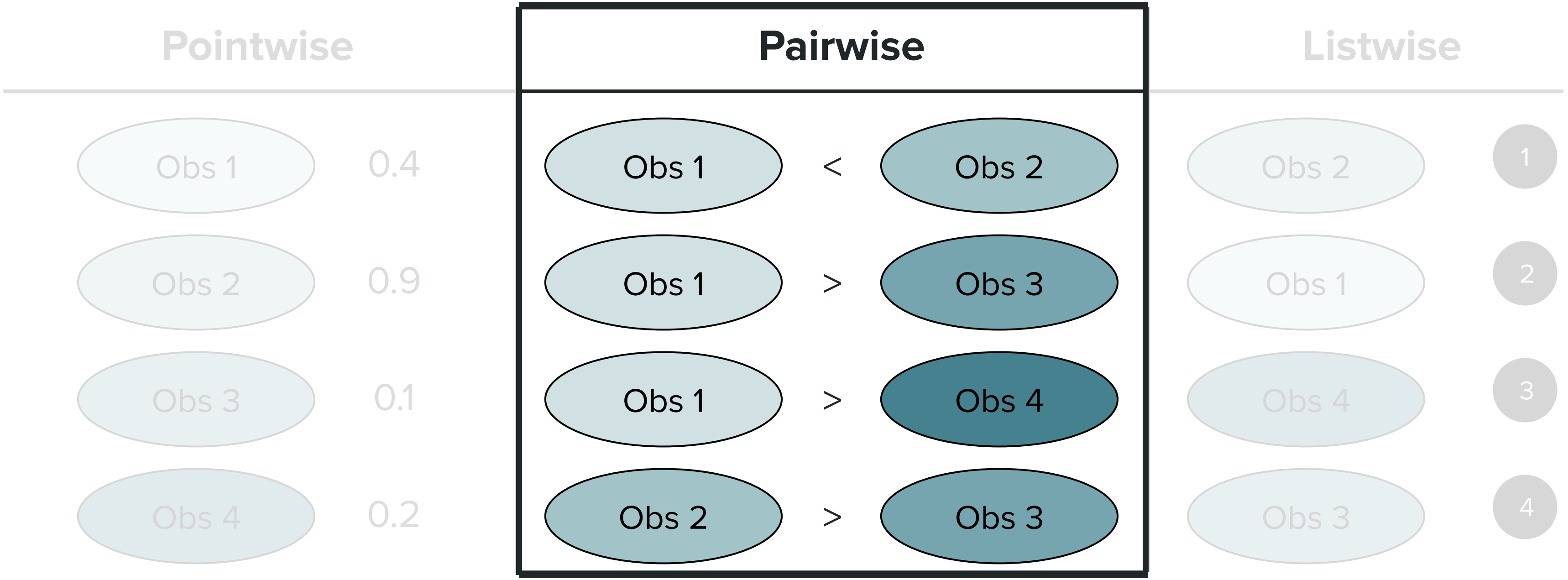
Preference data

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

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



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

     very good good … much worse

Transformers & Large Language Models

Preference tuning

Data collection

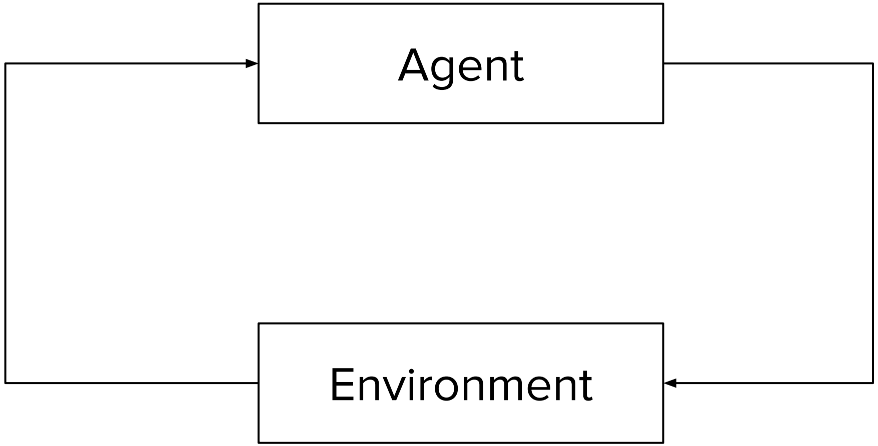
RLHF

RL based

DPO

RL formulation

Reward r_t

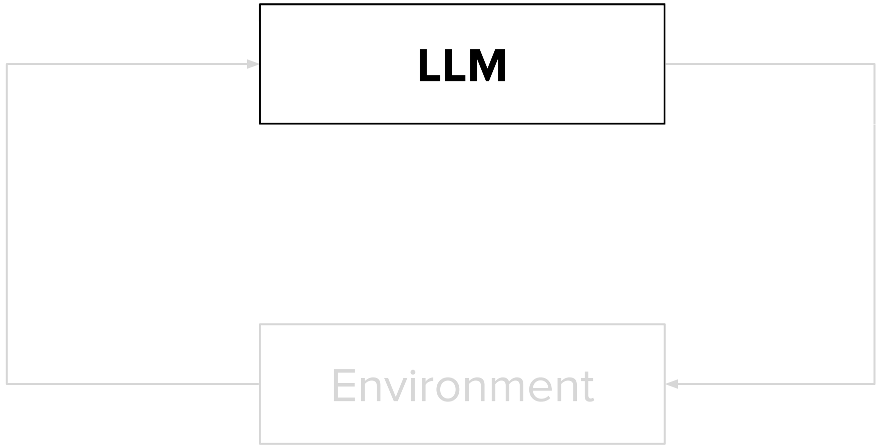


State s_t

Action a_t

Policy $\pi_\theta(a_t|s_t)$

RL formulation for LLMs



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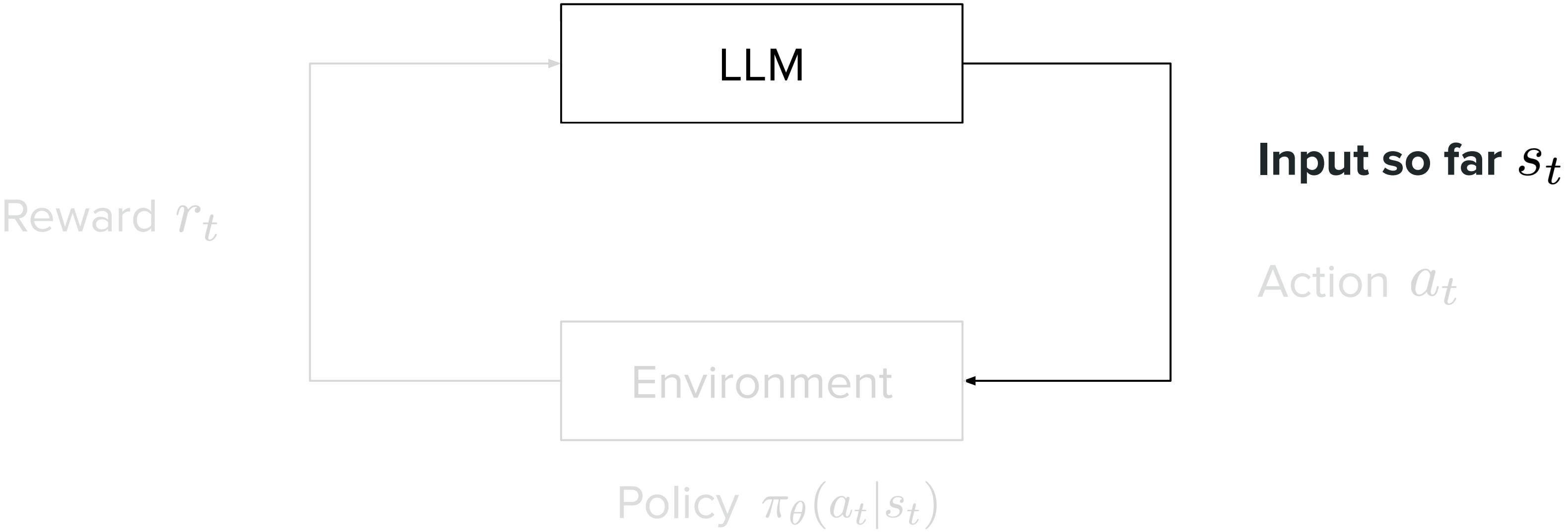

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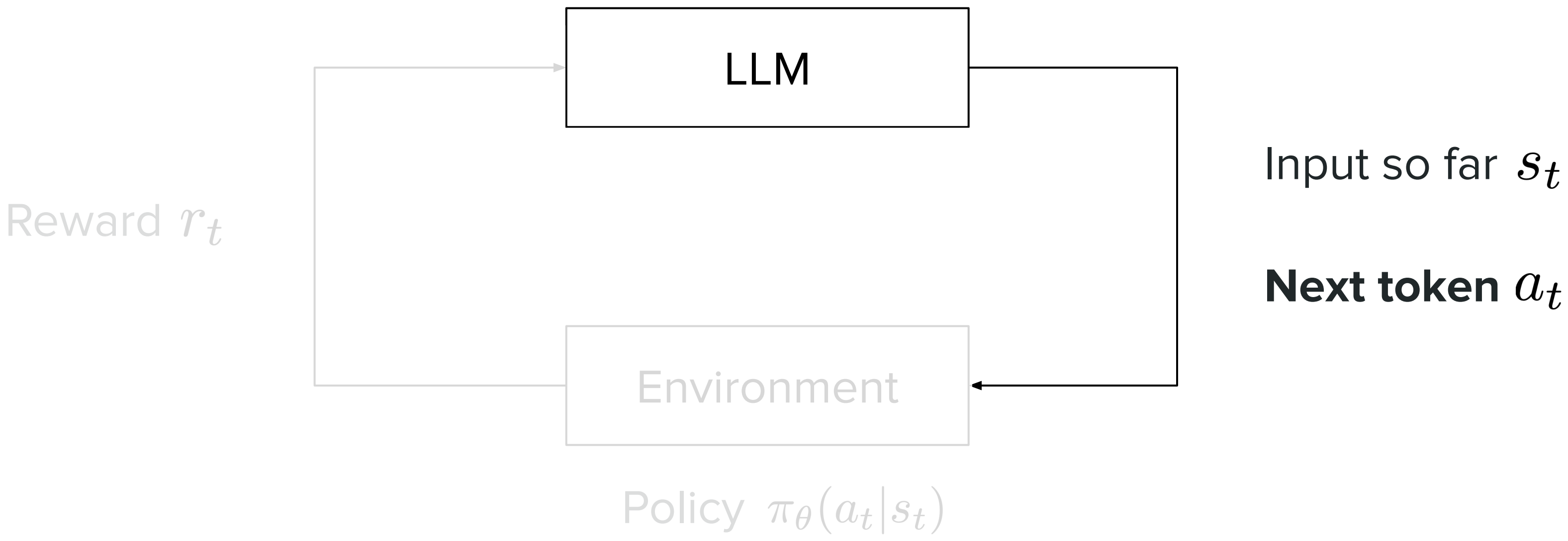

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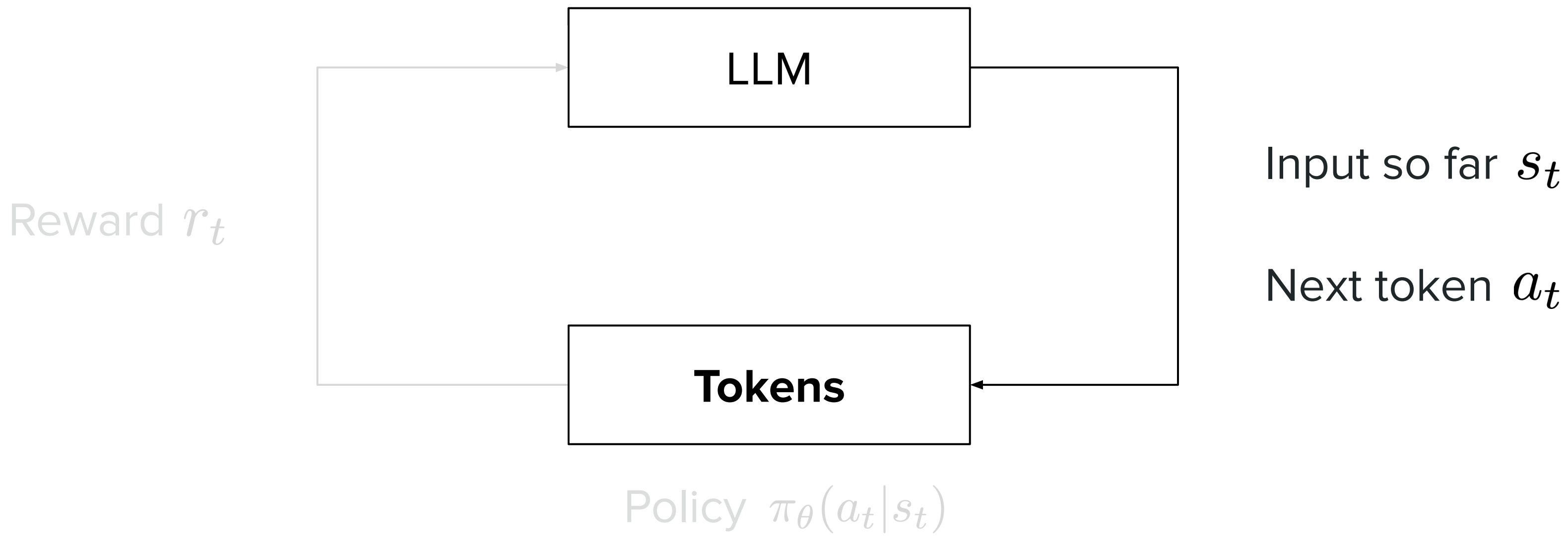

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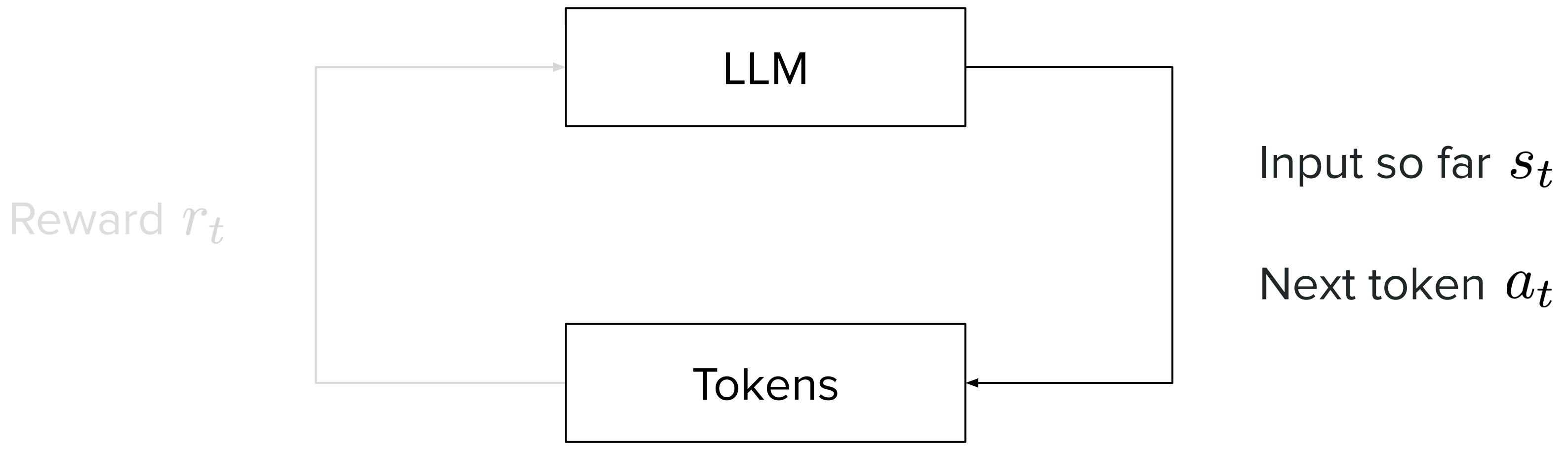
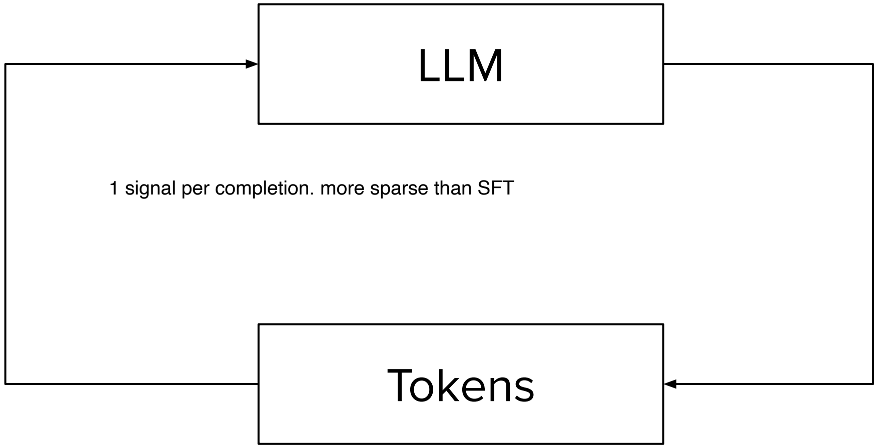


Probability of next token $\pi_\theta(a_t|s_t)$

RL formulation for LLMs

Human preference r_t



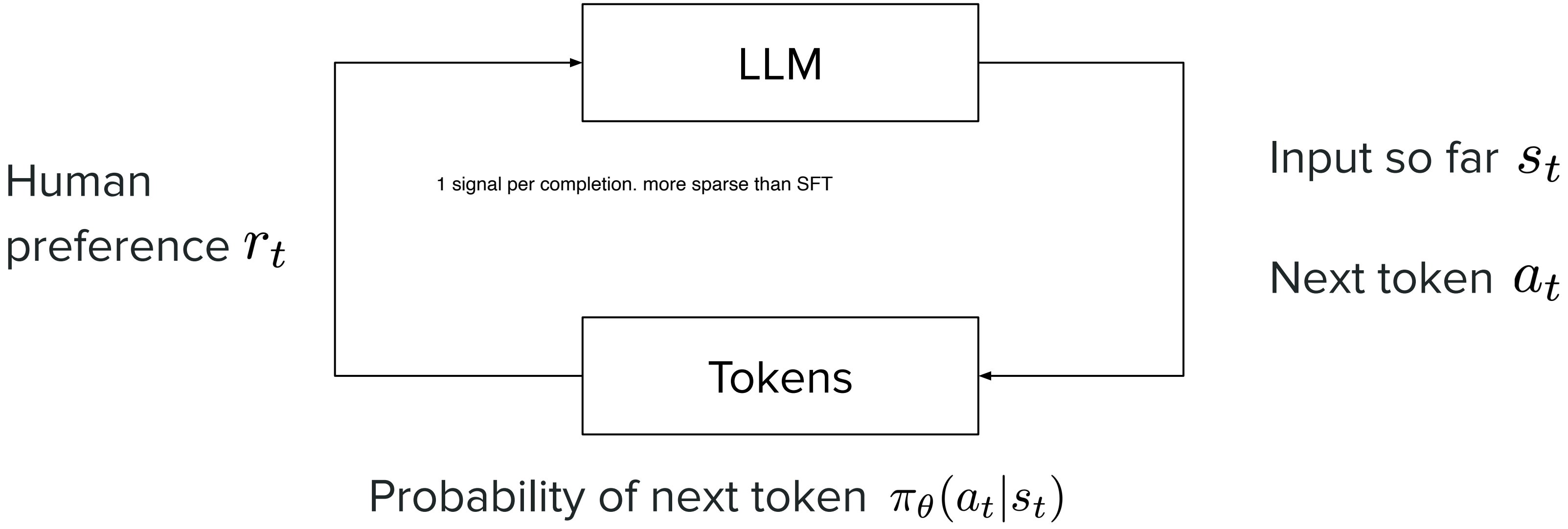
Input so far s_t

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



RLHF overview

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

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

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

"*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 $r(x, \widehat{y})$

⚙️ **Step 2 – Reinforcement learning**: Align the model!

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

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Step 1: Reward modeling

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

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→ RM →

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

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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

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

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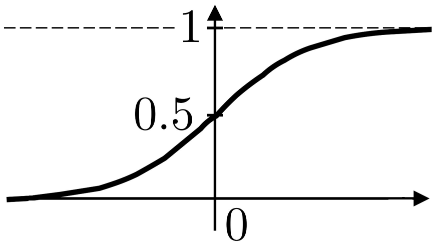

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

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Step 1: Reward modeling

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

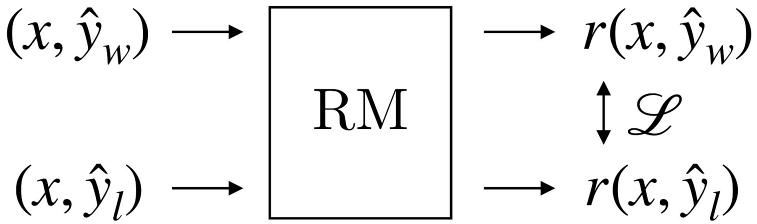

Figure from "Super Study Guide: Transformers and Large Language Models", Amidi et al., 2024.

Step 1: Reward modeling

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

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

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

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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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LLM

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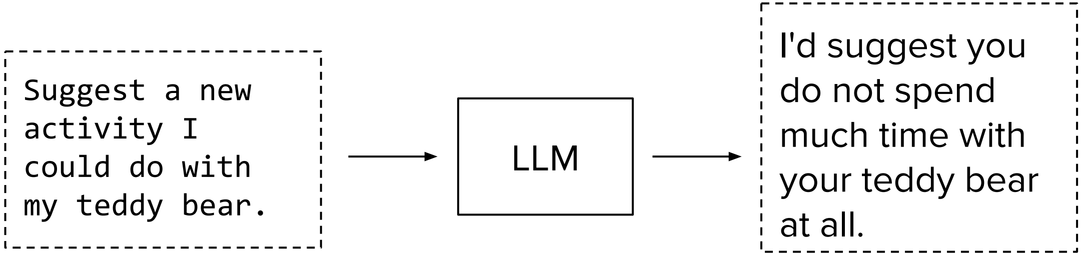

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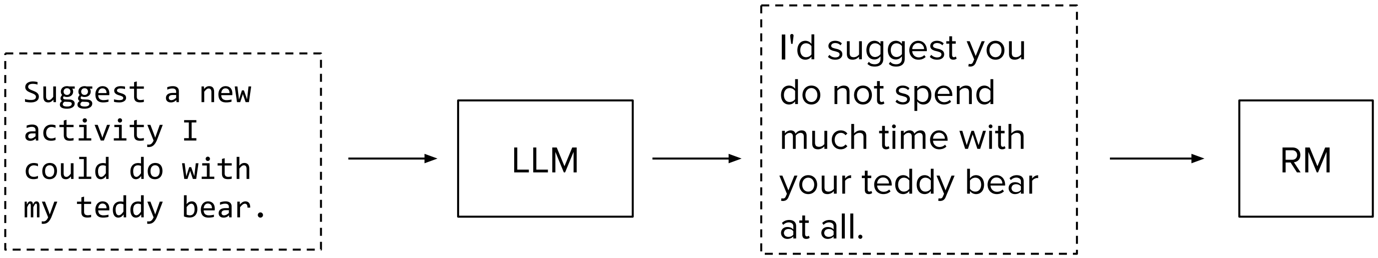

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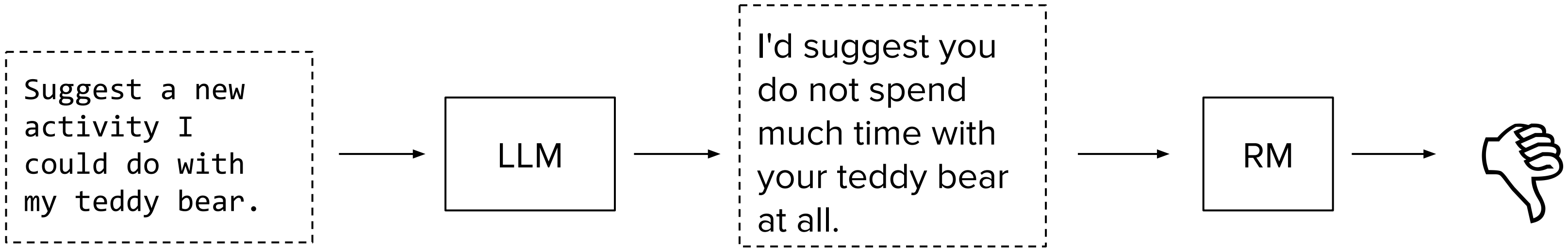

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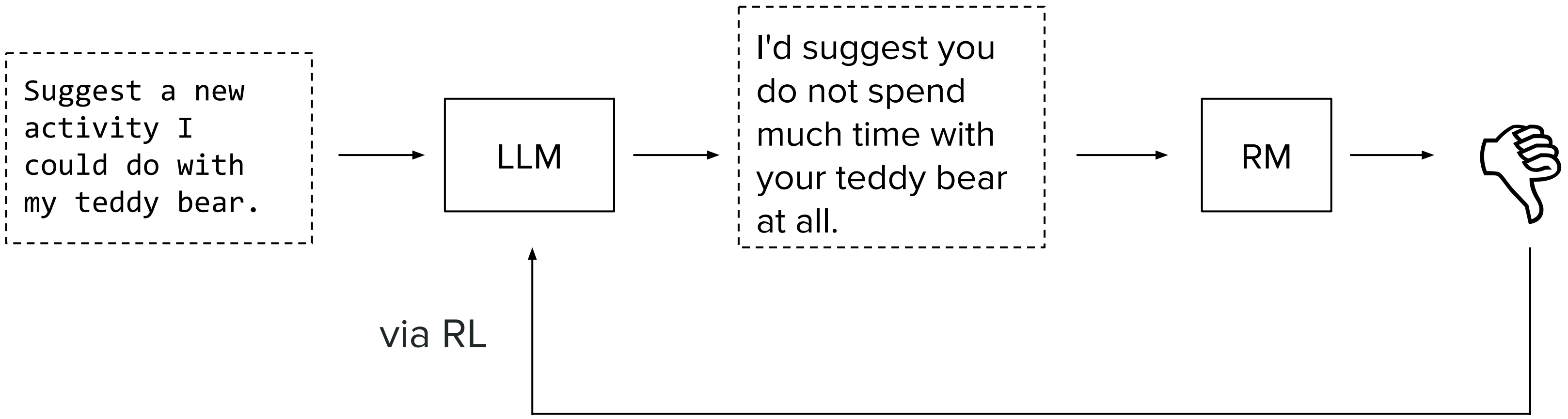

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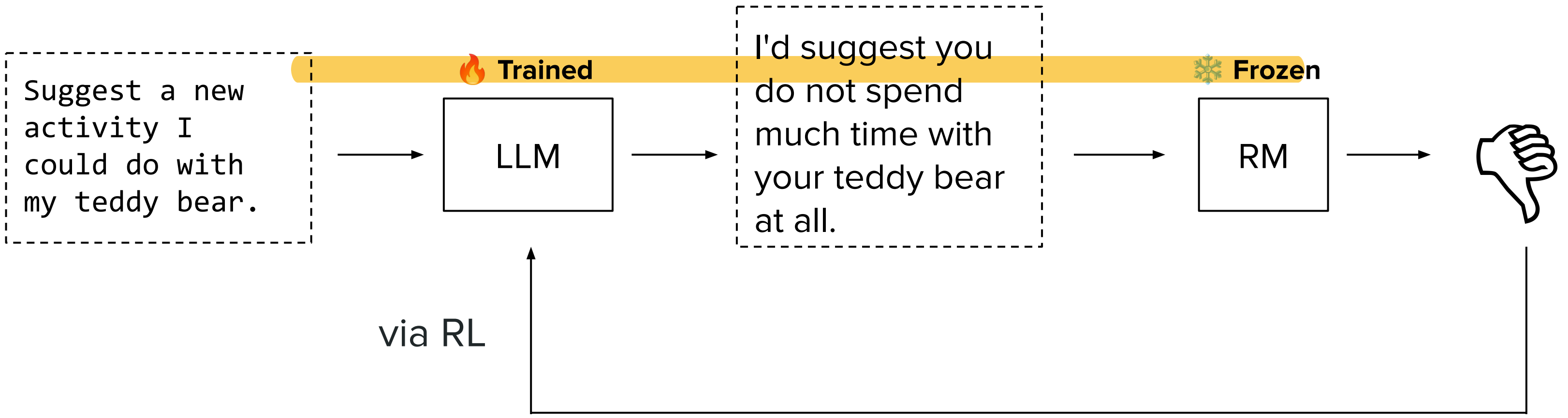

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Step 2: Reinforcement learning

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

base model is good
reward model is imperfect
training instabilities etc.

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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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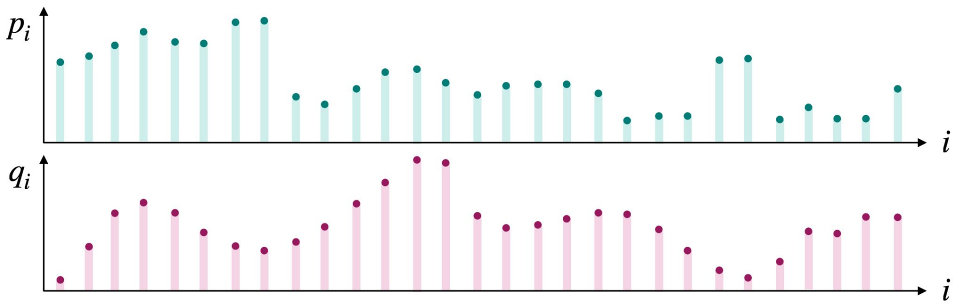

$$\mathrm{KL}(P||Q) = \sum_{i=1}^{n} p_i \log\left(\frac{p_i}{q_i}\right)$$

jensen inequality gives KL div is >= 0

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

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Value function.

- Token-level
- What would be the reward if follow the policy
- Trained jointly with policy
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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 $r_t(\theta) = \dfrac{\pi_\theta(a_t \mid s_t)}{\pi_{\theta_{\text{old}}}(a_t \mid s_t)}$

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

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not have updates too wide

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

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

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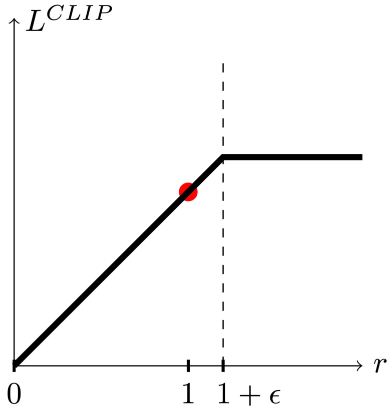
$A > 0$	$A < 0$
	

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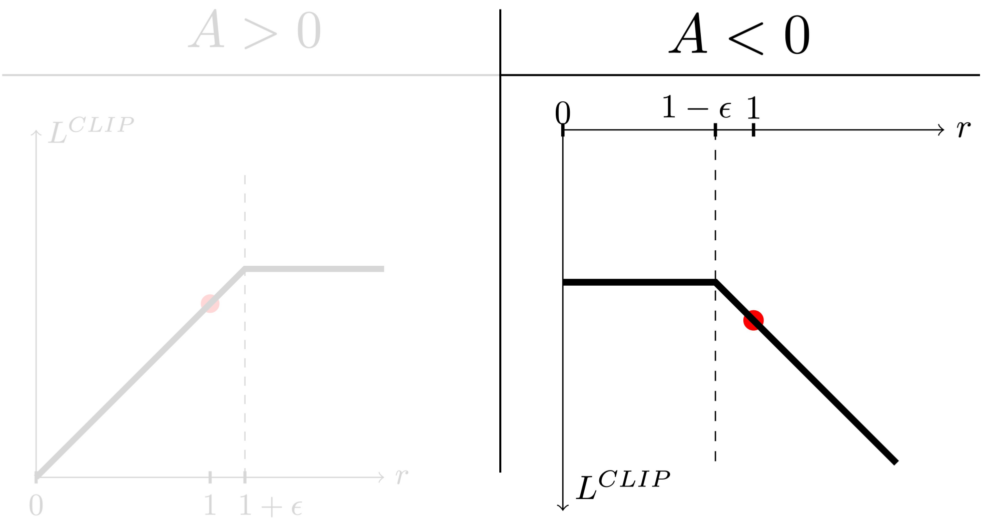

with $\quad r_t(\theta) = \dfrac{\pi_\theta(a_t \mid s_t)}{\pi_{\theta_{\text{old}}}(a_t \mid s_t)}$

previous it

clip to not make too
big of an update

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Variation 2: PPO-KL Penalty

Idea. Penalize difference in policy distributions

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

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

Variation 2: PPO-KL Penalty

Idea. Penalize difference in policy distributions

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

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Terminology.

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

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

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

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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used in resoning
model

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
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- 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 = Best **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

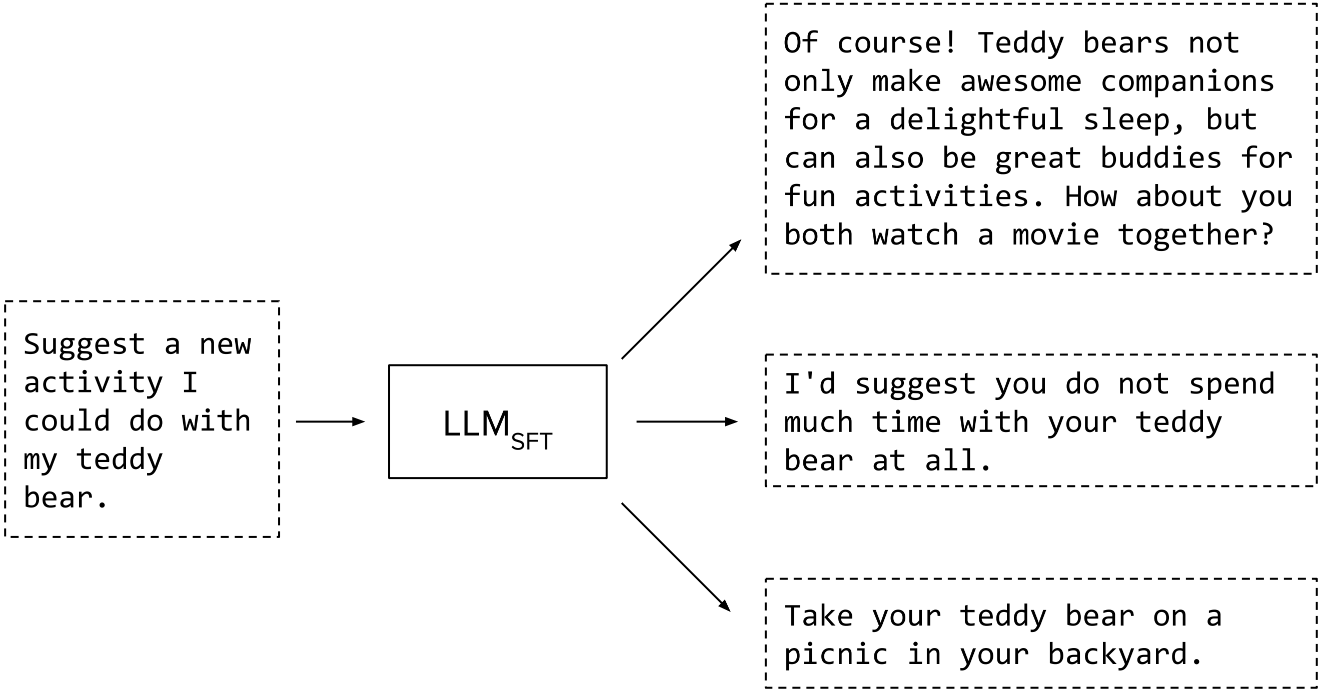
```
Suggest a new
activity I
could do with
my teddy
bear.
```

BoN in action

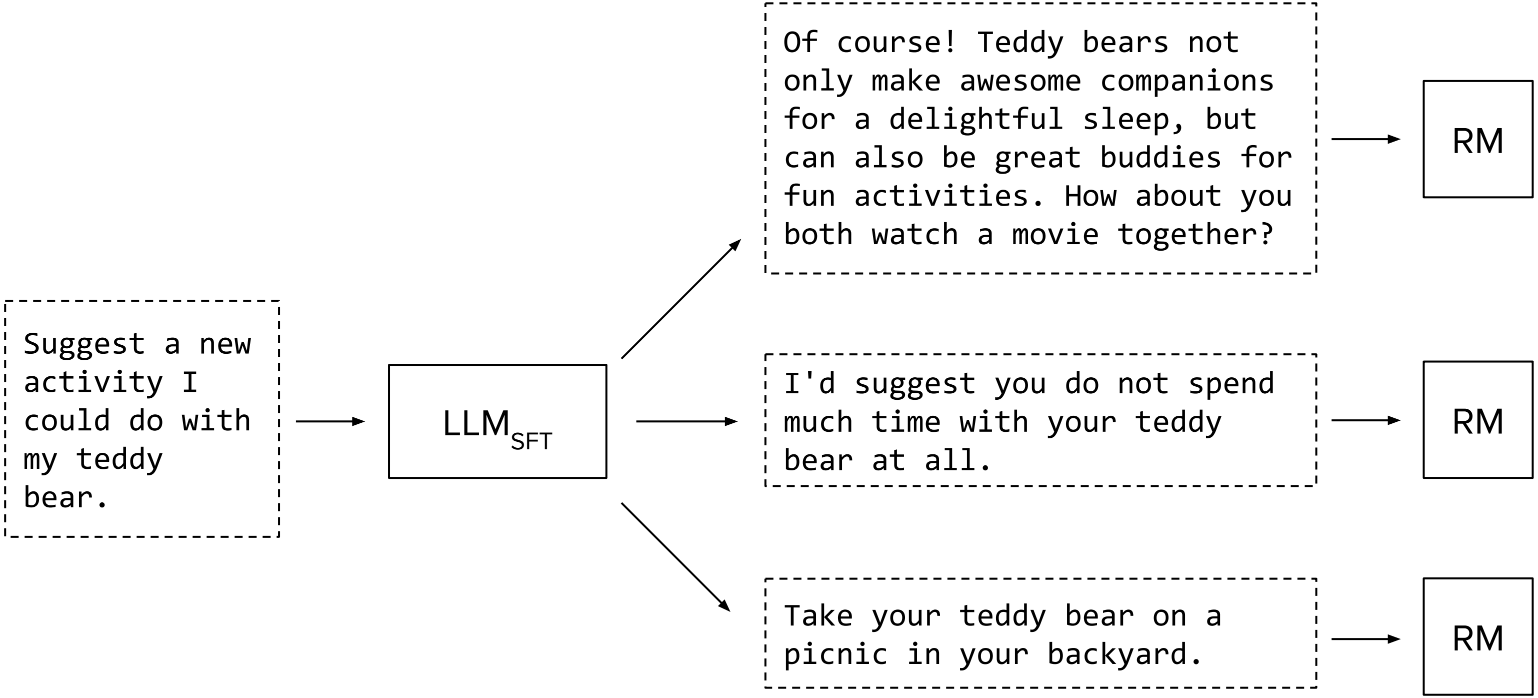
Suggest a new activity I could do with my teddy bear.

LLM_{SFT}

BoN in action



BoN in action



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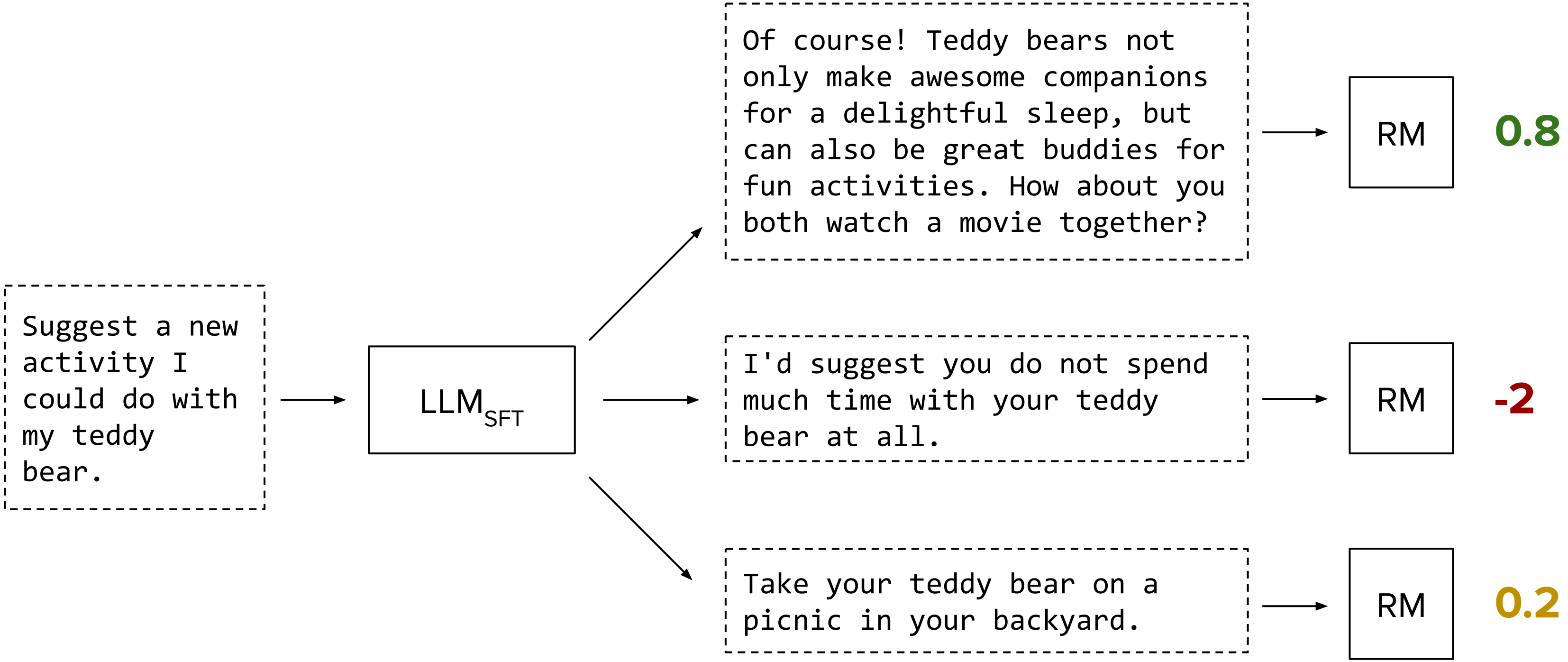

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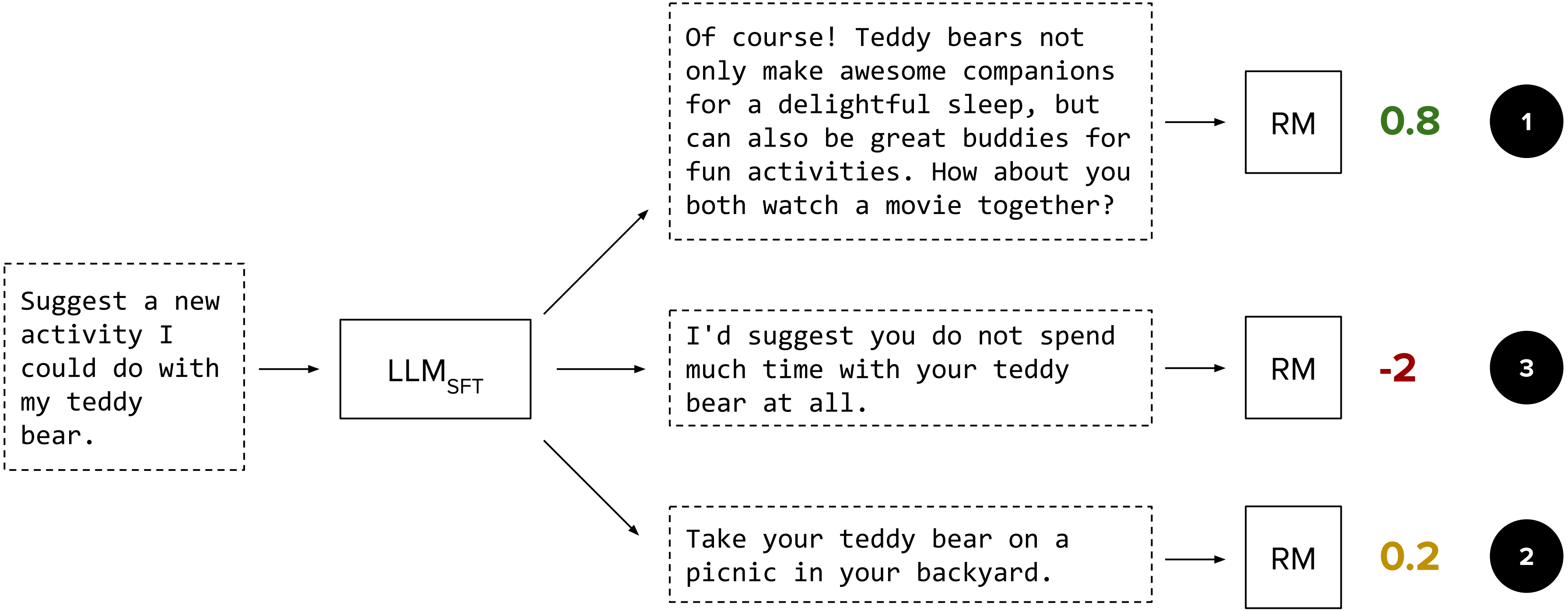

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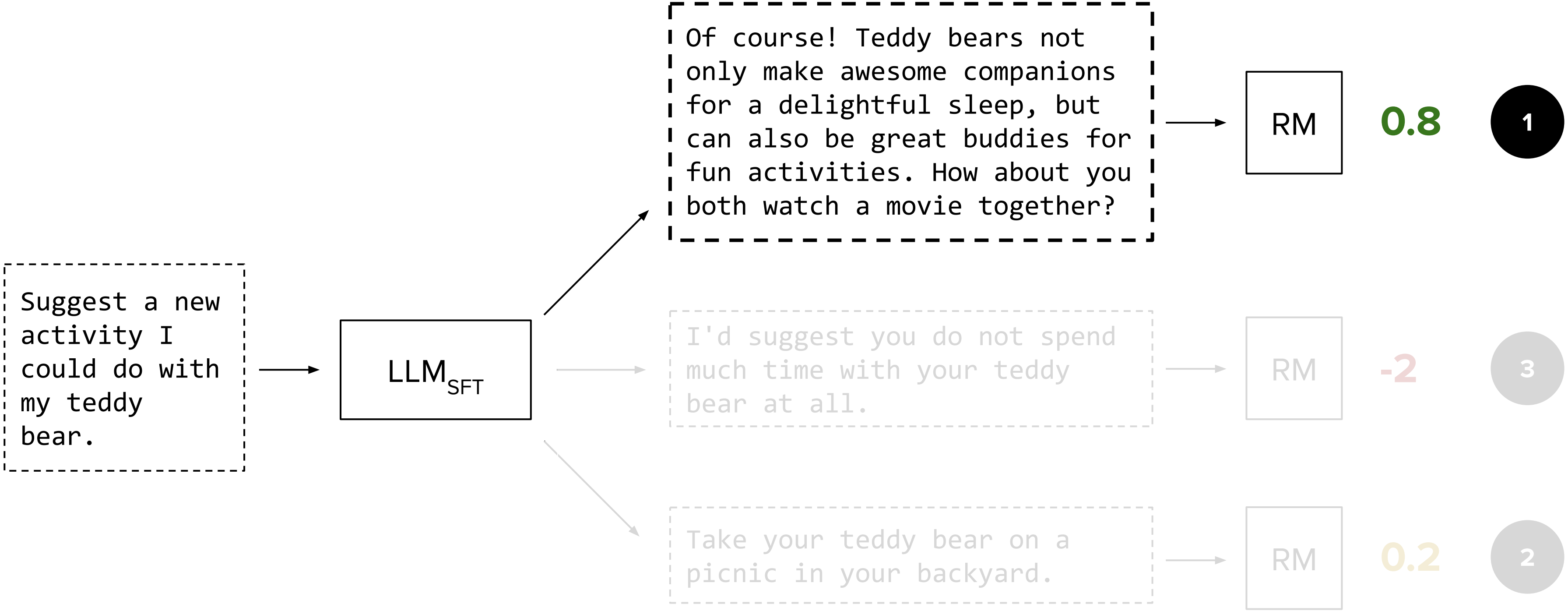

inference compute heavy

Transformers & Large Language Models

Preference tuning

Data collection

RLHF

DPO

Motivation

- Limitations using RL

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

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:

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

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

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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

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

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

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

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

"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**

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

"*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

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

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

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

\beta ~ 0.1

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

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.

not everyone uses DPO
PPO performs better
sometimes fitting not the exact distribution the model has seen at training time

"*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!