

Scalable Post-Training Optimization for Large Language Models

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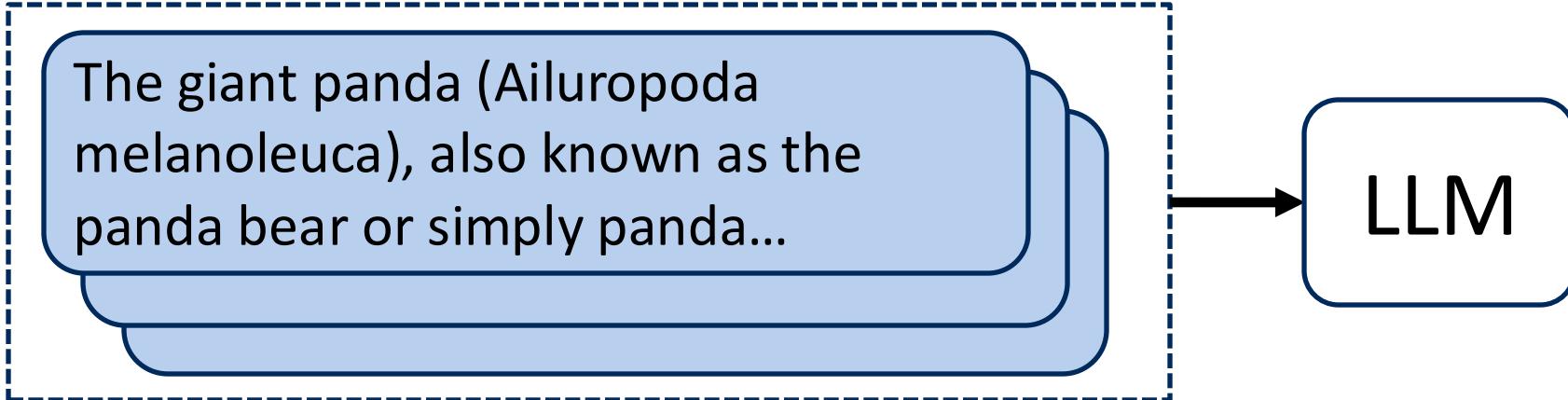
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December 11, 2025

LLM training pipeline

Stage 1: Pretraining (Learn rich knowledge from raw texts)



Stage 2: SFT (Align LLM with instruction format)

Question: Why is the sky blue?
Answer: The sky appears blue because of
...

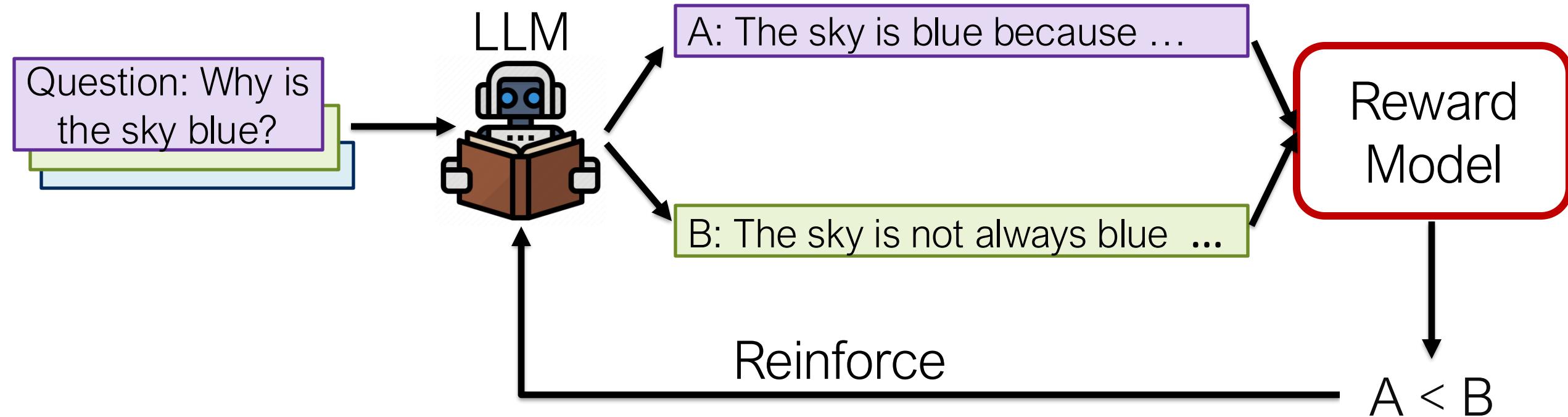
Stage 3: Post-training (RLHF, knowledge distillation)

Question: Why is the sky blue?
y1: The sky appears blue because ...
y2: The sky is not always blue ...

Outline

- Aligning with online preference optimization (BPO)
- Iterative refinement with fine-grained feedback (LLMRefine)
- Learning Optimized Sample Compute Allocation (OSCA)
- Speculative Knowledge Distillation

Learning from Reward / Quality-Estimation Metric(QE)



PPO training

RL objective:

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



Maximize reward

Training stability +
Avoid reward hacking

Constrained optimization

Issues with PPO:

1. Many hyperparameters to tune
2. Involve four different models: ref model, old model, optimized model, reward model

Reward modeling in RLHF

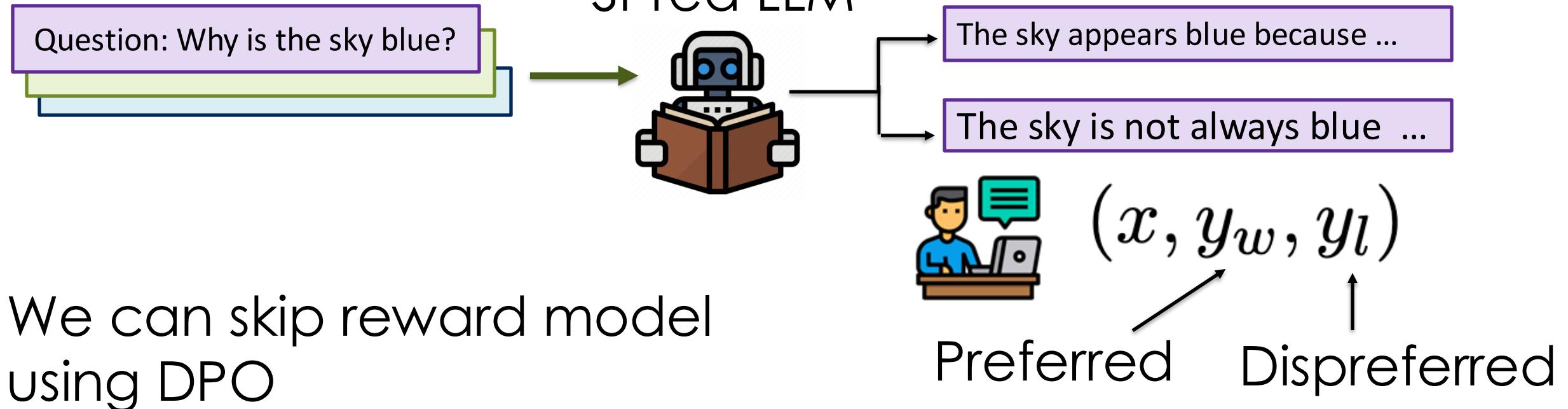
$(x, y_w, y_l) \rightarrow$ Reward Model

$$p^*(y_1 \succ y_2 \mid x) = \frac{\exp(r^*(x, y_1))}{\exp(r^*(x, y_1)) + \exp(r^*(x, y_2))}. \text{ Bradley-Terry Model}$$

$$\mathcal{L}_R(r_\phi, \mathcal{D}) = -\mathbb{E}_{(x, y_w, y_l) \sim \mathcal{D}} [\log \sigma(r_\phi(x, y_w) - r_\phi(x, y_l))]$$

Training language models to follow instructions with human feedback

Direct Preference Optimization



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

Derivation of DPO

$$r(x, y) = \beta \log \frac{\pi_r(y|x)}{\pi_{ref}(y|x)} + \beta \log Z(x)$$

Represent reward r using optimal policy π_r

$$p^*(y_1 > y_2 | x) = \frac{\exp(r^*(x, y_1))}{\exp(r^*(x, y_1)) + \exp(r^*(x, y_2))} = \frac{1}{1 + \frac{\exp(r^*(x, y_2))}{\exp(r^*(x, y_1))}} =$$

$$\frac{1}{1 + \exp\left(\beta \log \frac{\pi_r(y_2|x)}{\pi_{ref}(y_2|x)} - \beta \frac{\pi_r(y_1|x)}{\pi_{ref}(y_1|x)}\right)}$$

Plug reward function into Bradley Terry model

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

Offline DPO variants

All DPO variants follow this

DPO loss:

$$-\log \sigma \left(\beta \log \frac{\pi_{\theta}(\mathbf{y}^+|\mathbf{x})\pi_{\theta^0}(\mathbf{y}^-|\mathbf{x})}{\pi_{\theta^0}(\mathbf{y}^+|\mathbf{x})\pi_{\theta}(\mathbf{y}^-|\mathbf{x})} \right)$$

$$r_{\phi}(y_w) - r_{\phi}(y_l) = \beta \left(\log \frac{\pi_{\theta}^*(y_w)}{\pi_{\text{ref}}(y_w)} - \log \frac{\pi_{\theta}^*(y_l)}{\pi_{\text{ref}}(y_l)} \right).$$

IPO loss:

$$\left(\log \left(\frac{\pi_{\theta}(\mathbf{y}^+|\mathbf{x})\pi_{\theta^0}(\mathbf{y}^-|\mathbf{x})}{\pi_{\theta}(\mathbf{y}^-|\mathbf{x})\pi_{\theta^0}(\mathbf{y}^+|\mathbf{x})} \right) - \frac{1}{2\beta} \right)^2$$

Avoids the overfitting from
DPO (Squared loss)

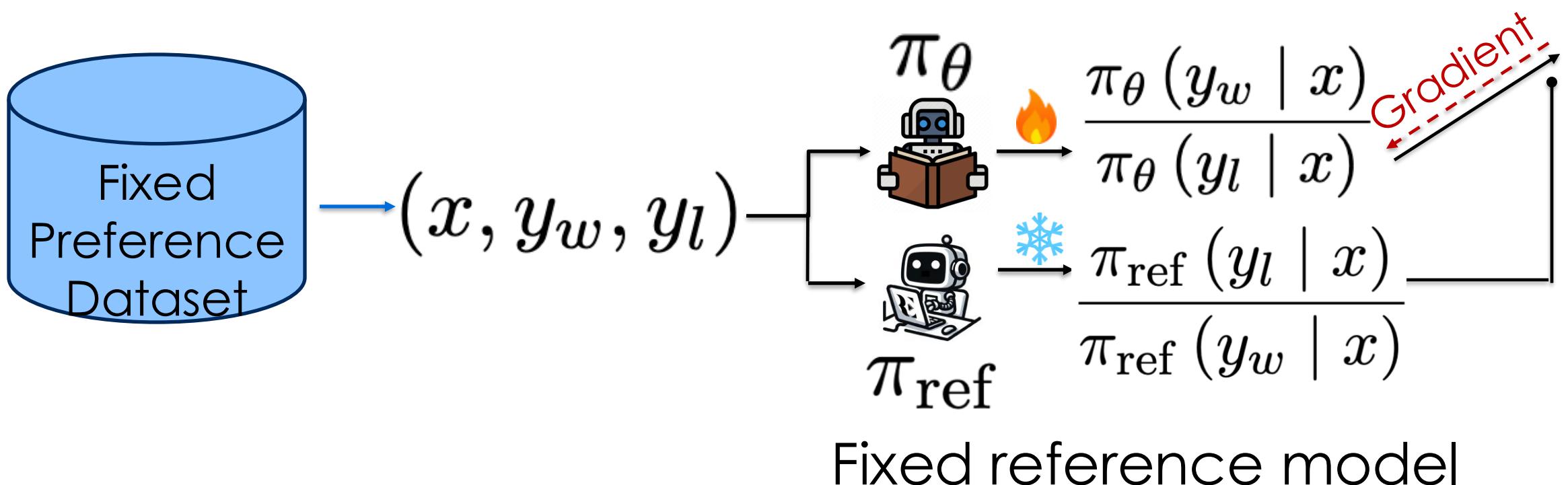
SLiC loss:

$$\max \left(0, 1 - \beta \log \left(\frac{\pi_{\theta}(\mathbf{y}^+|\mathbf{x})\pi_{\theta^0}(\mathbf{y}^-|\mathbf{x})}{\pi_{\theta}(\mathbf{y}^-|\mathbf{x})\pi_{\theta^0}(\mathbf{y}^+|\mathbf{x})} \right) \right)$$

Hinge loss

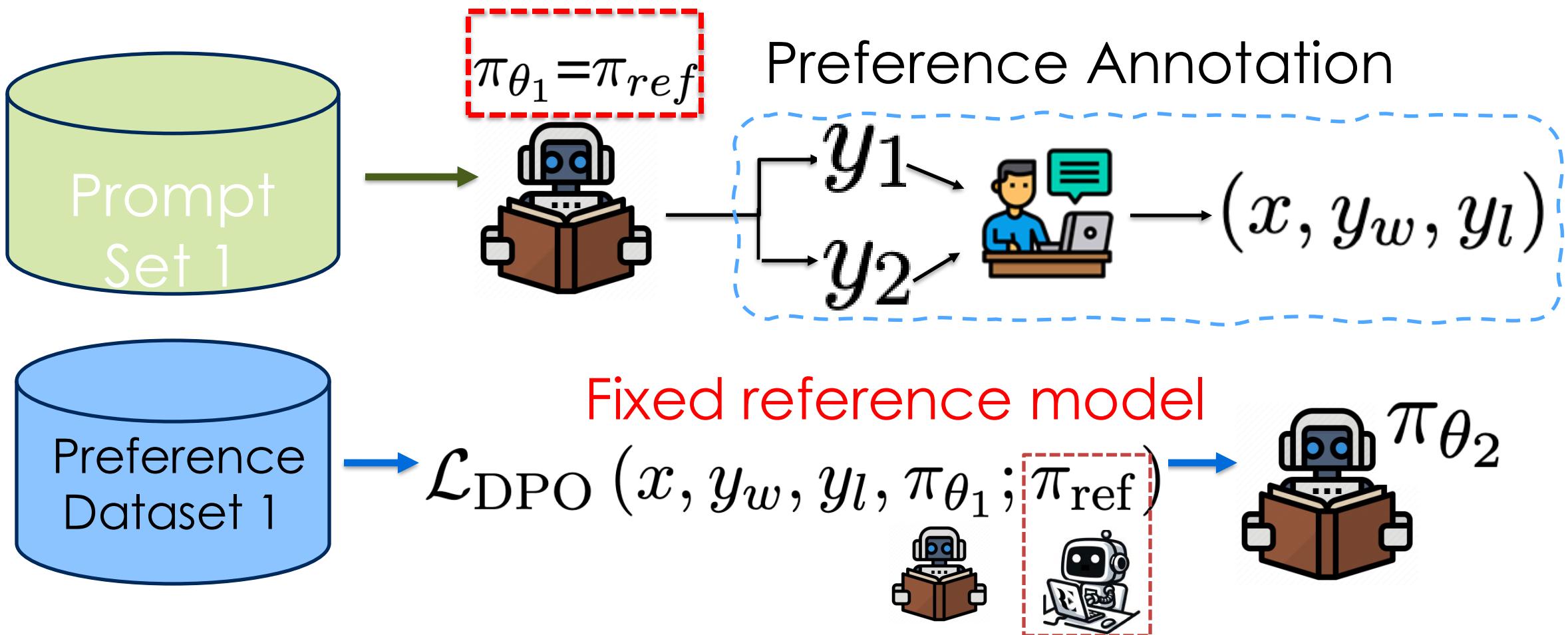
Illustration of DPO

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



Limitation of offline DPO (and online DPO)

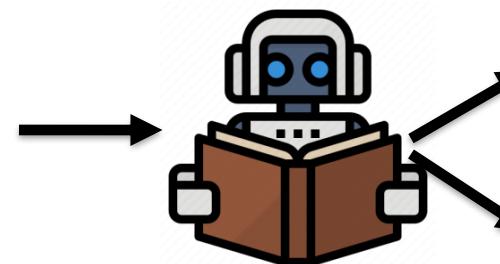
Synthetic data distribution shifts



Data distribution shift during training

Iter 1

Prompt : Translate this Assamese sentence into English...



I don't know this language

π_{ref}

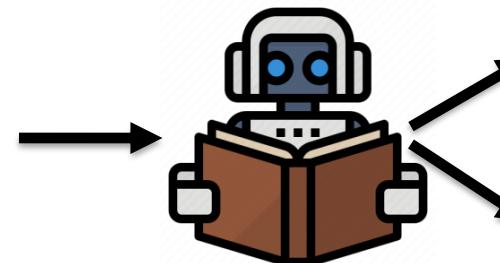


In the past, in the past, in the past



Iter 2

Prompt : Translate this Assamese sentence into English...



It was to last for the next 40 years ...

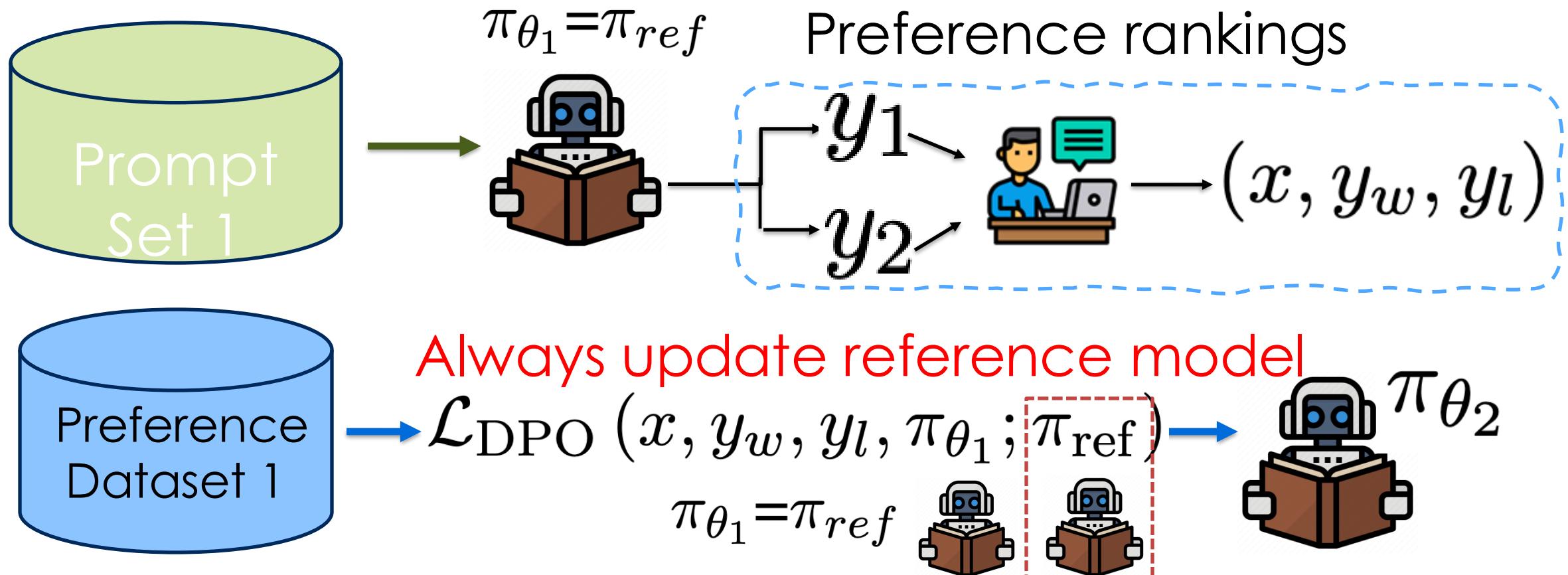
?

This has been going on for 40 years ...

Introducing BPO (B=Behavior)

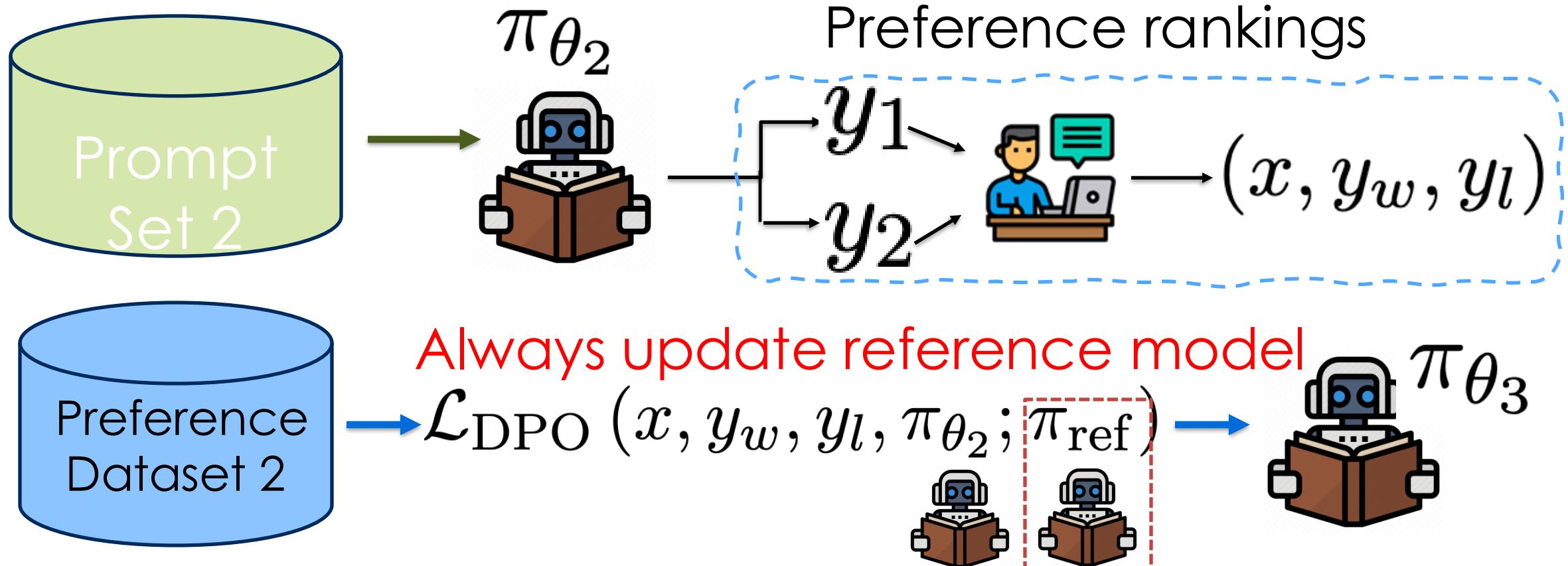
- Data collection needs to be online
- The reference model needs to be updated and has to be close to the behavior LLM

BPO

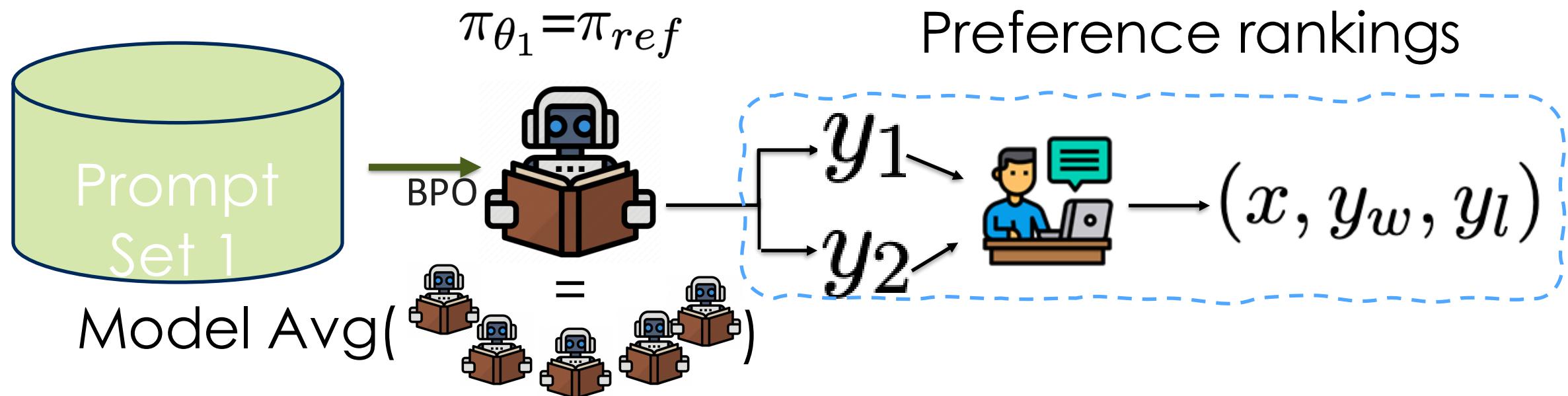


BPO

use new behavior model to generate samples

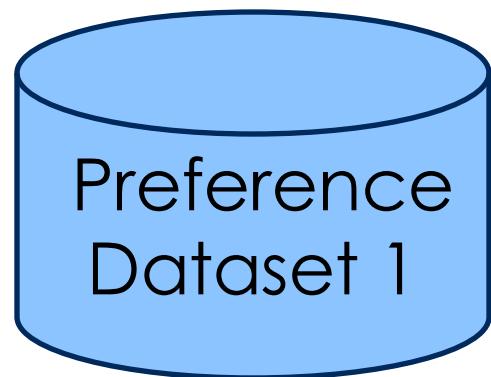


Practical implementation of BPO (Lora ensemble)



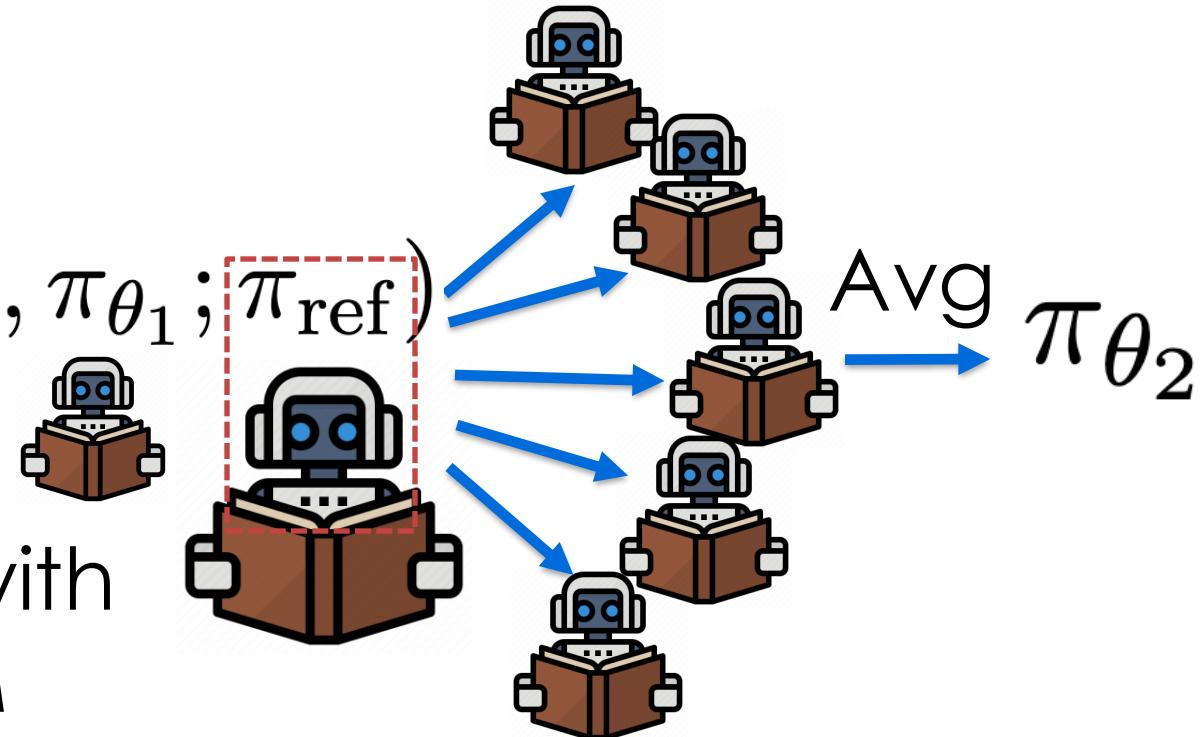
We use model averaged LoRA weights to perform sampling

Practical implementation of BPO (Lora ensemble)



$$\mathcal{L}_{\text{DPO}}(x, y_w, y_l, \pi_{\theta_1}; \pi_{\text{ref}})$$

We update reference model with
Model averaged behavior LLM



Each lora weight is
updated
independently

Why ref=behavior may not work?

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

$$\nabla_\theta \mathcal{L}_{\text{DPO}}(\pi_\theta; \pi_{\text{ref}}) =$$

$$-\beta \mathbb{E}_{(x, y_w, y_l) \sim \mathcal{D}} \left[\underbrace{\sigma(\hat{r}_\theta(x, y_l) - \hat{r}_\theta(x, y_w))}_{\text{higher weight when reward estimate is wrong}} \left[\underbrace{\nabla_\theta \log \pi(y_w | x)}_{\text{increase likelihood of } y_w} - \underbrace{\nabla_\theta \log \pi(y_l | x)}_{\text{decrease likelihood of } y_l} \right] \right]$$



$$\text{where } \hat{r}_\theta(x, y) = \beta \log \frac{\pi_\theta(y|x)}{\pi_{\text{ref}}(y|x)}$$

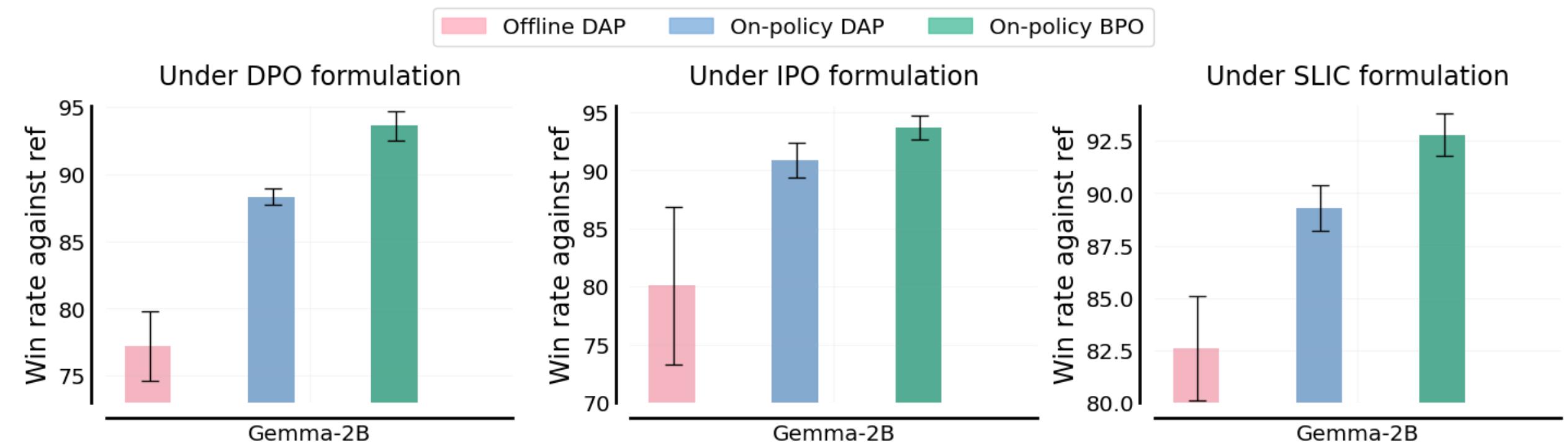
This term degenerates to constant 0.5

When ref=behavior

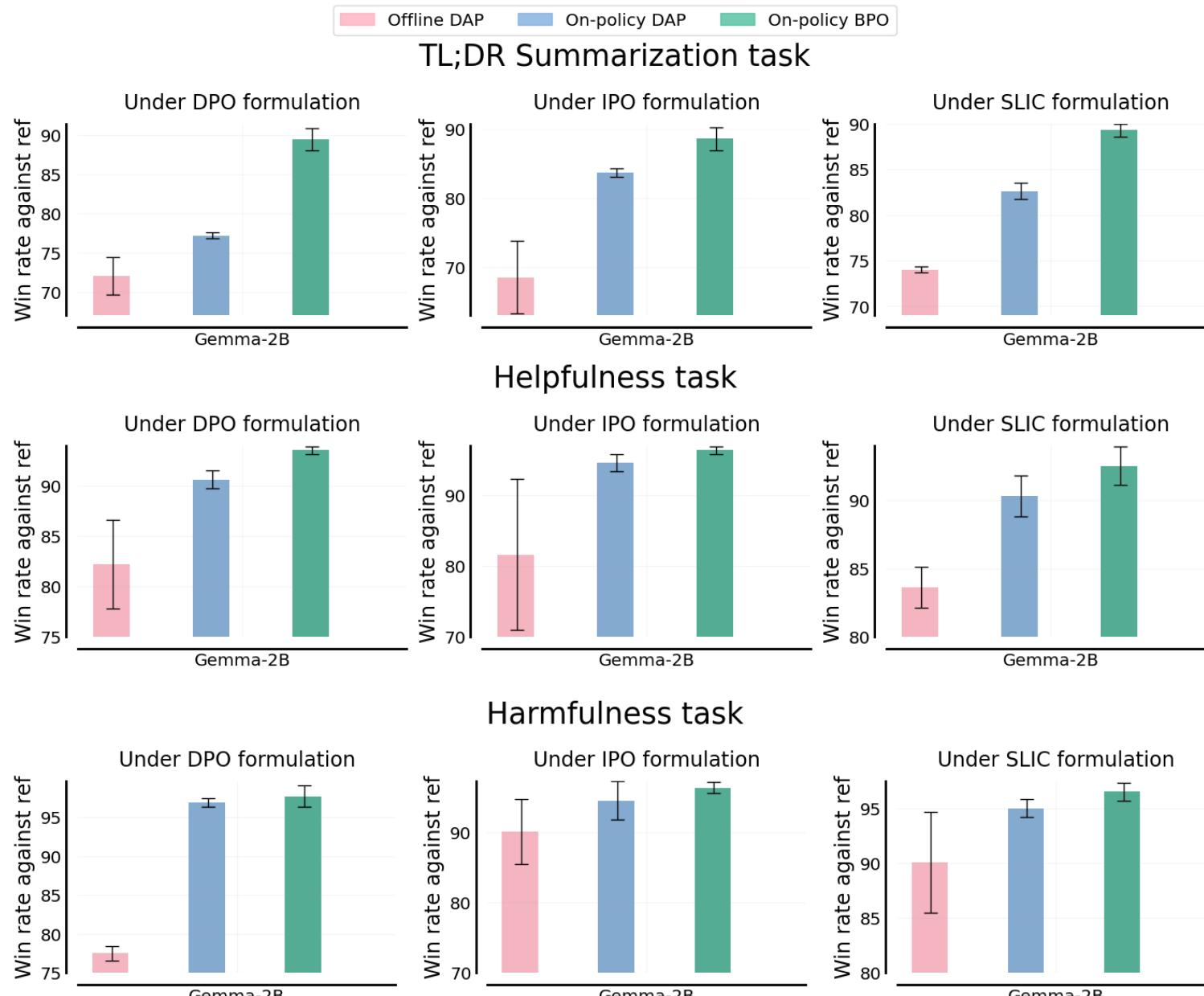
Evaluation on TLDR dataset

- Tasks:
 - TLDR, helpfulness and harmfulness
- Baselines:
 - DPO, SLIC, IPO in offline, online and on-policy settings
- Base model: Gemma-2B
- Preference simulator (Oracle): RM-deberta (In practice, it should be human)

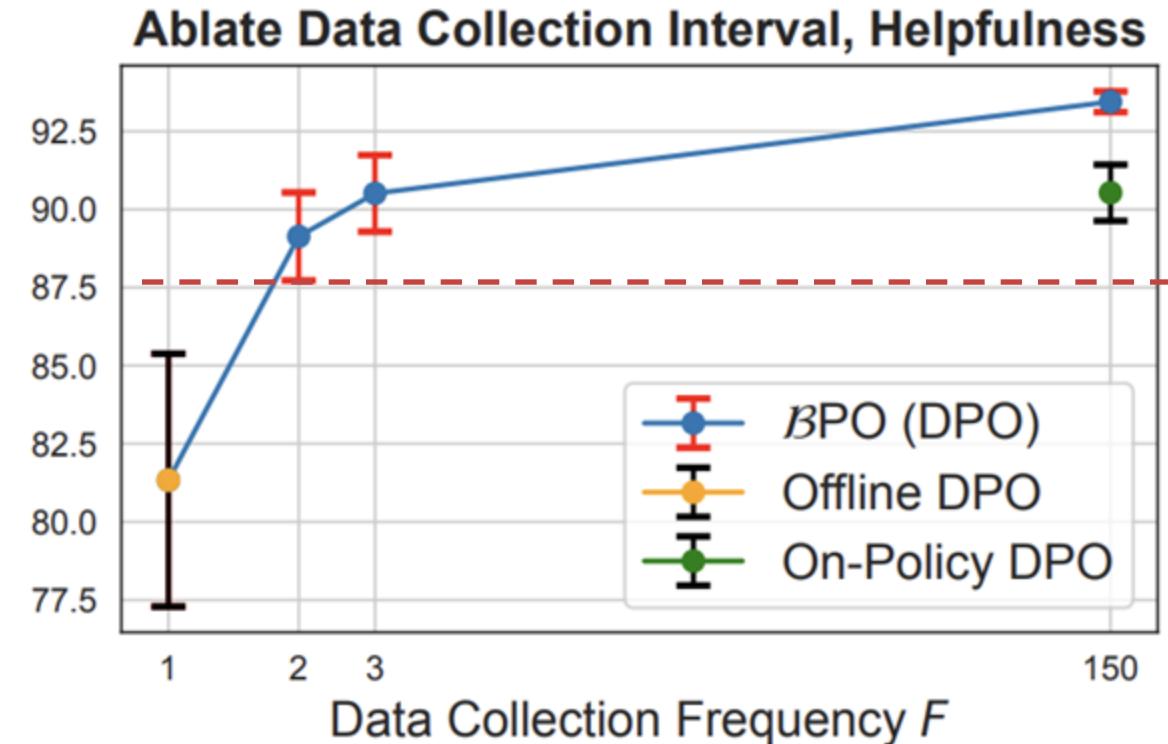
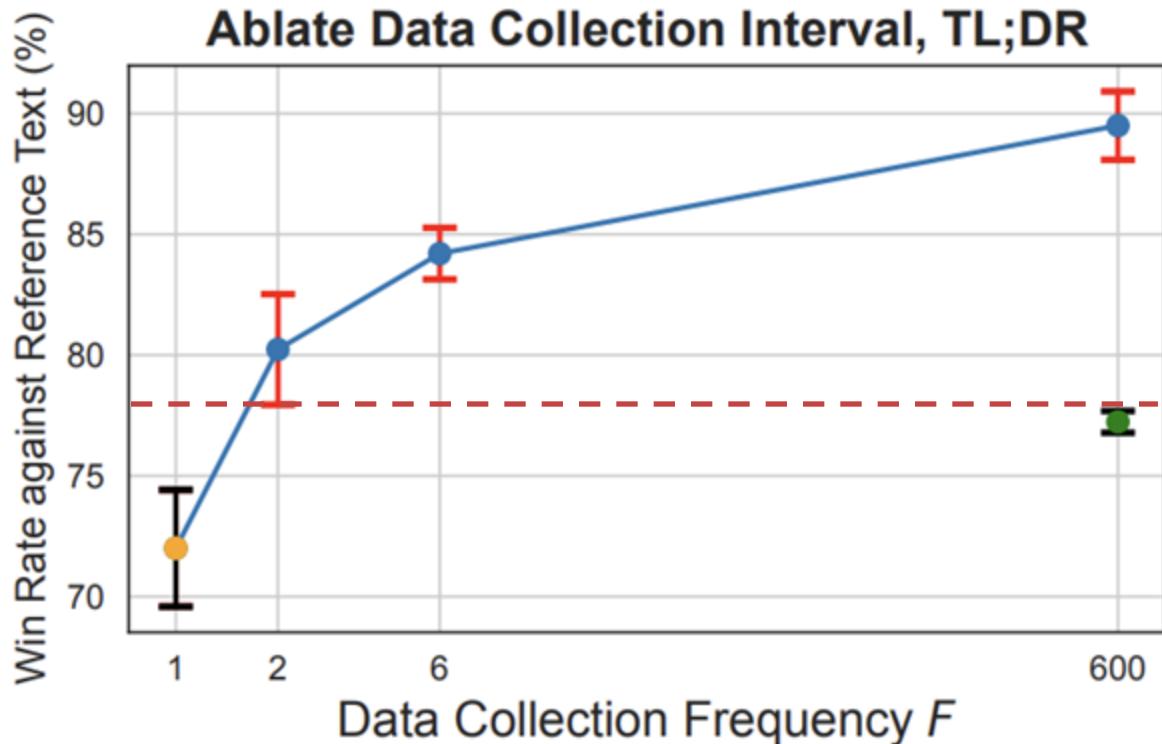
BPO outperforms online and offline alignment methods



BPO outperforms baselines across three tasks



BPO adapts to different data collection frequencies



BPO Highlight



- Reference model should stay close to the behavior LLM and create better online LLM alignment
- Practical applicability: We empirically show our online BPO with ≥ 2 data collection steps can significantly improve offline baselines
- The effectiveness of BPO stems from proximity to the behavior model, rather than improvements in the reference model's quality.

Outline

- Aligning with online preference optimization (BPO)
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Can we use fine-grained feedback to guide LLM?

Input: Translate "新冠疫情危机爆发" into English.



LLM's output:

the outbreak of the new crown crisis

What feedback can we give to LLM?

Can we use fine-grained feedback to guide LLM?

Input: Translate "新冠疫情危机爆发" into English.



LLM's output:

the outbreak of the new crown crisis

Ask LLM to improve?

Source:新冠疫情危机爆发

Translation: the outbreak of the new crown crisis

Please Improve current translation.



Can we use fine-grained feedback to guide LLM?

Input: Translate "新冠疫情危机爆发" into English.



LLM's output:

the outbreak of the new crown crisis

Use binary feedback to guide LLM?

Source:新冠疫情危机爆发

Translation: the outbreak of the new crown crisis

Your translation contains errors. Please improve current translation.



Can we use fine-grained feedback to guide LLM?

Input: Translate "新冠疫情危机爆发" into English.



LLM's output:

the outbreak of the new crown crisis

Use scalar feedback to guide LLM?

Source:新冠疫情危机爆发

Translation: the outbreak of the new crown crisis

Your translation has score of 70/100. Please improve current translation.



Can we use fine-grained feedback to guide LLM?

Input: Translate "新冠疫情危机爆发" into English.



LLM's output:

the outbreak of the new crown crisis

Use fine-grained feedback to guide LLM!

Source:新冠疫情危机爆发

Translation: the outbreak of the new crown crisis

"new crown" is a major terminology error. Please improve current translation.



InstructScore's Fine-grained Explanation

Input: Translate "新冠疫情
危机爆发" into English.

Candidate: The outbreak of the **new crown** crisis



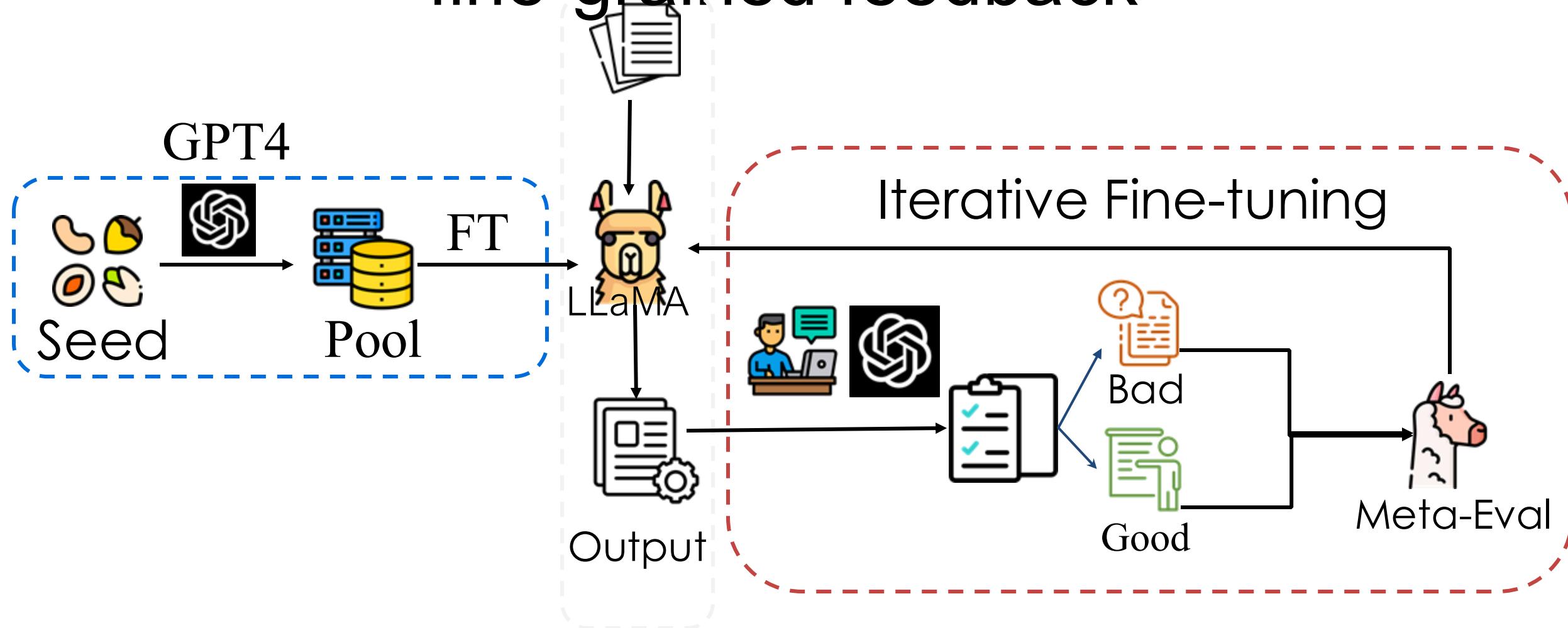
Error location: new crown

Error type: Terminology is used inconsistently

Major/Minor: Major

Explanation: The term "new crown" is not the correct term for "Covid-19".

InstructScore-QE (source-based) to provide fine-grained feedback



Introducing LLMRefine

Source:新冠疫情危机爆发

Translation: the outbreak of the new crown crisis

"new crown" is a major terminology error. Please improve current translation.

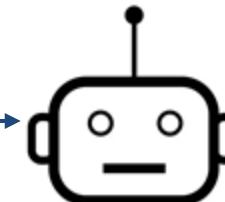


Reject

resample
from LLM
Accept



LLM's proposal:
the outbreak of the new crisis



Repeat above steps for n iterations



LLM's final output:
the outbreak of the Covid-19 crisis

Source Translation: 新冠疫情危机爆发

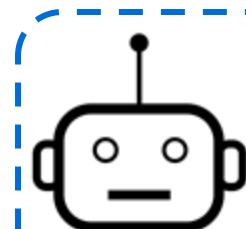


LLMRefine Algorithm

Repeat n times

Obtain feedback F_i from error pinpoint

Sample revision c_i based on feedback f_i and last generation y_{i-1}



$$P_{accept} = \min(1, e^{\frac{s(F(c_i)) - s(F(y_{i-1}))}{n * T_i}})$$

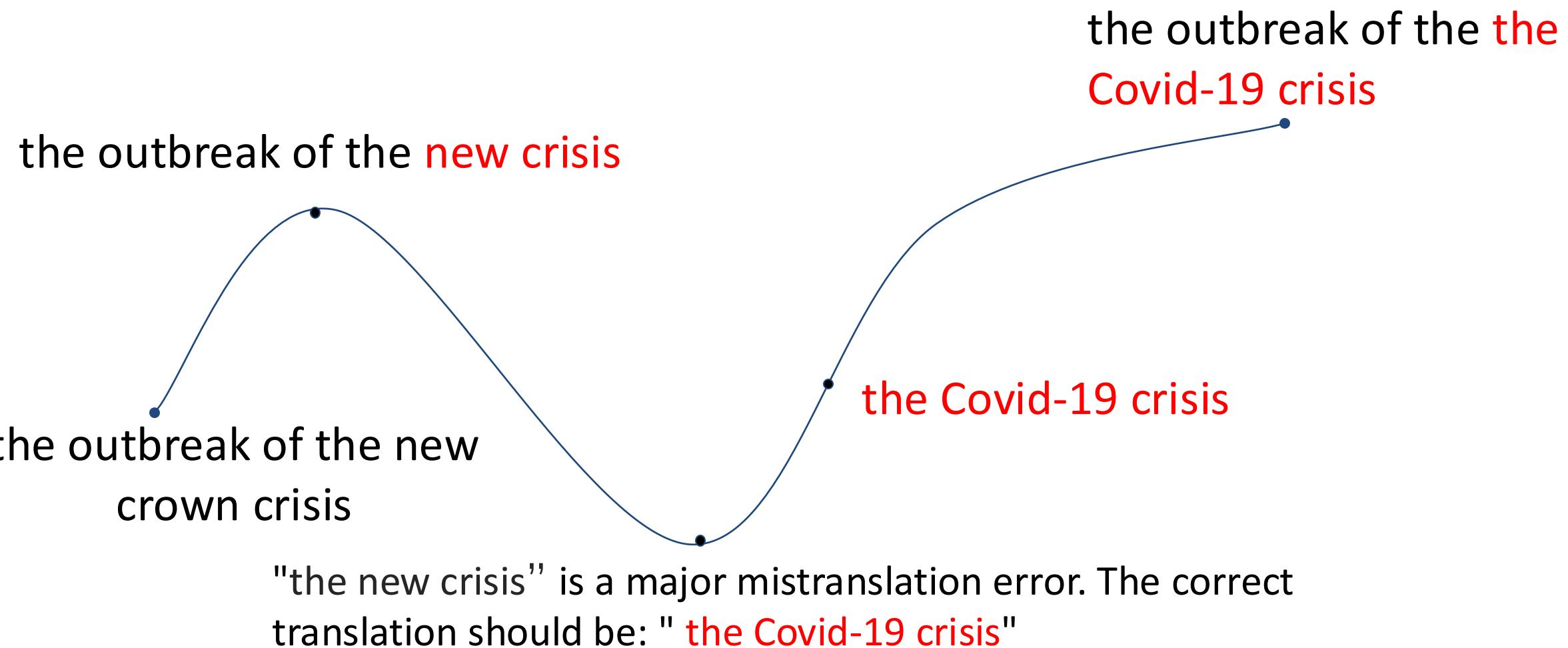


Accept new revision

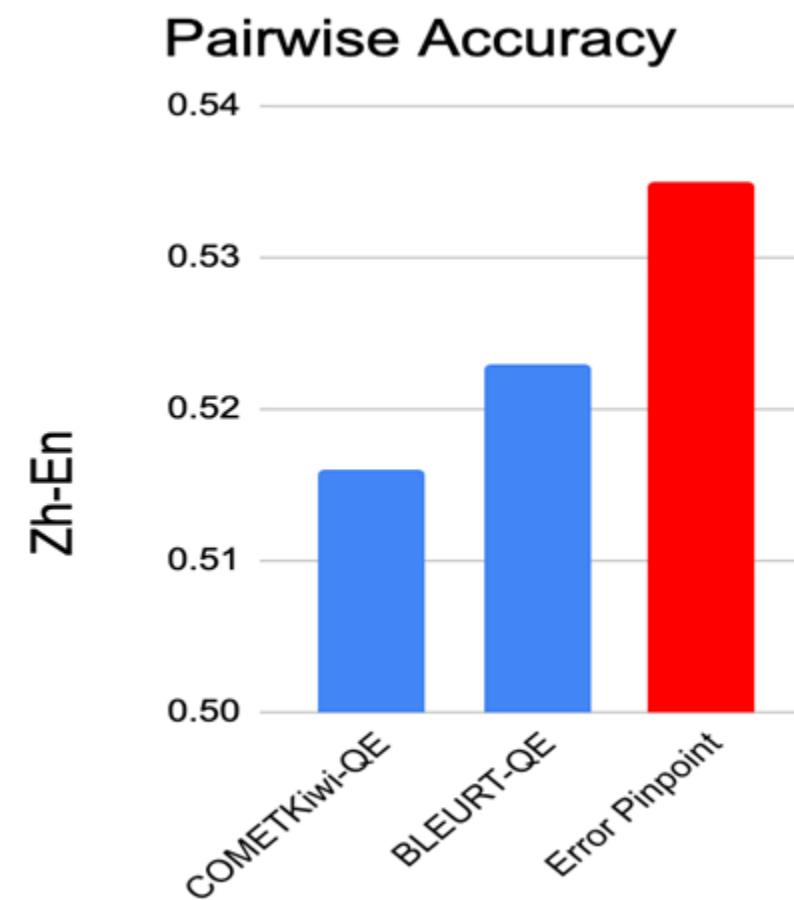
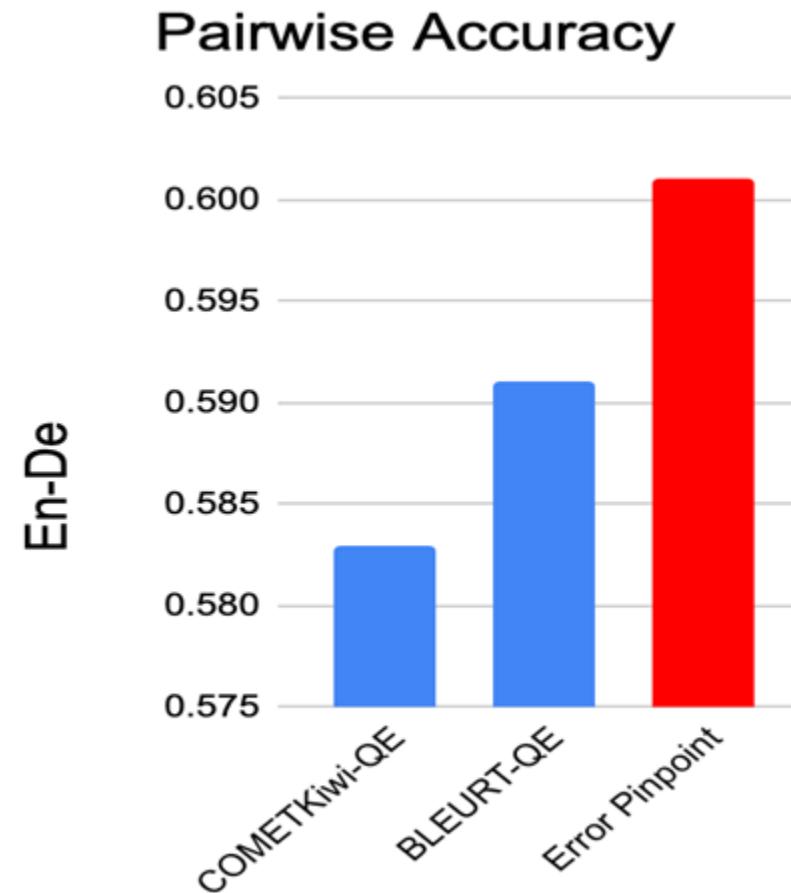
Keep the last step candidate

$$T_{i+1} = \max(T_i - c * T_i, 0)$$

Source Translation: 新冠疫情危机爆发

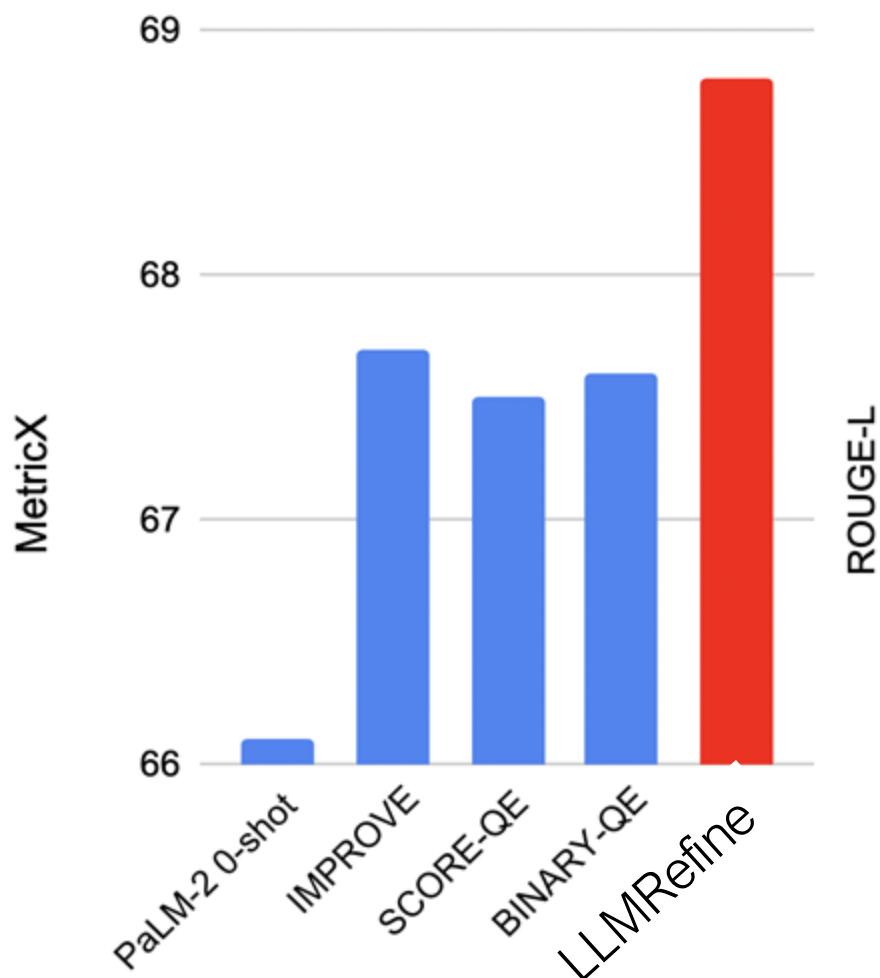


RQ1: How well does our error pinpoint model align with human annotations of generation quality?

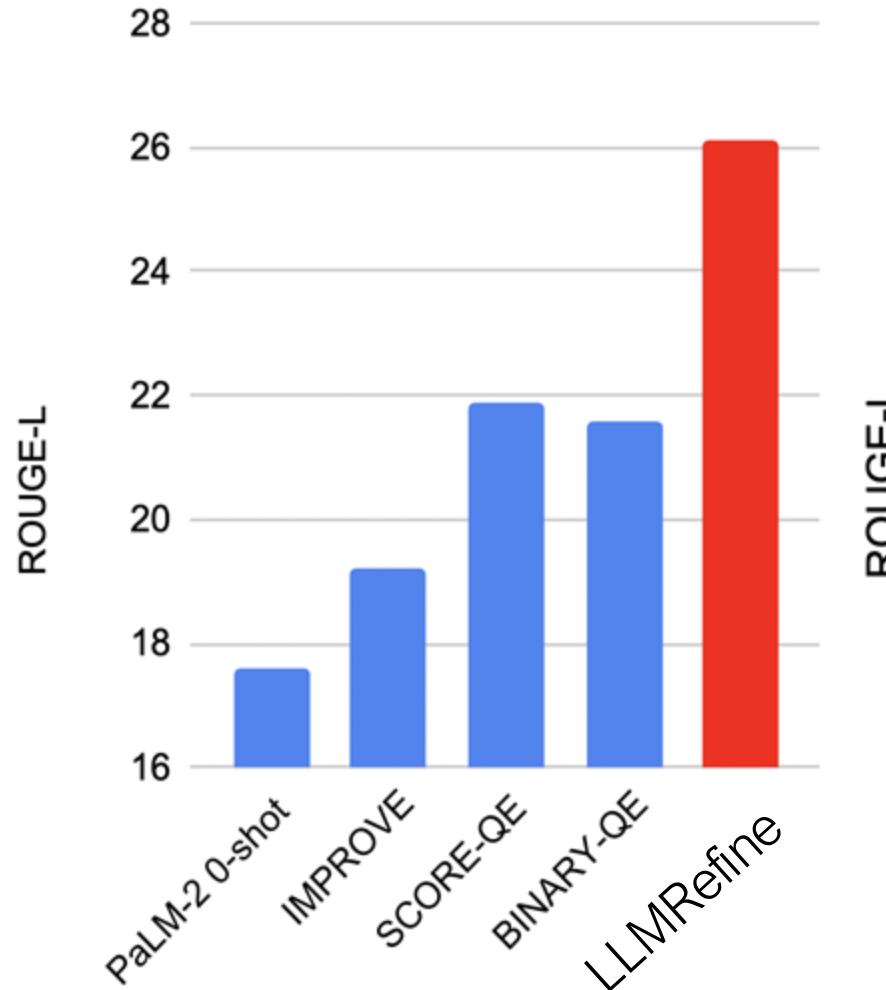


LLMRefine results in better translations than coarse feedback

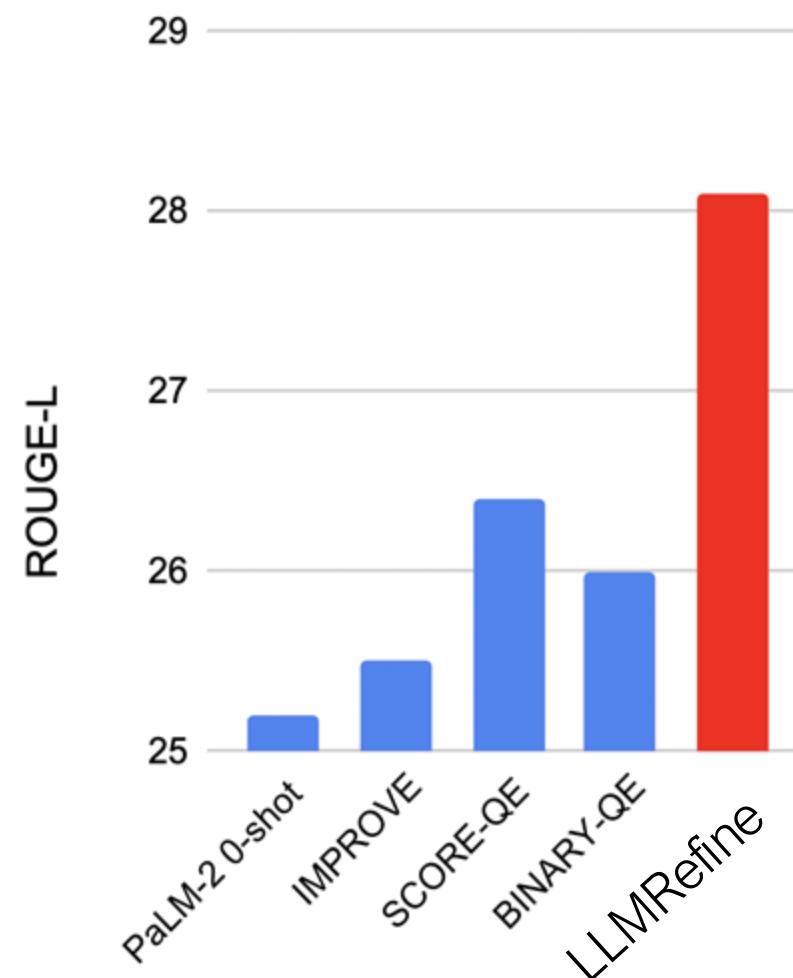
Chinese-to-English Translation



Long form QA (ASQA)



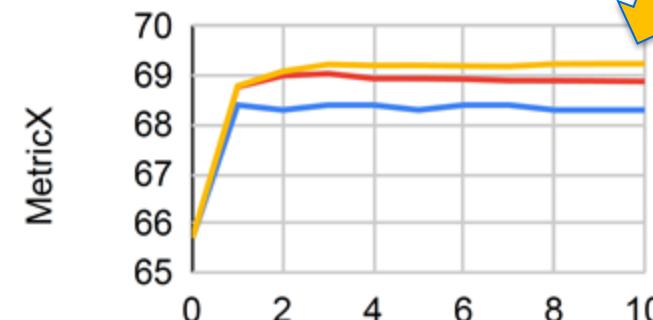
Topical Summ



Simulated Annealing works in LLMRefine

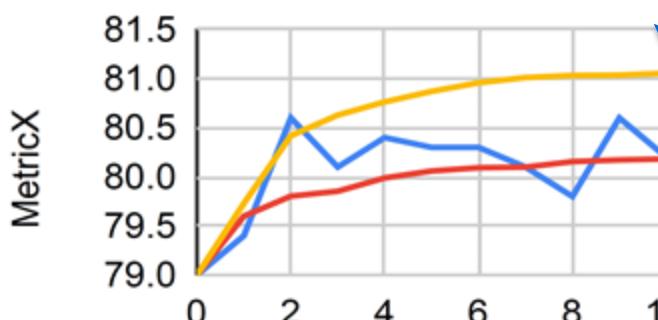
WMT23 Zh-En

— Always Accept — Uphill Algorithm
— Simulated Annealing



WMT22 En-De

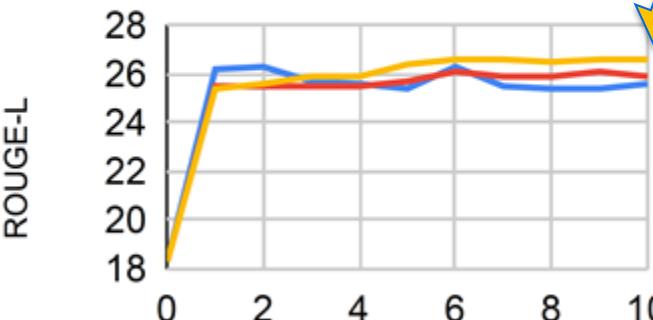
— Always Accept — Uphill Algorithm
— Simulated Annealing



Translation
Summarization
Long form QA

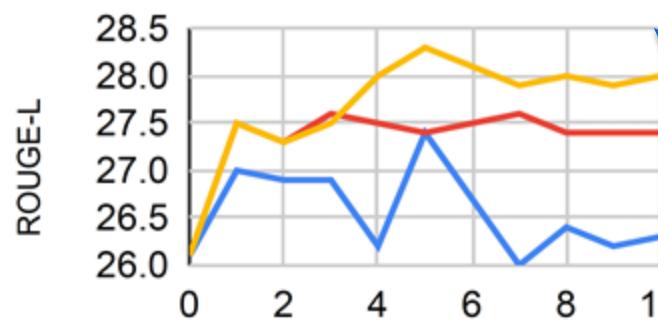
Iteration
ASQA

— Always-accept — Uphill Algorithm
— Simulated Annealing

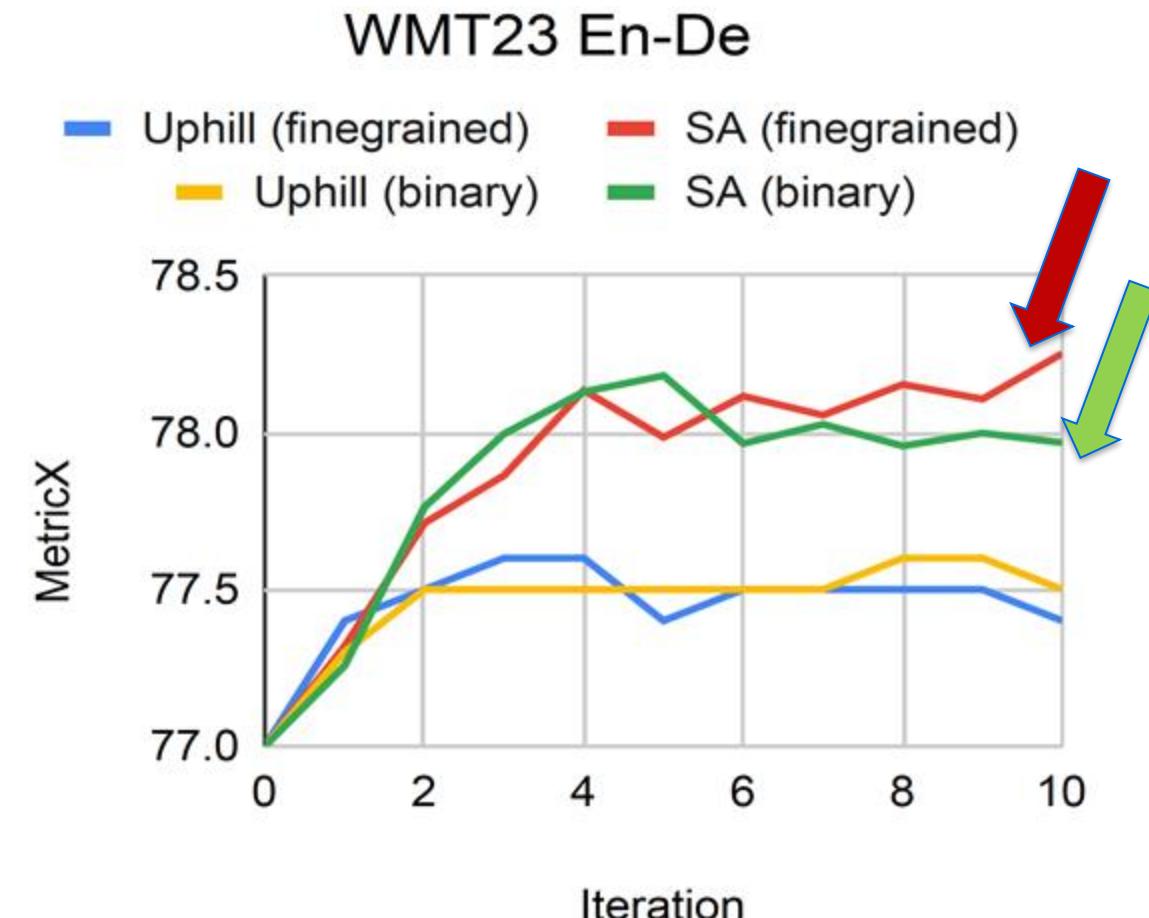
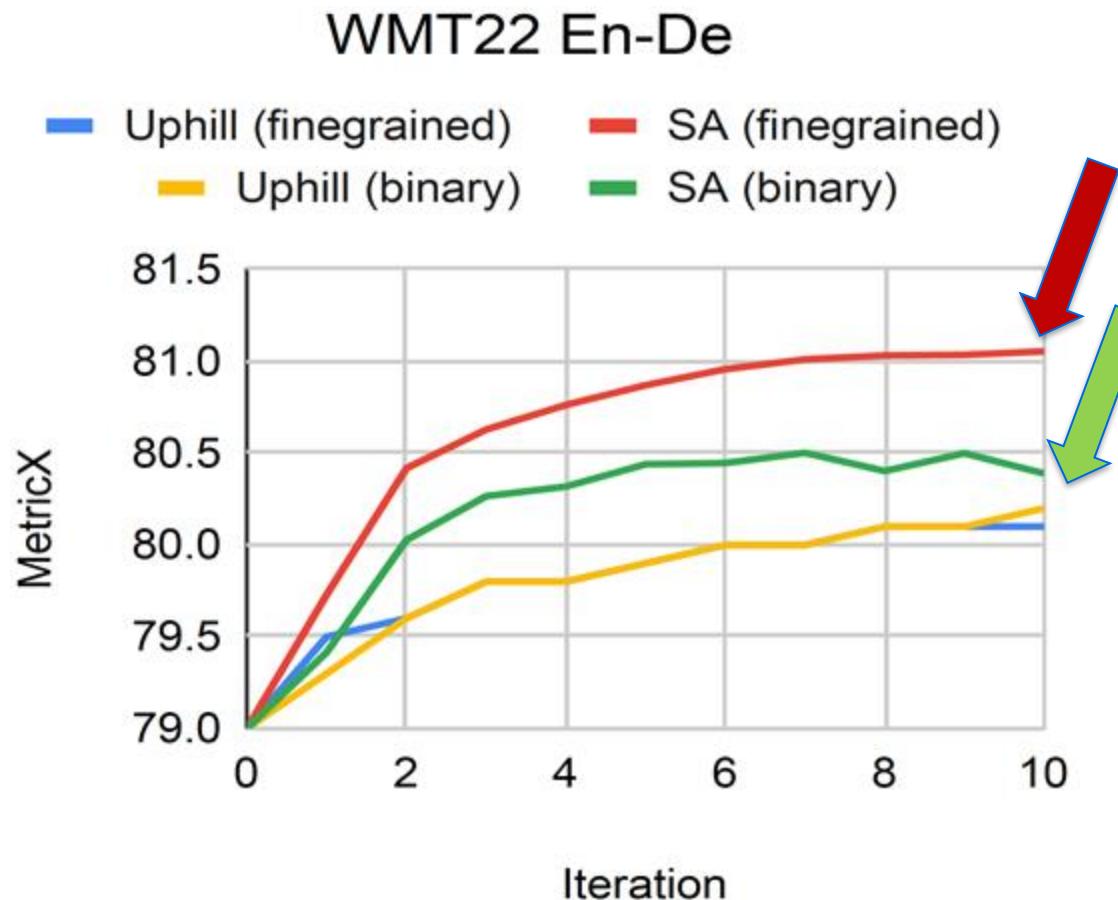


Iteration
Summarization

— Always-accept — Uphill Algorithm
— Simulated Annealing



Simulated annealing can boost performance of both coarse and fine-grained feedback



Human Evaluation further validates our results

Our fine-grained has all win/lose ratios greater than 1

WMT22 En-De	Win/lose ratio
0-shot	2.34
Improve	2.44
BLEURT-Score-QE	2.79
BLEURT-Binary-QE	1.76
Score-QE	1.23
Binary-QE	1.84

Our SA has all win/lose ratios greater than 1

WMT22 En-De	Win/lose ratio
Always-Accept	1.56
Greedy Uphill	1.38

Key insights of LLMRefine

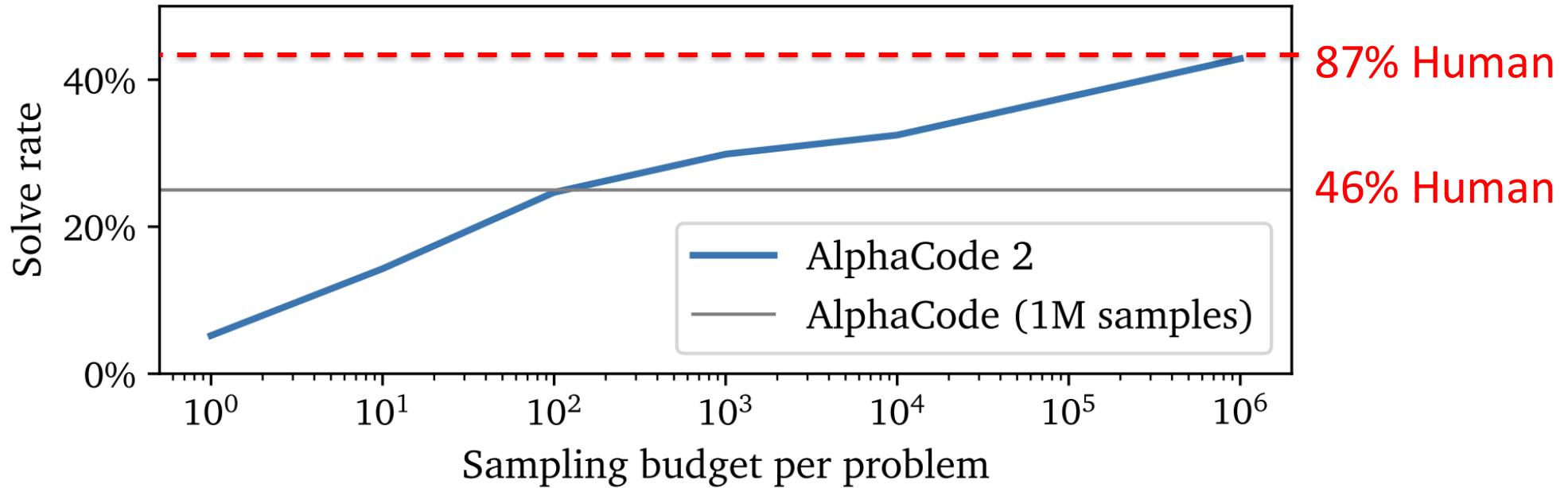
- Binary feedback is not enough
- Fine-grained feedback is better
- Algorithmic iterative refinement is superb



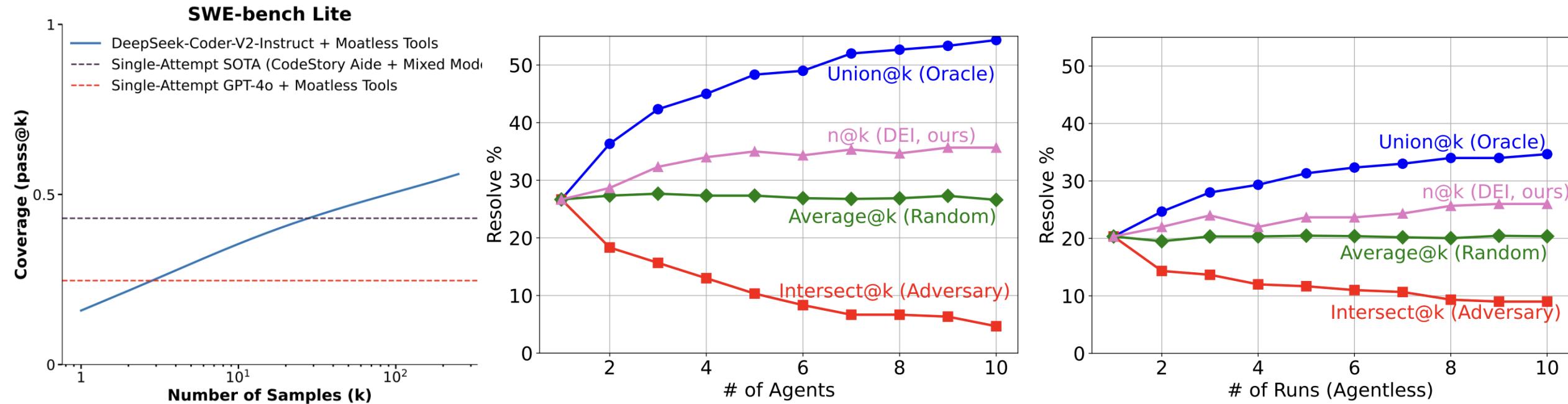
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Inference-Time Scaling Law



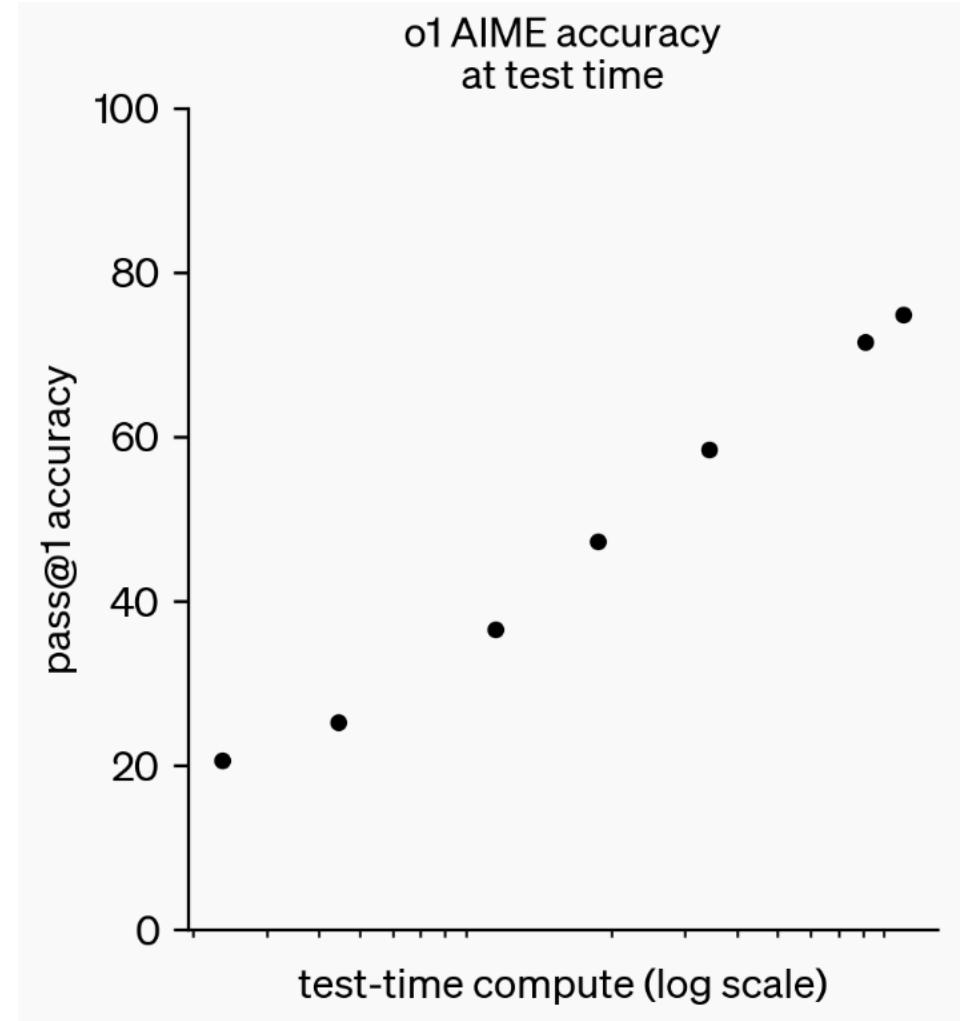
Inference-Time Scaling Law



same for Agentic Tasks like SWE-Bench.
More agents, more runs → Better solve rate.

Inference-Time Scaling Law

- Solve rates scale log-linearly with longer CoT.

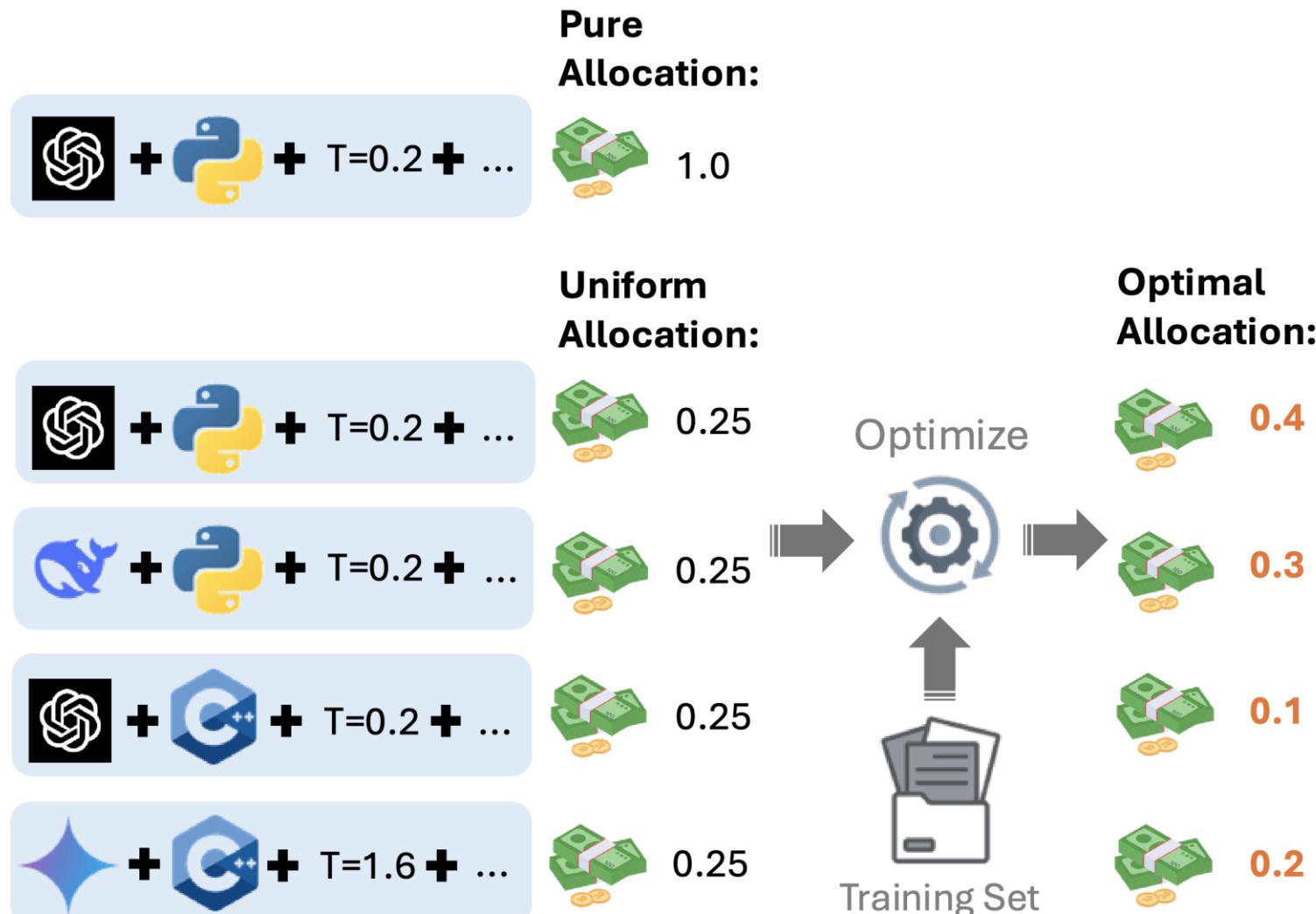


Sample Compute Allocation Problem for LLM Inference

- Allocate the total amount of compute (# samples, # tokens, FLOPs) C.
- Sampling configurations (i.e. inference hyperparameters):
 - Model to use: gpt-4o, gemini, deepseek, qwen, ...
 - Temperature:
 - Output language: python / C++ / Chinese / English
- Pure Strategy
 - one config uses all compute
- Mixed Strategy

USE CASE	TEMPERATURE
Coding / Math	0.0
Data Cleaning / Data Analysis	1.0
General Conversation	1.3
Translation	1.3
Creative Writing / Poetry	1.5

Sample Compute Allocation



Mixed Strategy could be better

- Two problems p_1 and p_2 , two inference settings d_1 and d_2 .
- $P(d_1 \text{ solving } p_1) = 10\%$, $P(d_2 \text{ solving } p_1) = 1\%$.
- $P(d_1 \text{ solving } p_2) = 1\%$, $P(d_2 \text{ solving } p_2) = 10\%$.
- Expected number of problems solved given 10 samples:
 - Pure strategy (select either d_1 or d_2): 37.3%
 - Mixed strategy (5 samples for d_1 & d_2): 43.8%
- **Better to use mixed strategy!**

Optimizing Sample Compute Allocation

- The task:

- Given a set of sampling configurations.
- Given a training problem set i.i.d. with the test.
- Given a compute budget C .
- Find the optimal allocation π that maximizes pass@ C .

$$\begin{aligned} & \max_{\pi} \mathbb{E}[\text{pass}@C] \\ &= \frac{1}{|\mathcal{D}|} \sum_{j=1}^{|\mathcal{D}|} \left(1 - \prod_{i=1}^{|\mathcal{H}|} (1 - p_{ij})^{\pi_i} \right), \end{aligned}$$

$$\text{s.t. } 0 \leq \pi_i \leq C,$$

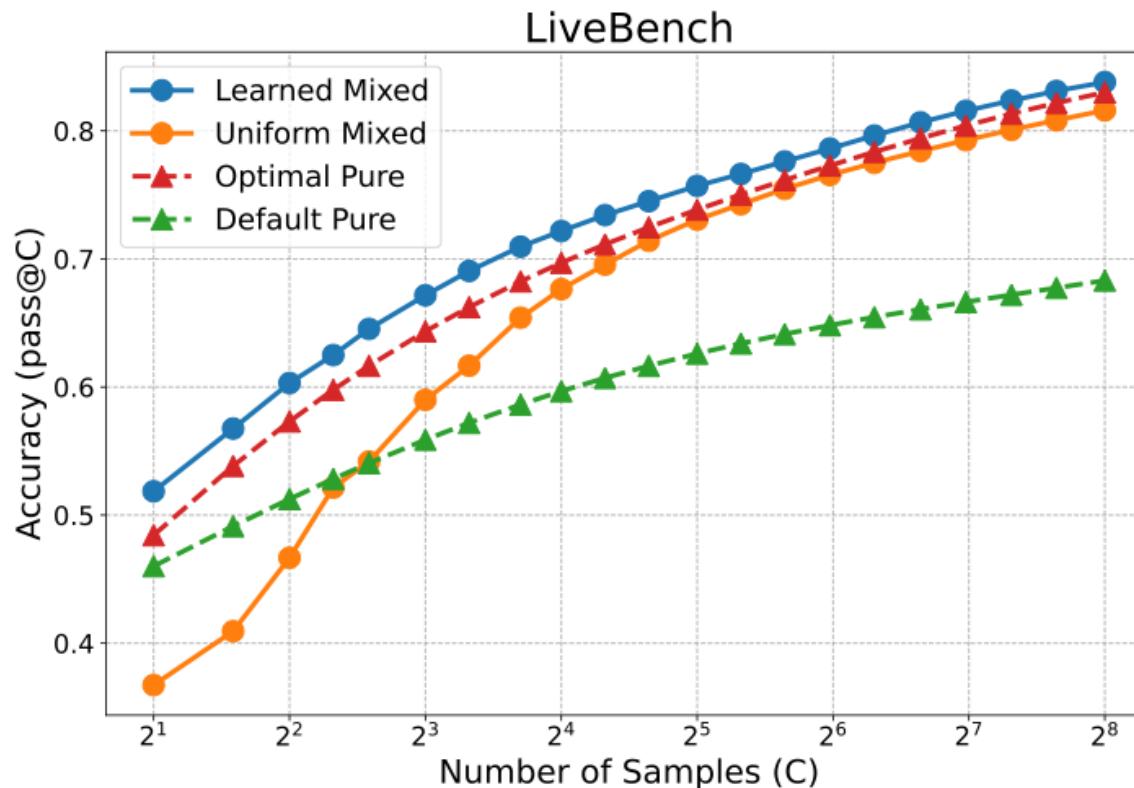
$$\sum_{i=1}^{|\mathcal{H}|} \pi_i = C, \pi_i \in \mathbb{N}.$$

OSCA: Learning to Scale Inference Optimally

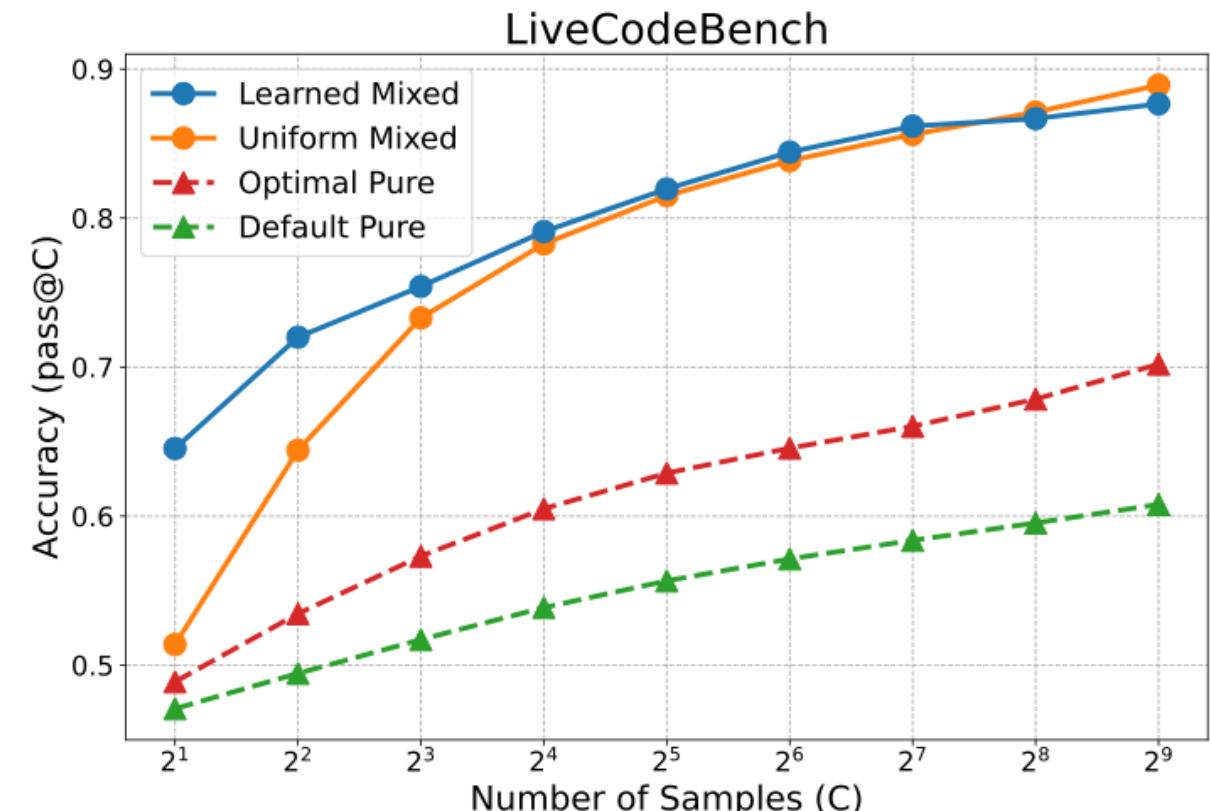
- If we ignore the integral constraints, this is a convex problem.
- We run hill climbing algorithm to find the solution.

$$\begin{aligned} & \max_{\pi} \mathbb{E}[\text{pass}@C] \\ &= \frac{1}{|\mathcal{D}|} \sum_{j=1}^{|\mathcal{D}|} \left(1 - \prod_{i=1}^{|\mathcal{H}|} (1 - p_{ij})^{\pi_i} \right), \\ & \text{s.t. } 0 \leq \pi_i \leq C, \\ & \sum_{i=1}^{|\mathcal{H}|} \pi_i = C, \pi_i \in \mathbb{N}. \end{aligned}$$

OSCA learned strategies excel!



Qwen2, LLaMA3, Deepseek-70B



GPT4o, Gemini, Deepseek

OSCA Learns to Scale Inference Optimally

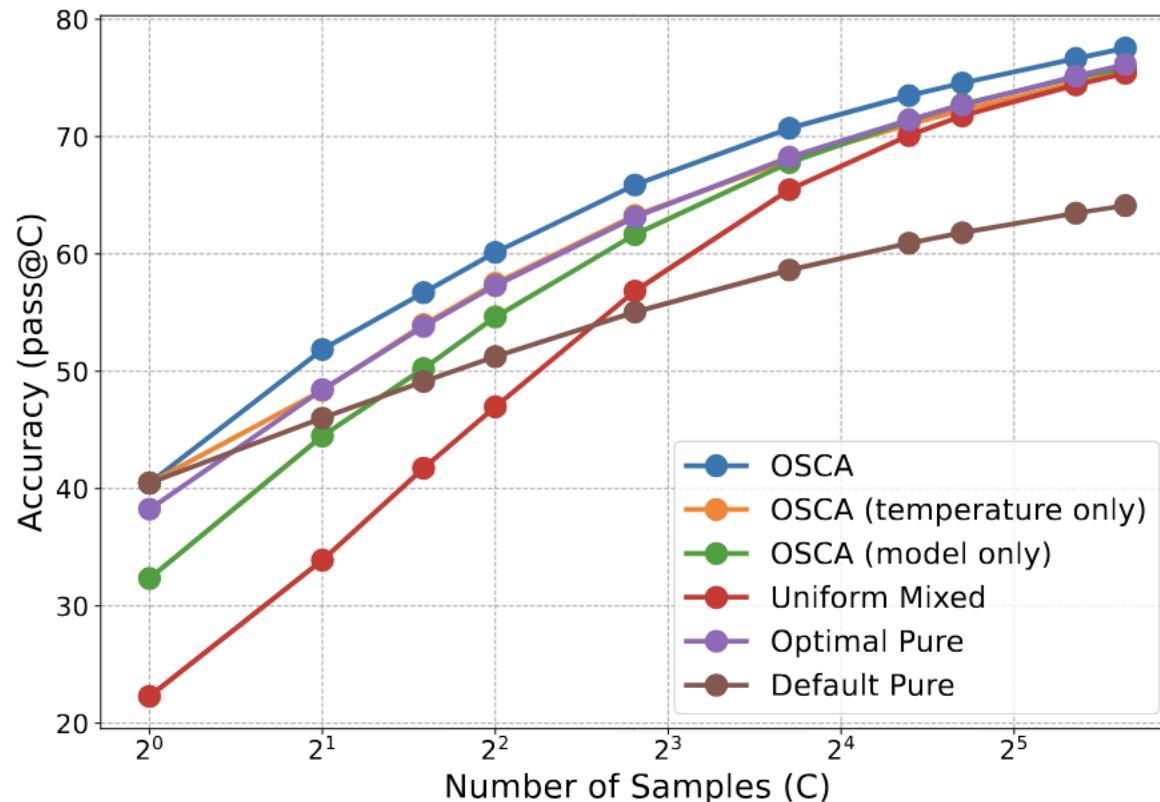


Figure 5: OSCA's pass rates on LiveBench when it is banned from allocating compute to multiple temperatures or multiple models.



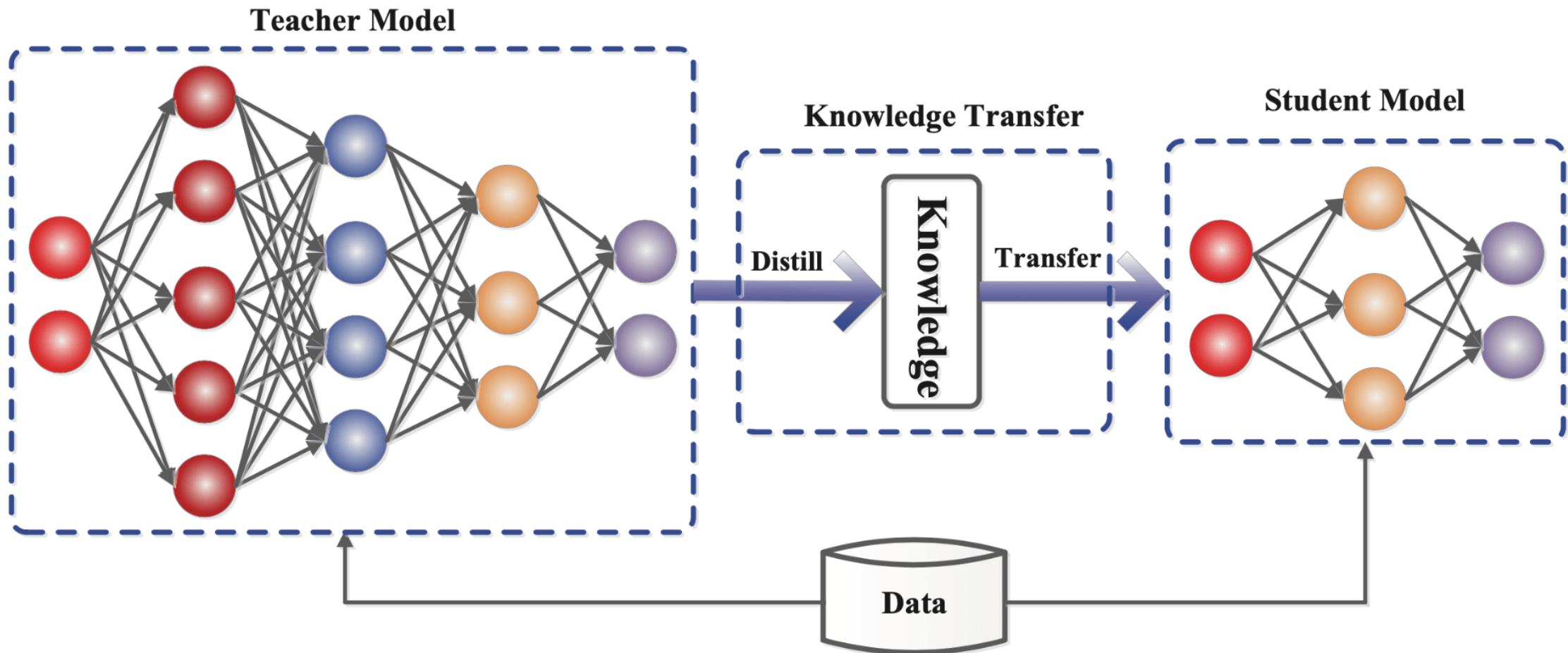
Highlight of OSCA

- LLM's problem solve-rate grows log-linearly with # of samples.
- Allocating compute to different inference settings could lead to huge improvement
- Estimating the passing rate for each problem and each configuration
- Hill-climbing to find the optimal allocation

Outline

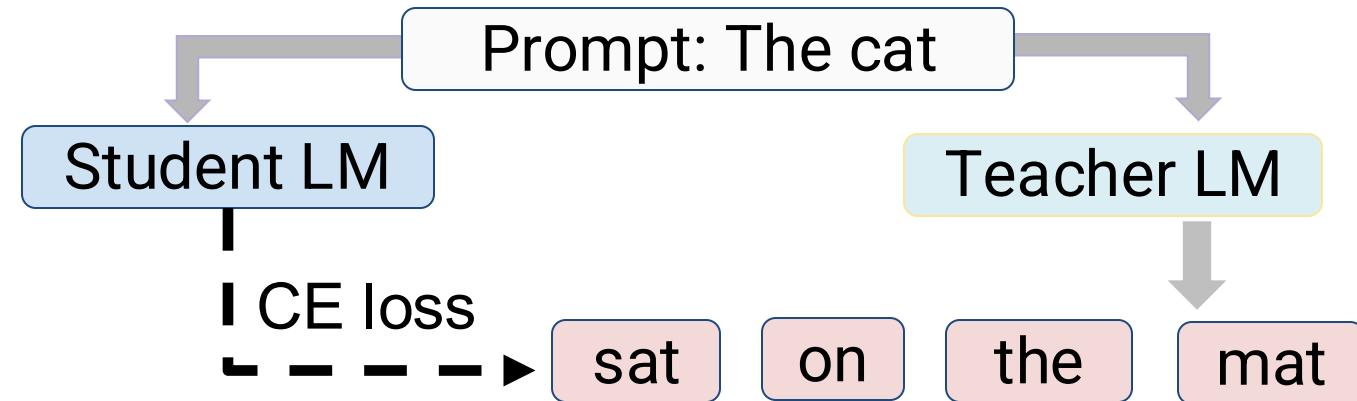
- Aligning with online preference optimization (BPO)
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- Speculative Knowledge Distillation

Knowledge Distillation

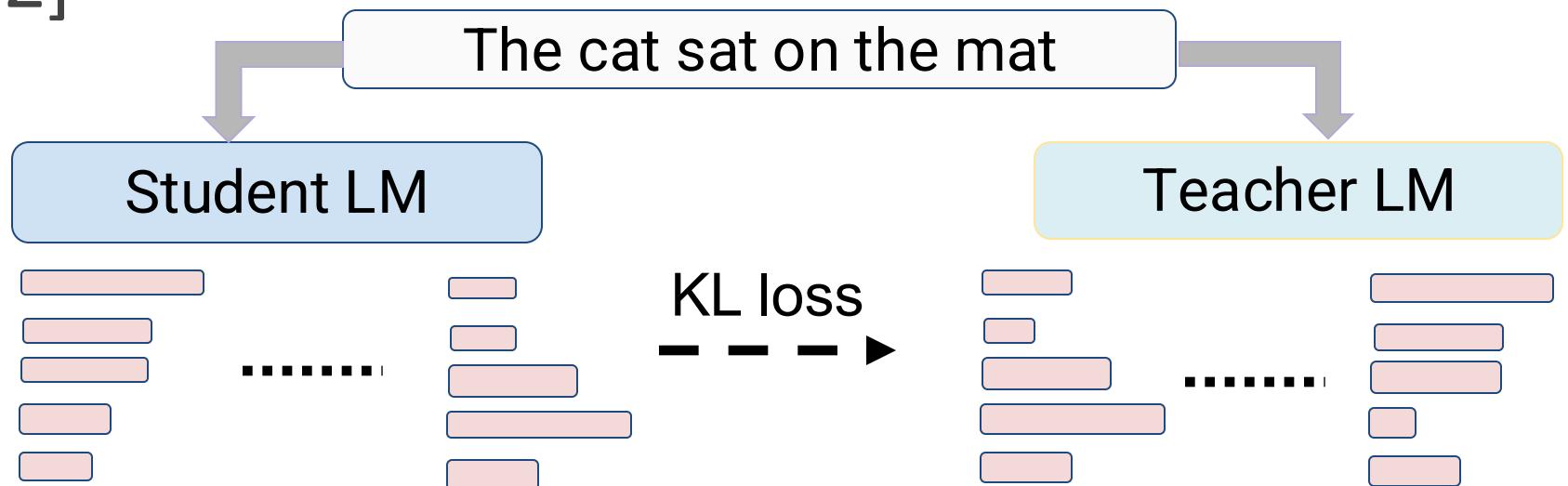


LLM Distillation Approaches

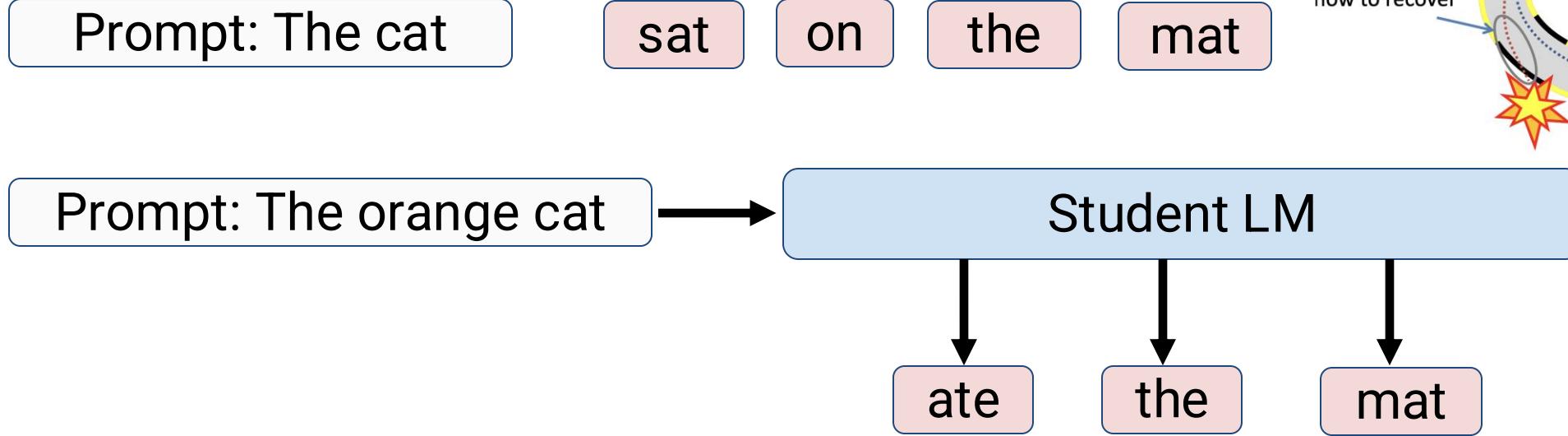
1) Sequence-Level KD [1]



2) Supervised KD [2]



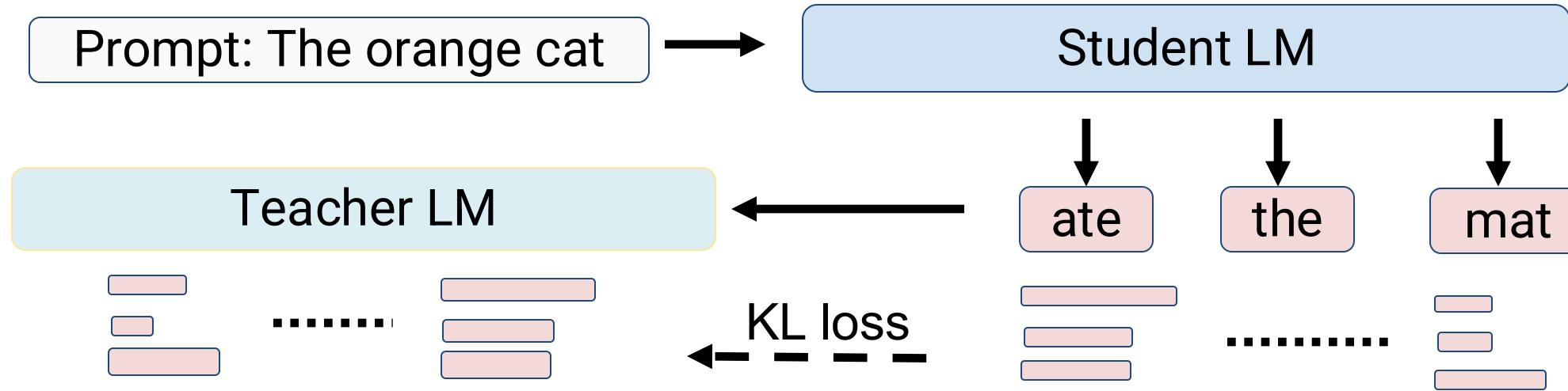
Drawbacks of supervised KD



Supervised KD

- Fixed dataset -> training and inference mismatch
- Student model never learns to correct previous mistakes

On-policy KD can help but not perfect!



On-policy KD

- Low quality student samples makes convergence harder
- Inaccurate assessment from teacher

On-policy KD generates low-quality samples

Prompt : Translate Assamese sentence into English.

Reference : It was to last for the next 40 years and would be fought for real, by proxy armies, on battlefields from Africa to Asia, in Afghanistan, Cuba and many other places.

On-policy (COMET: 36) : This has been a long war, and has been fought in the past, in the past.....

SKD (COMET: 72): This has been going on for 40 years and is still ongoing, with the possibility of war, a civil war, Afghans in the Balkans, Ethiopia, Kenya, Somalia, and possibly even the United States

On-policy samples are OOD to teacher

Student Gemma-2b-it	On-policy	SKD (Interleaved)	Supervised KD
Teacher PPL	46.8	10.8	1.57

Teacher samples are OOD to student

Student Gemma-2b-it	On-policy	SKD (Interleaved)	Supervised KD
Student PPL	44.0	358	5606.3

Speculative KD: Interleaved text sampling

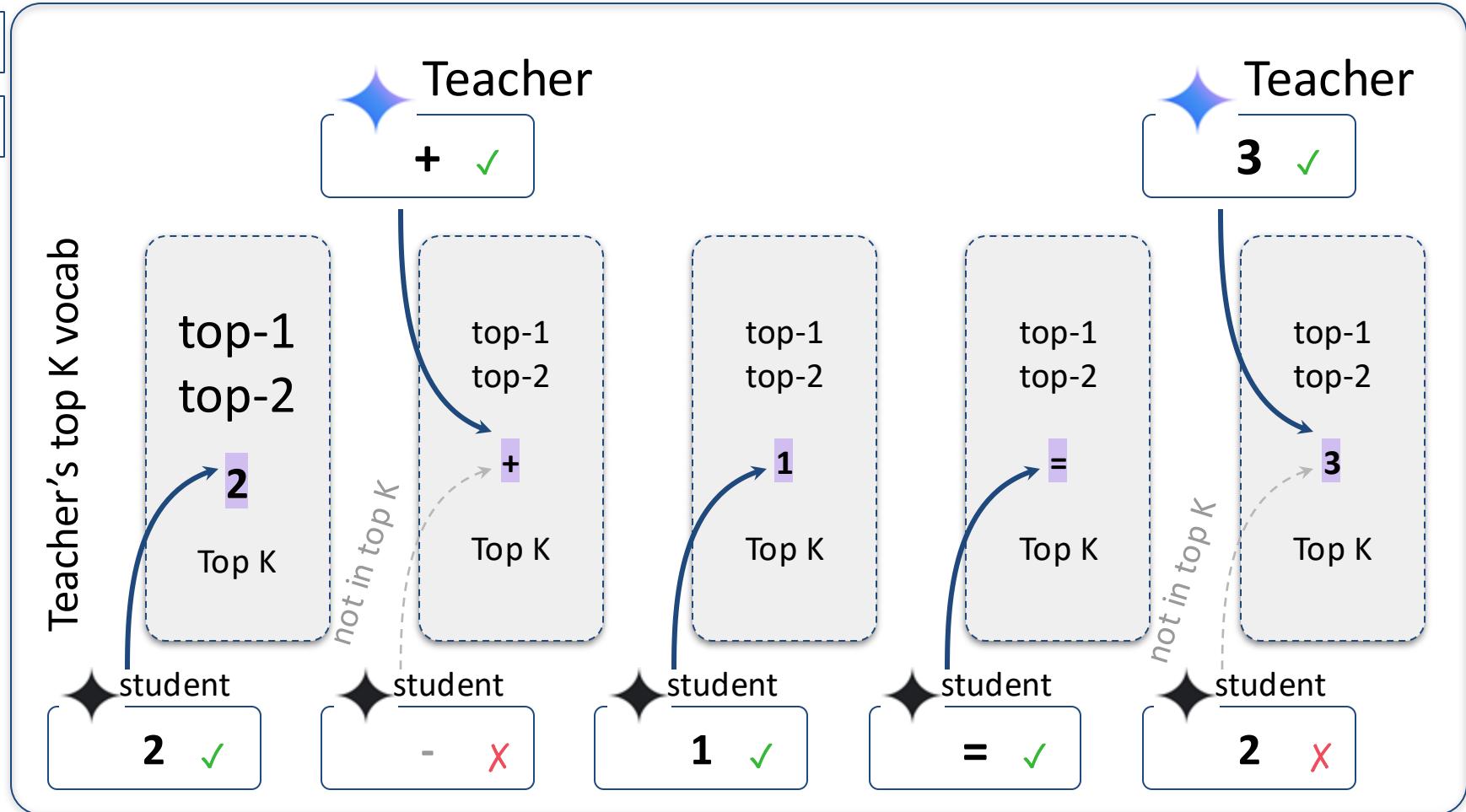
Input

Bob ate two apples yesterday and ate one apple today.
How many apples did he eat? Think step by step.

Output

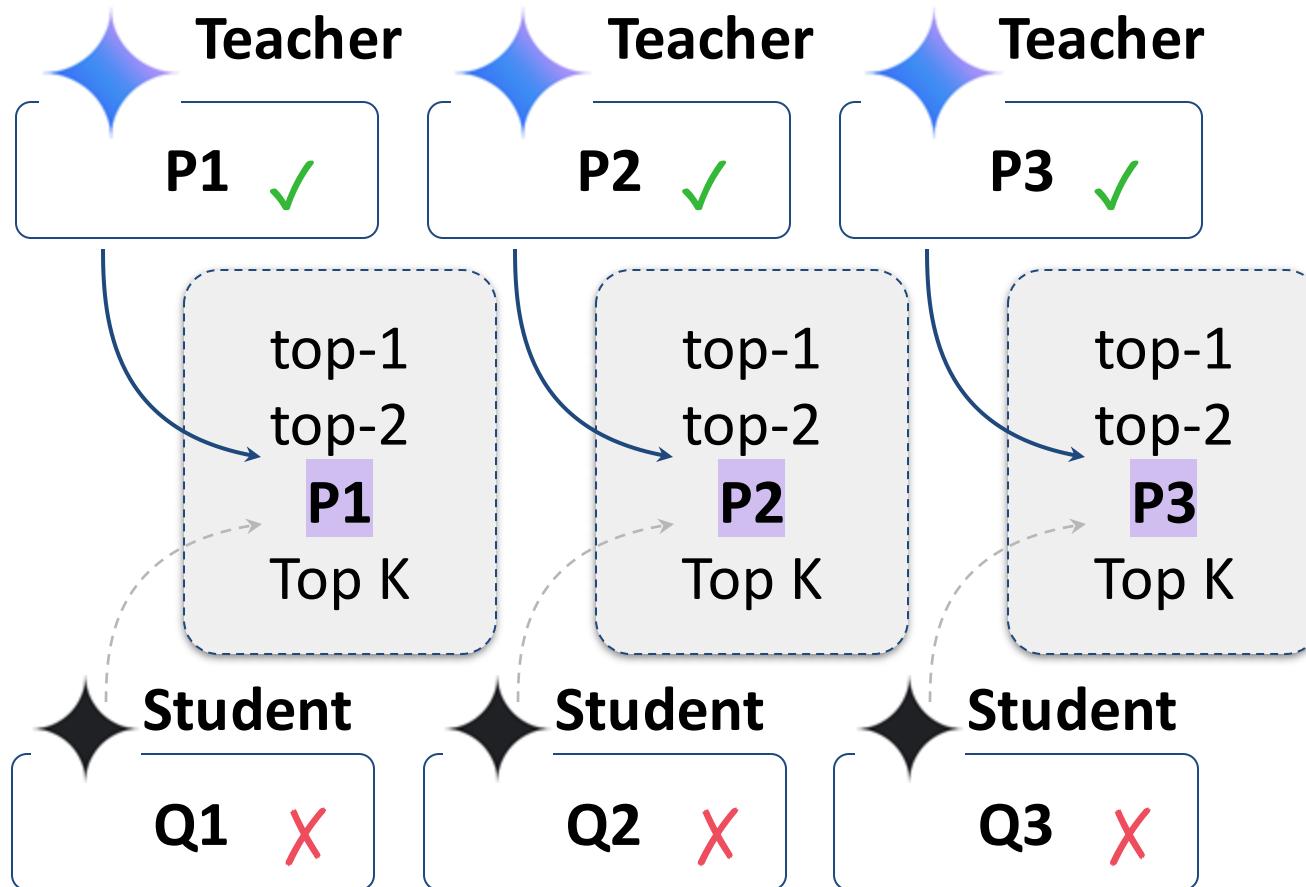
On-Policy KD: $2-1=2$

SKD (ours): $2+1=3$



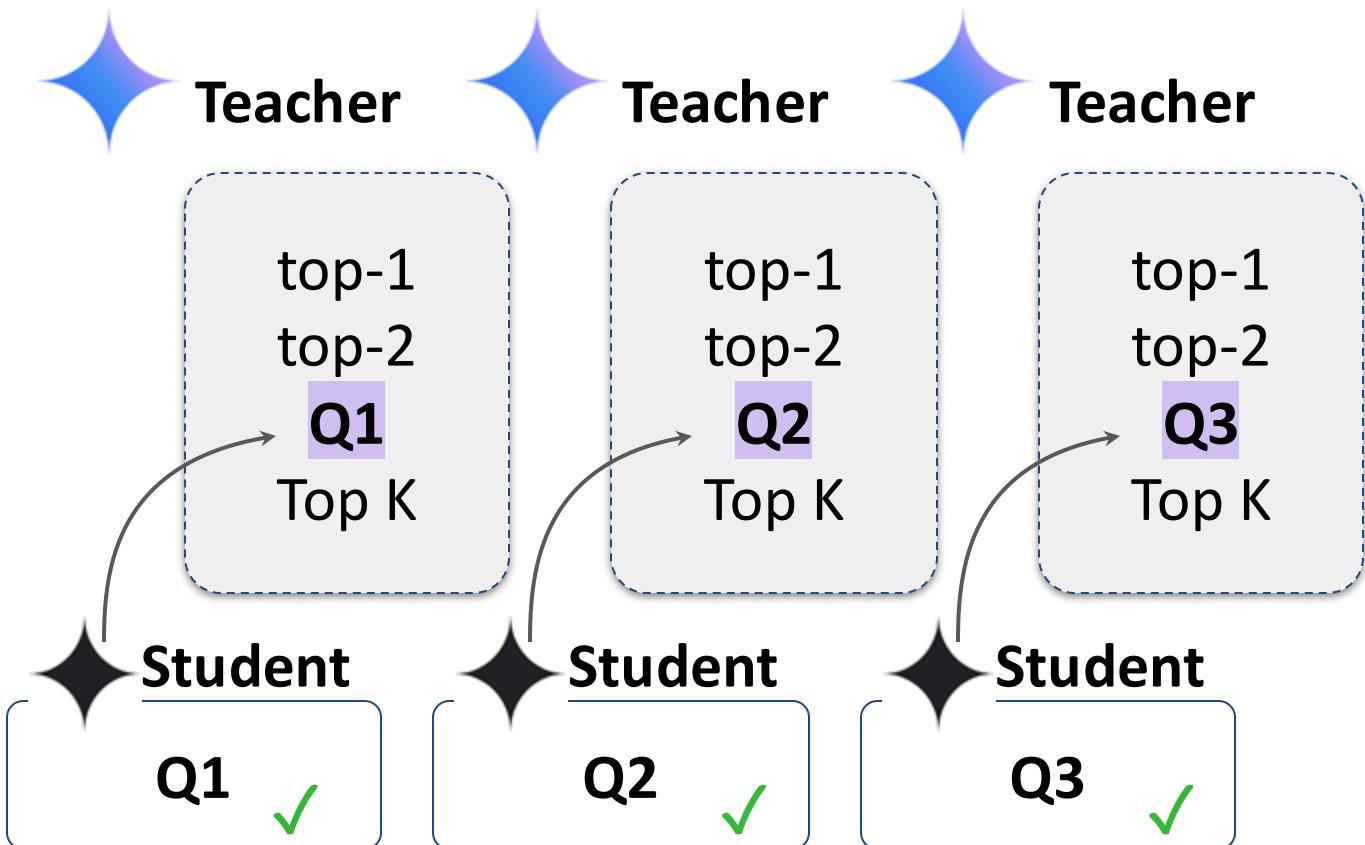
SKD degenerates to Supervised KD

SKD degenerates to **Supervised KD** when the teacher rejects all tokens proposed by the student



SKD degenerates to On-policy KD

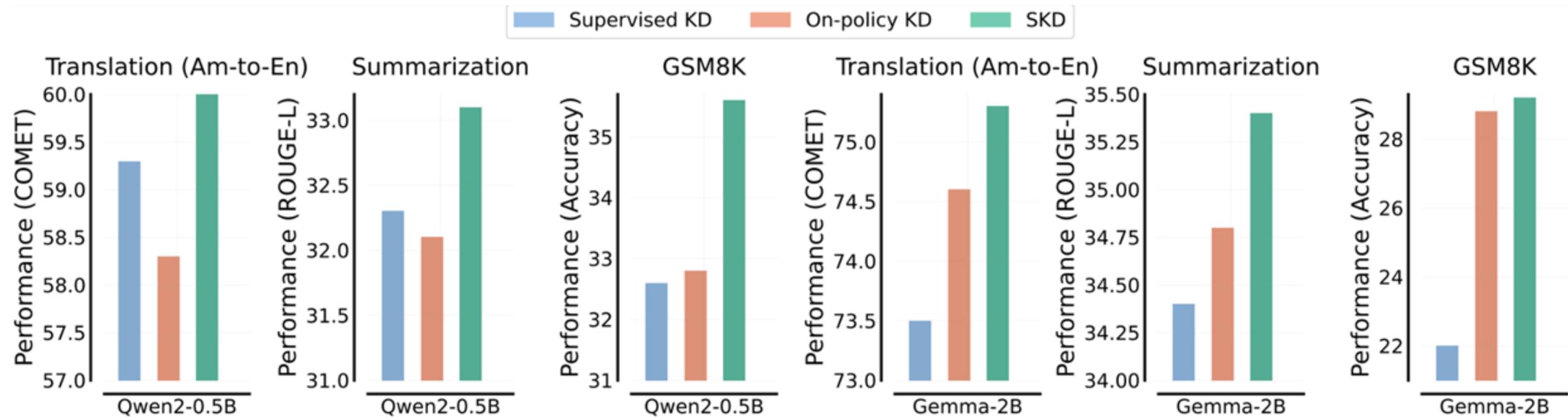
SKD degenerates to **On-policy KD** when the teacher accepts all tokens proposed by the student



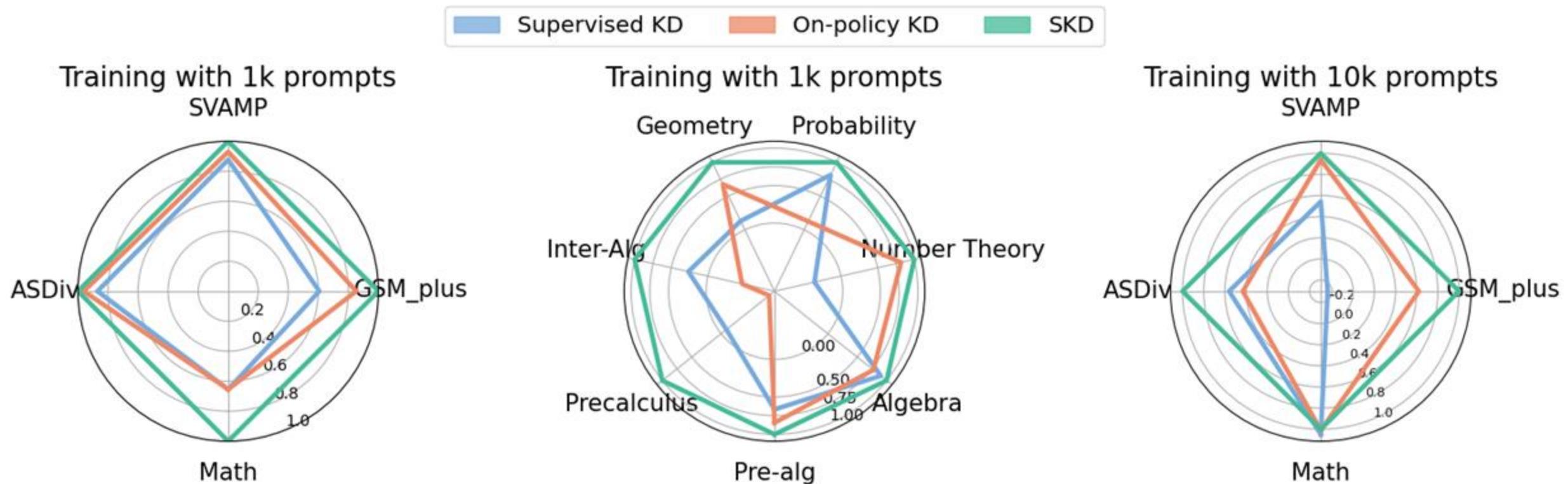
Evaluation Setup

- Tasks:
 - Translation (Am-En), Dialogue summarization,
 - Arithmetic reasoning (GSM-8k) and Math instruction following task
- Baselines:
 - SFT, Supervised KD, on-policy KD and ImitKD
- Base Model:
 - Teacher: Gemma-7B and Qwen2-7B
 - Student: Gemma-2B and Qwen2-0.5B

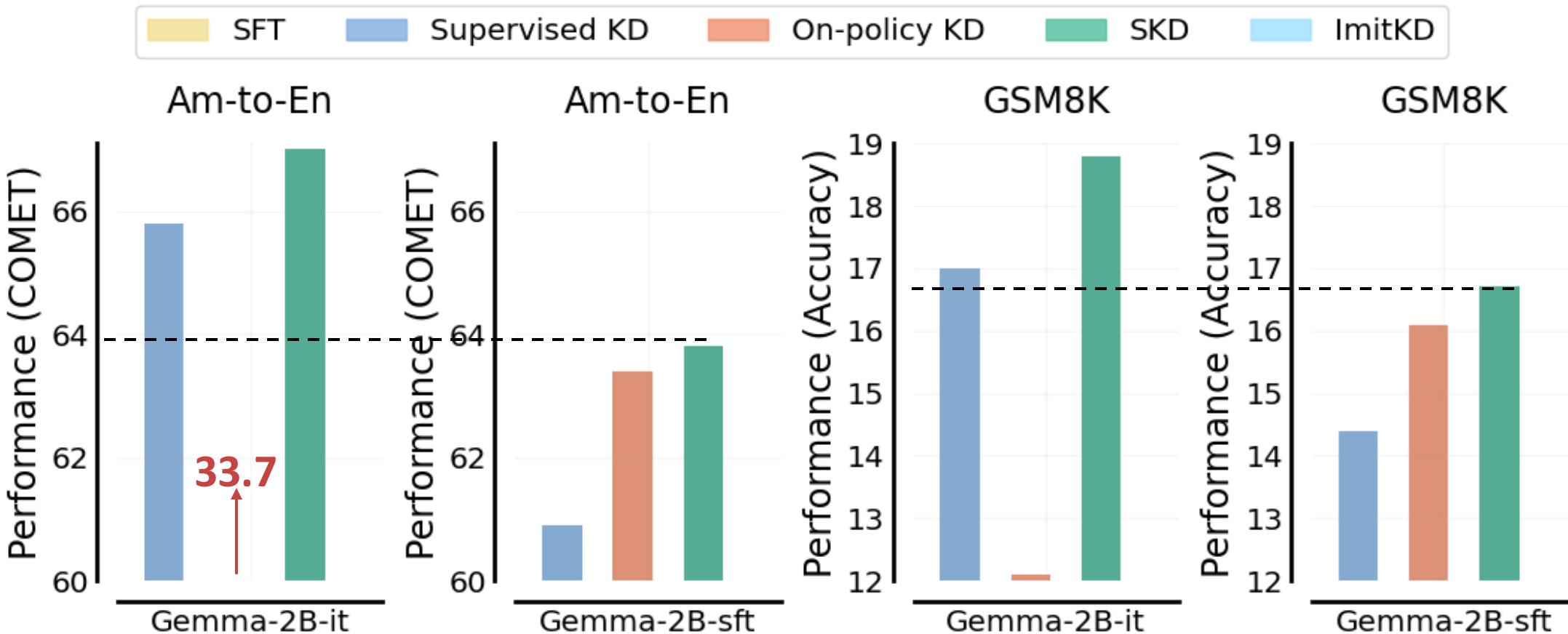
SKD outperform all baselines in task-specific distillation



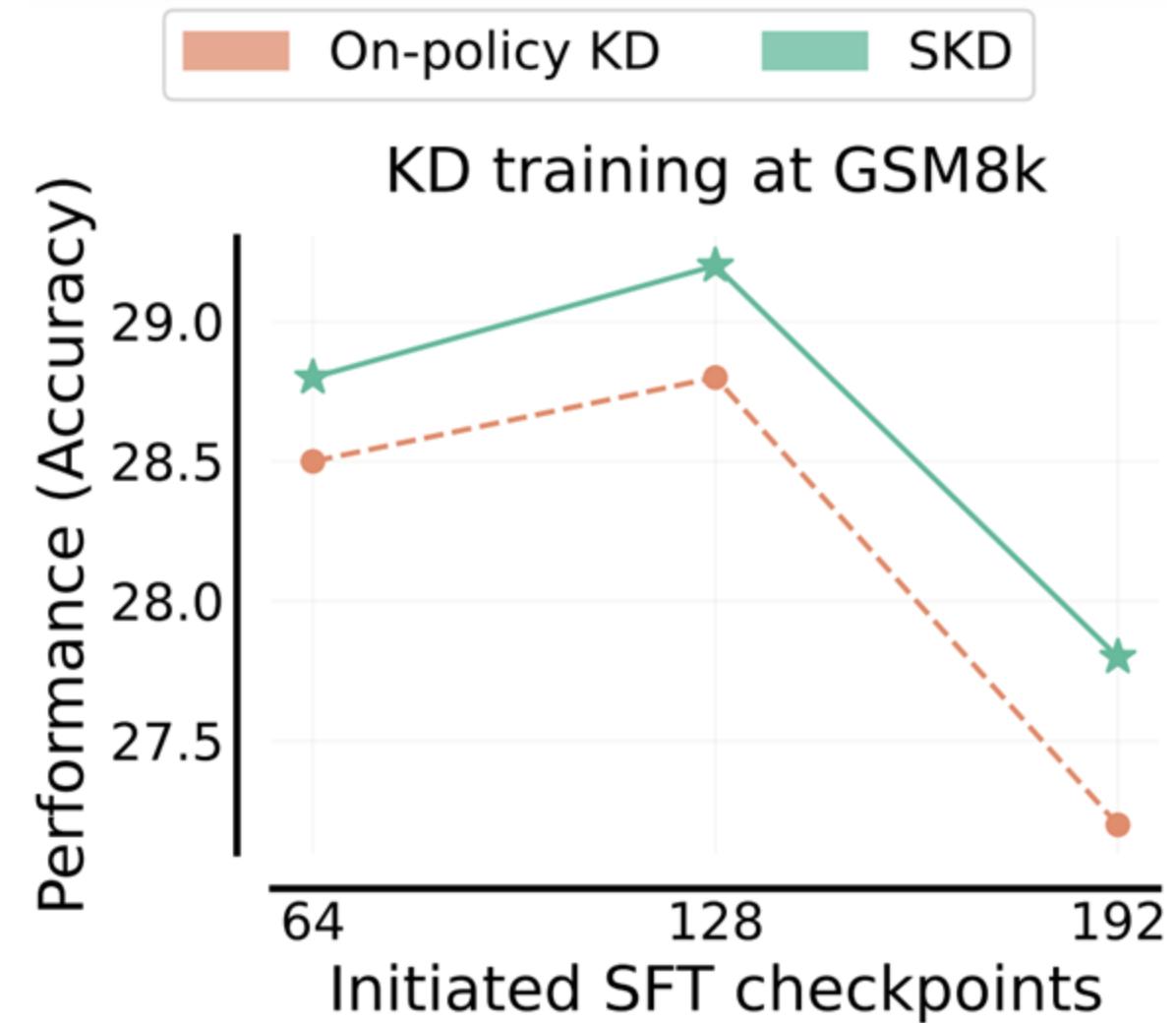
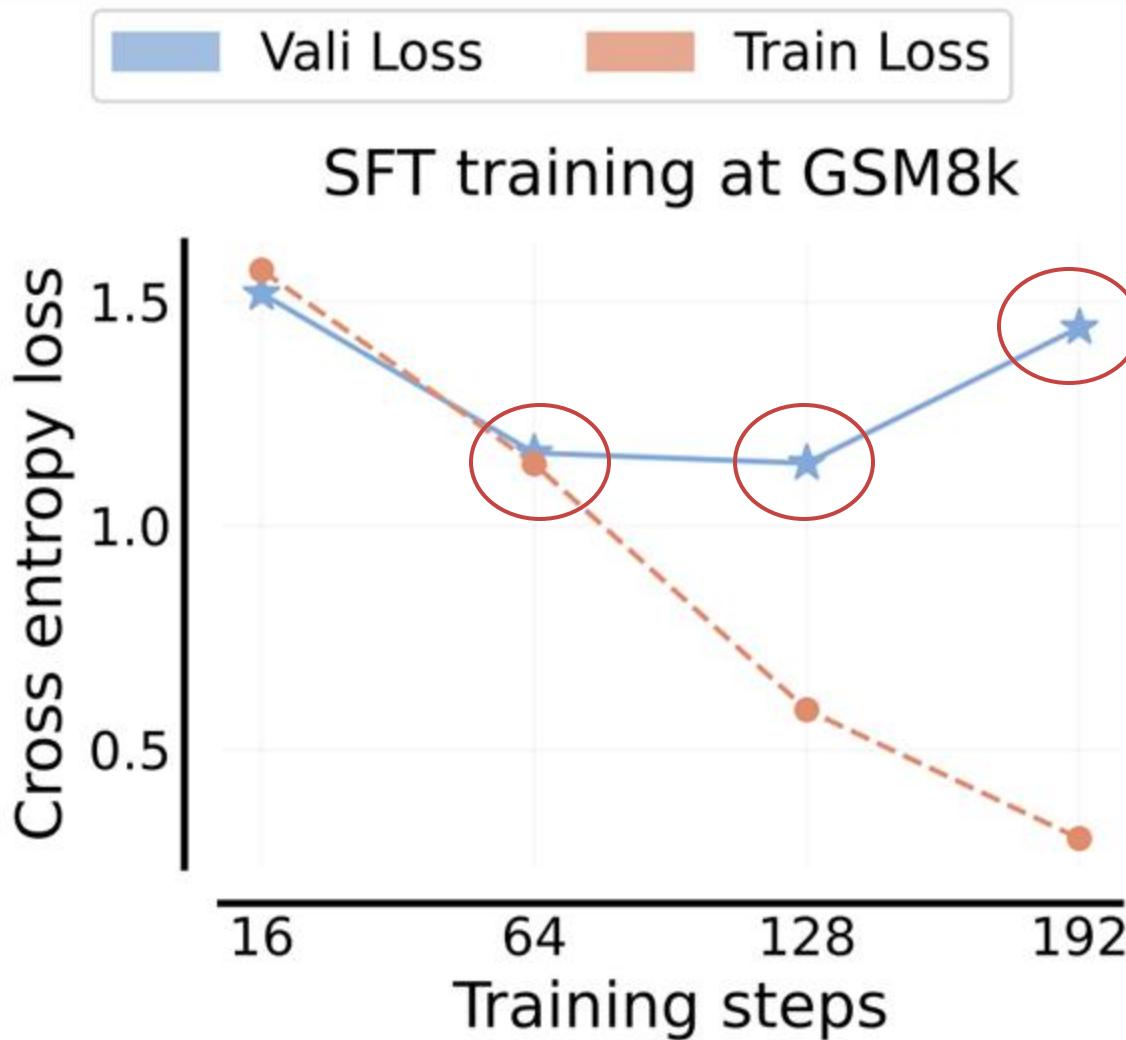
SKD outperforms all baselines in task-agnostic distillation



SKD outperforms all baselines under low data regime (100 data points)



Overfitting at SFT stage is bad for KD



Highlights of SKD

- SKD mitigate training-inference mismatch
- SKD reduces low-quality samples from poor student
- Superior performance than supervised KD and on-policy KD across various text generation tasks in both task-specific and task-agnostic scenarios.
- More robust to different initialization.

Summary and Takeaway

- Aligning with online preference optimization (BPO)
 - online and on-policy alignment is better
- Iterative refinement with fine-grained feedback (LLMRefine)
 - simulated annealing with fine-grained feedback improves LLM
- Learning Optimized Sample Compute Allocation (OSCA)
 - sample compute configuration as hyperparameters to optimize
- Speculative Knowledge Distillation for LLM
 - an adaptive version of supervised seq and on-policy distillation

Reference

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- Wenda Xu, Jiachen Li, William Yang Wang, Lei Li. BPO: Staying Close to the Behavior LLM Creates Better Online LLM Alignment. EMNLP 2024.
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