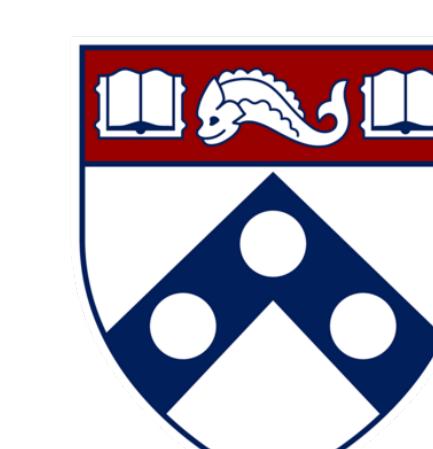


# One-Shot Safety Alignment for Large Language Models via Optimal Dualization

Xinmeng Huang\*†  
Osbert Bastani

Shuo Li\*†  
Hamed Hassani

Edgar Dobriban  
Dongsheng Ding†



Penn  
UNIVERSITY OF PENNSYLVANIA



## MOTIVATION

### Safety requirements for language models (LM)

1. **MUST NOT** contain offensive or discriminatory content
2. **MUST NOT** fabricate content and spread misinformation
- ...

### Constraining LMs w/ safety requirements

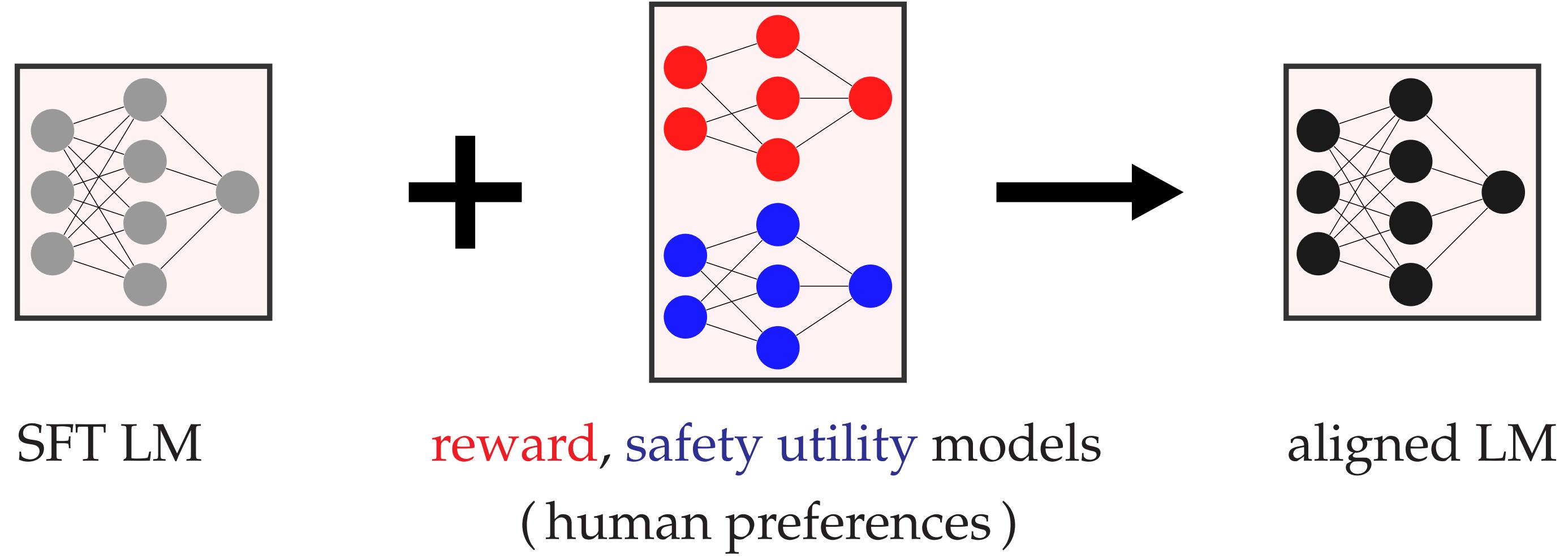
- Safe RLHF (ICLR 2024)
- Constrained RLHF (ICLR 2024)
- Constrained DPO (arXiv 2023)
- SACPO (arXiv 2024)

**Hurdle** • instability of iterative training • no optimality certificate

Can we align LMs w/ safety constraints in a **one-shot** way?

## PROBLEM FORMULATION

### LM alignment via human feedback



- $(x, y) \in \mathcal{X} \times \mathcal{Y}$  – (prompt, response)
- $\pi_{\text{ref}}(\cdot | x) \in \Delta(\mathcal{Y})$  – SFT LM
- $r(x, y), g_j(x, y), j = 1, \dots, m$  – reward, safety utility models

### Constrained alignment problem

$$\begin{aligned} \max_{\pi \in \Pi} \quad & \mathbb{E}_x [\mathbb{E}_{y \sim \pi(\cdot | x)} [r(x, y)] - \beta \text{KL}(\pi(\cdot | x) \| \pi_{\text{ref}}(\cdot | x))] \\ \text{s.t.} \quad & \mathbb{E}_x [\mathbb{E}_{y \sim \pi(\cdot | x)} [g_j(x, y)] - \mathbb{E}_{y \sim \pi_{\text{ref}}(\cdot | x)} [g_j(x, y)]] \geq b_j \\ \bullet \quad & \Pi - \text{LM policy set} \quad \bullet \quad b_j - \text{safety margin} \quad j = 1, \dots, m \end{aligned}$$

## OPTIMAL DUALIZATION

### Dual problem

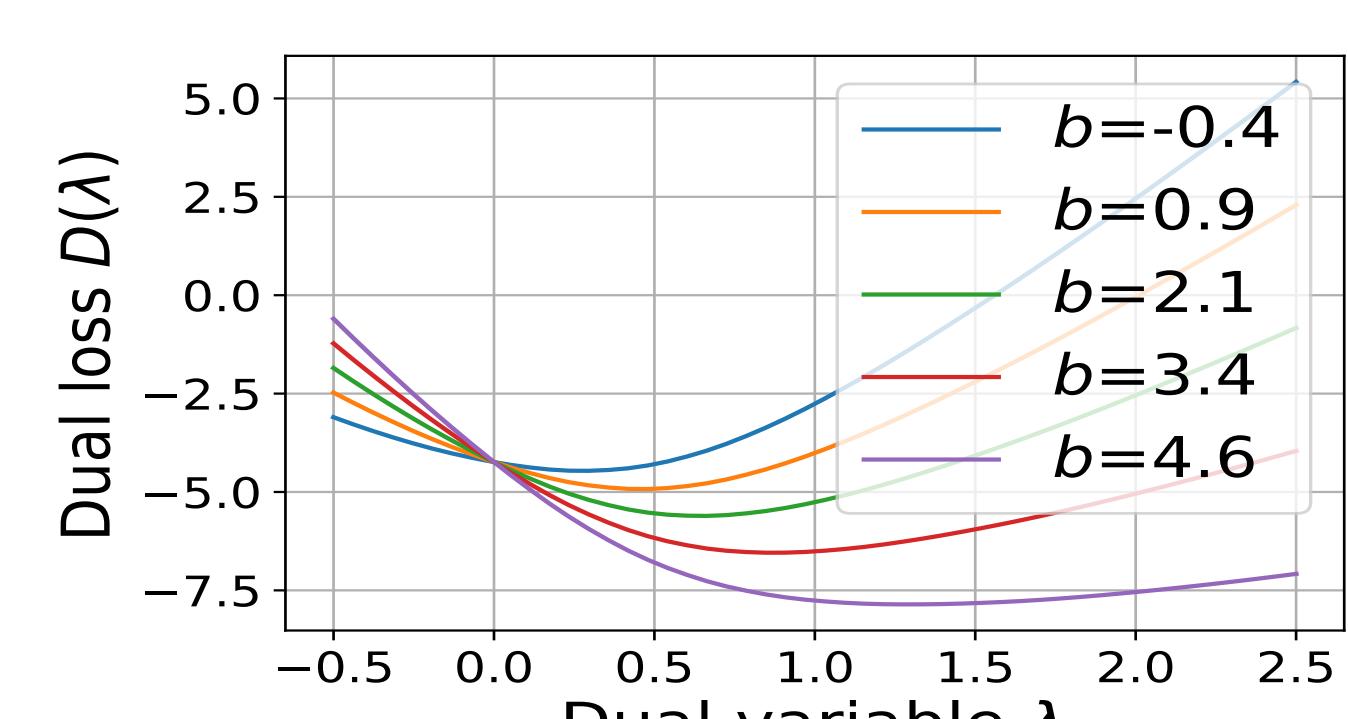
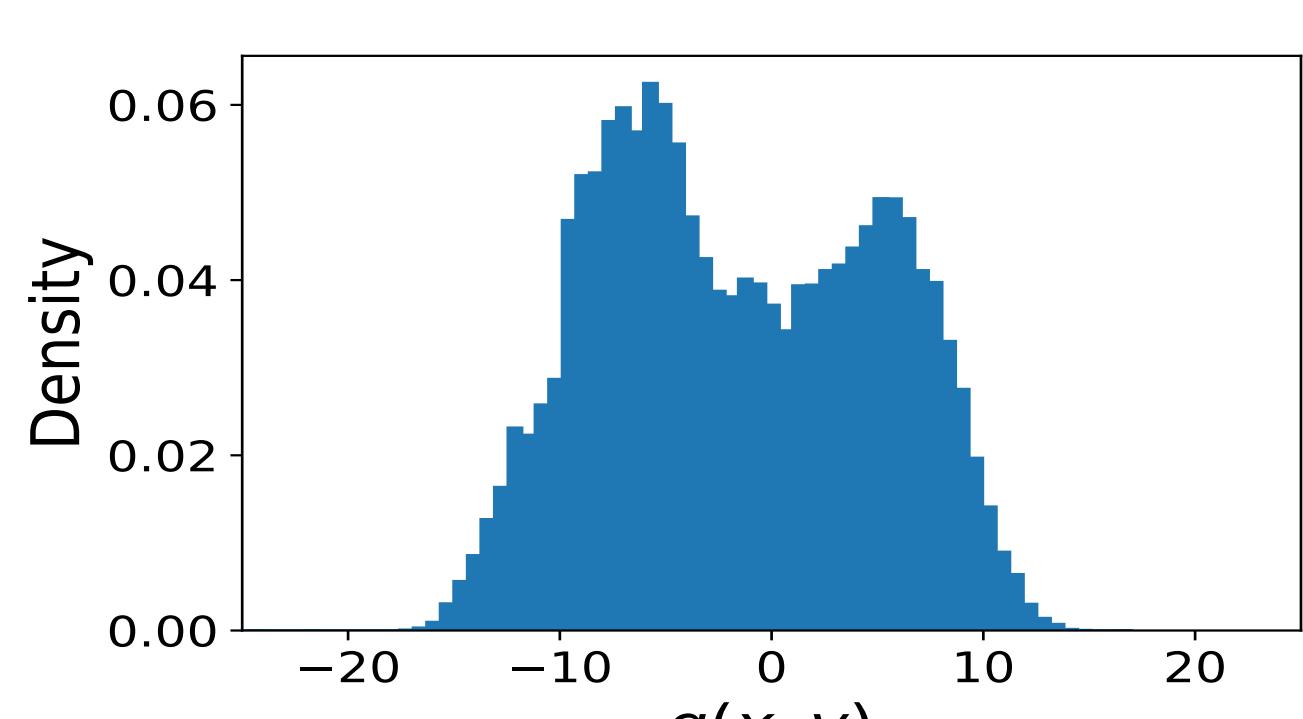
$$\underset{\lambda \geq 0}{\text{minimize}} \quad D(\lambda) := \underset{\pi \in \Pi}{\text{maximize}} \quad L(\pi, \lambda)$$

- $L(\pi, \lambda)$  – Lagrangian
- $= \mathbb{E}_x \mathbb{E}_{y \sim \pi(\cdot | x)} [r(x, y)] - \beta \text{KL}(\pi(\cdot | x) \| \pi_{\text{ref}}(\cdot | x))$  objective
- $+ \sum_{j=1}^m \lambda_j \mathbb{E}_x \mathbb{E}_{y \sim \pi(\cdot | x)} [h_j(x, y)]$  safety violation
- $h_j(x, y) := g_j(x, y) - \mathbb{E}_{\pi_{\text{ref}}} [g_j(x, y)] - b_j$  – shifted safety utility
- $L(\pi^*, 0) = D(\lambda^*)$  for an optimal pair  $(\pi^*, \lambda^*)$  – **strong duality**

### Explicit dual function

$$D(\lambda) = \beta \mathbb{E}_x \left[ \ln \mathbb{E}_{y \sim \pi_{\text{ref}}(\cdot | x)} \left[ \exp \left( \frac{r(x, y) + \lambda^\top h(x, y)}{\beta} \right) \right] \right]$$

- $(\pi^*, \lambda^*)$  – **uniqueness** of optimal primal-dual pair
- $D$  – smooth & **strongly convex** at the unique  $\lambda^*$



## ONE-SHOT SAFETY ALIGNMENT

### Constrained Alignment via dualizatioN (CAN)

**Stage 1** Optimal dual:  $\lambda^* = \arg \min_{\lambda \geq 0} D(\lambda)$

**Stage 2** Update LM:  $\pi^* = \arg \max_{\pi \in \Pi} L(\pi, \lambda^*)$

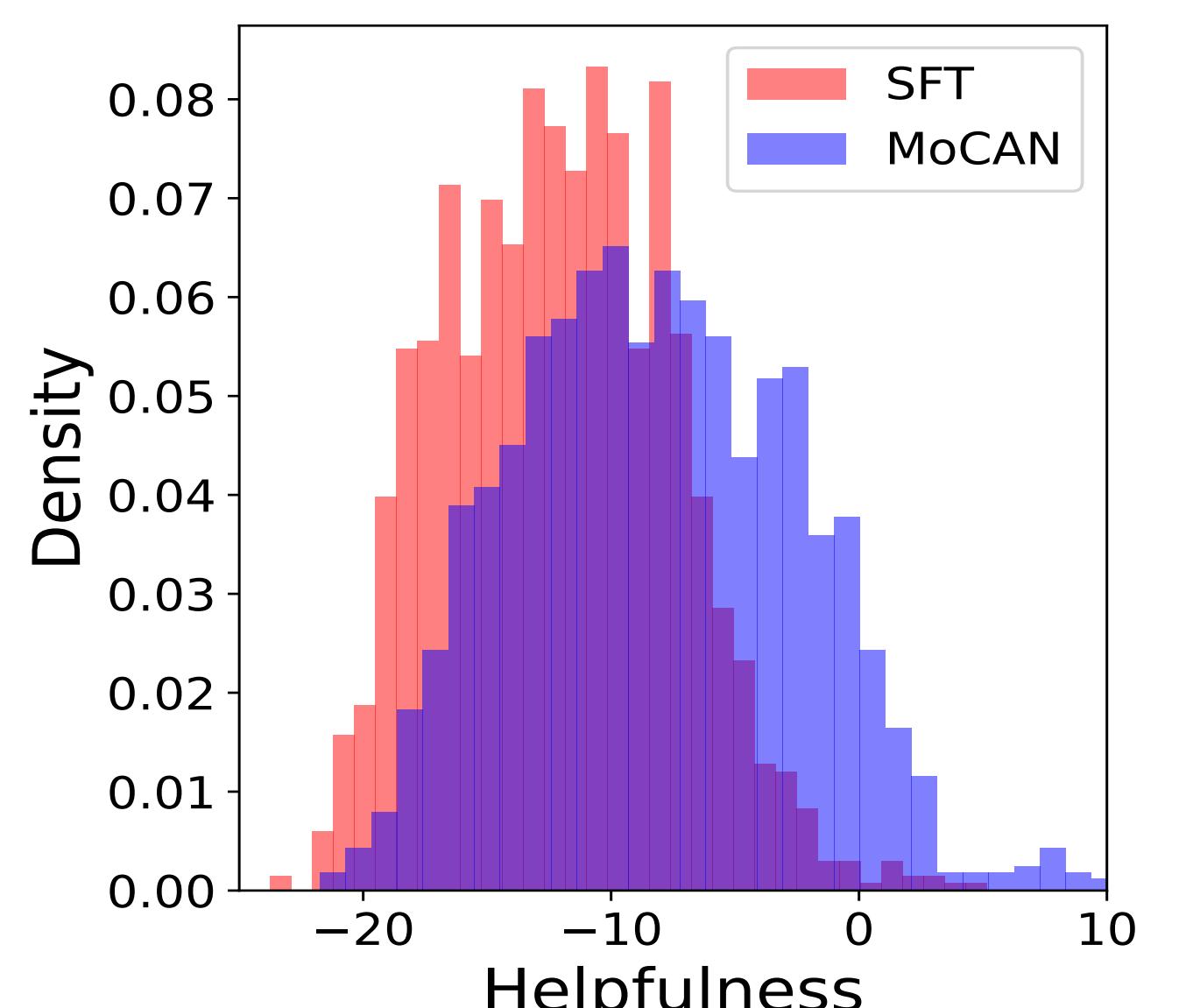
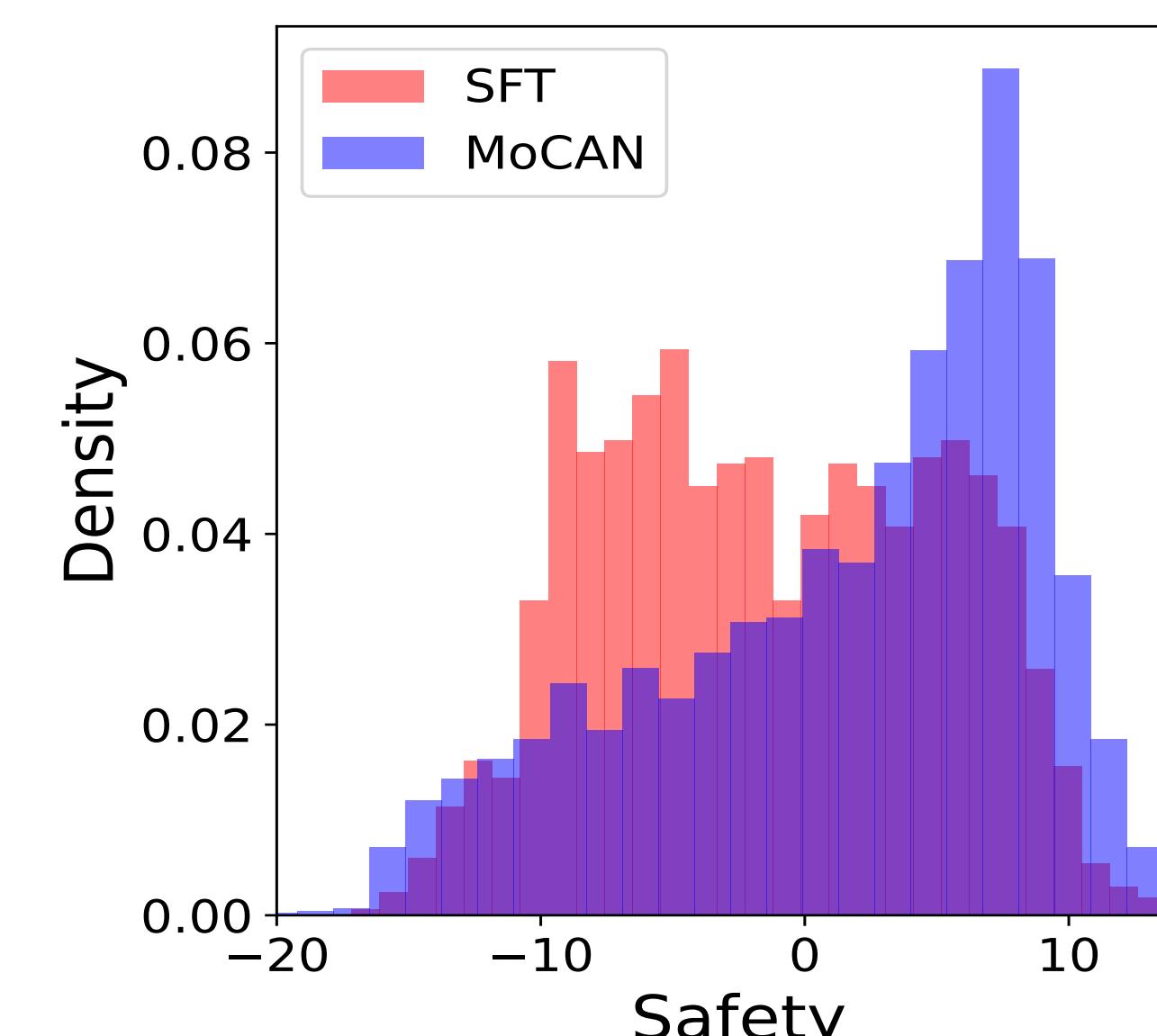
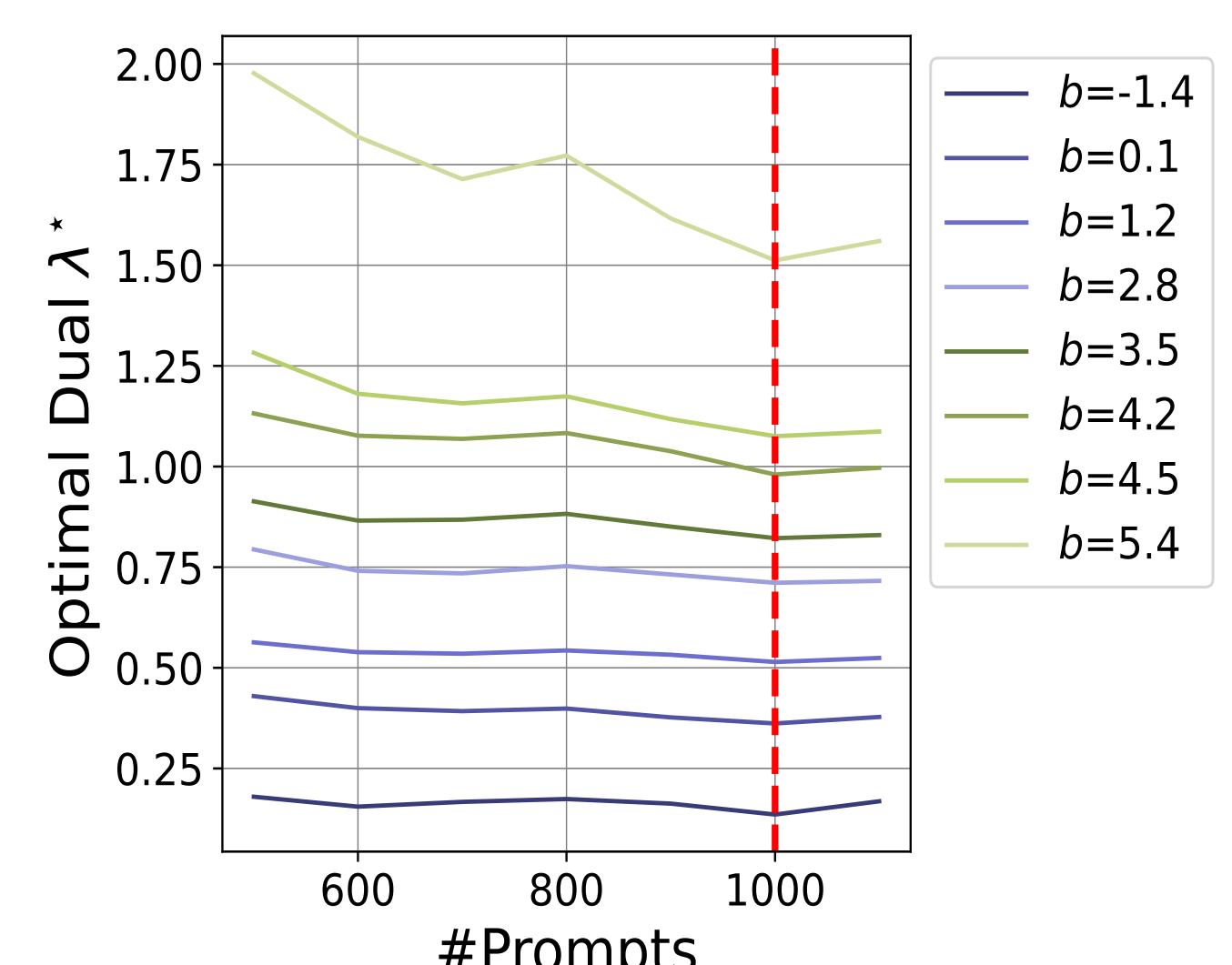
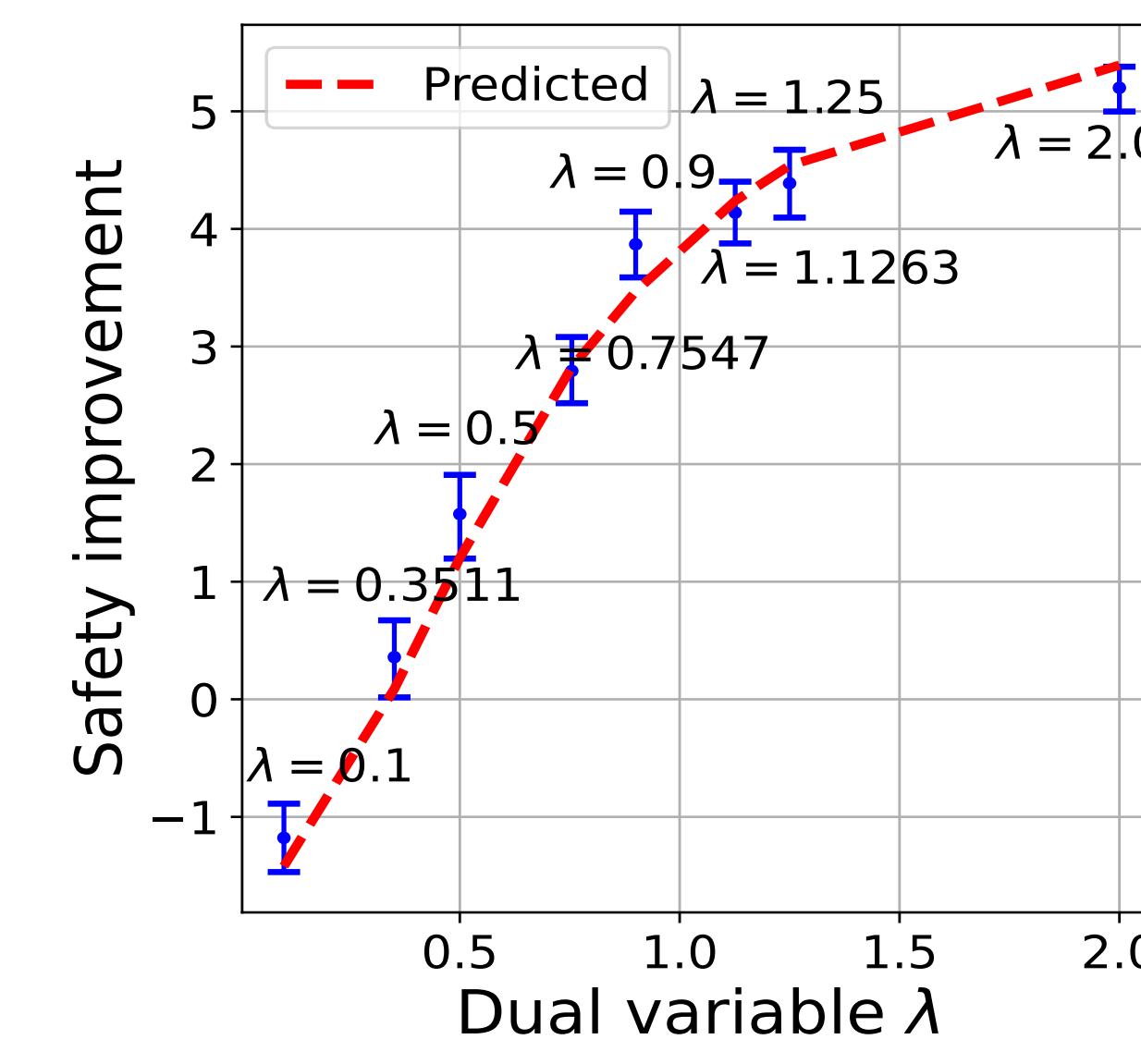
smooth convex optimization & unconstrained alignment

**Advantages** • optimality of LM • stability of safety training

## PRACTICAL IMPLEMENTATION & EVALUATION

### Model-based CAN (MoCAN)

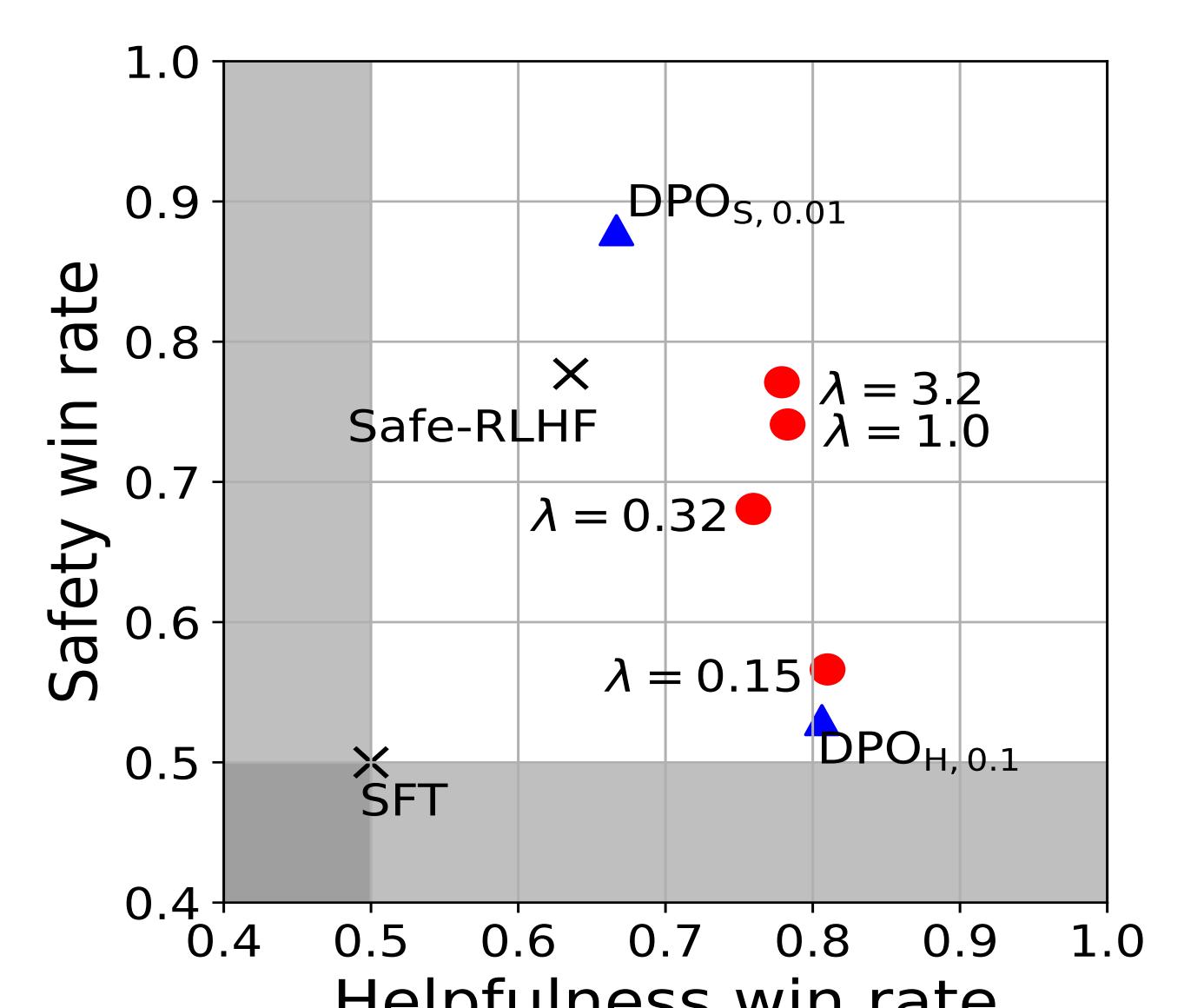
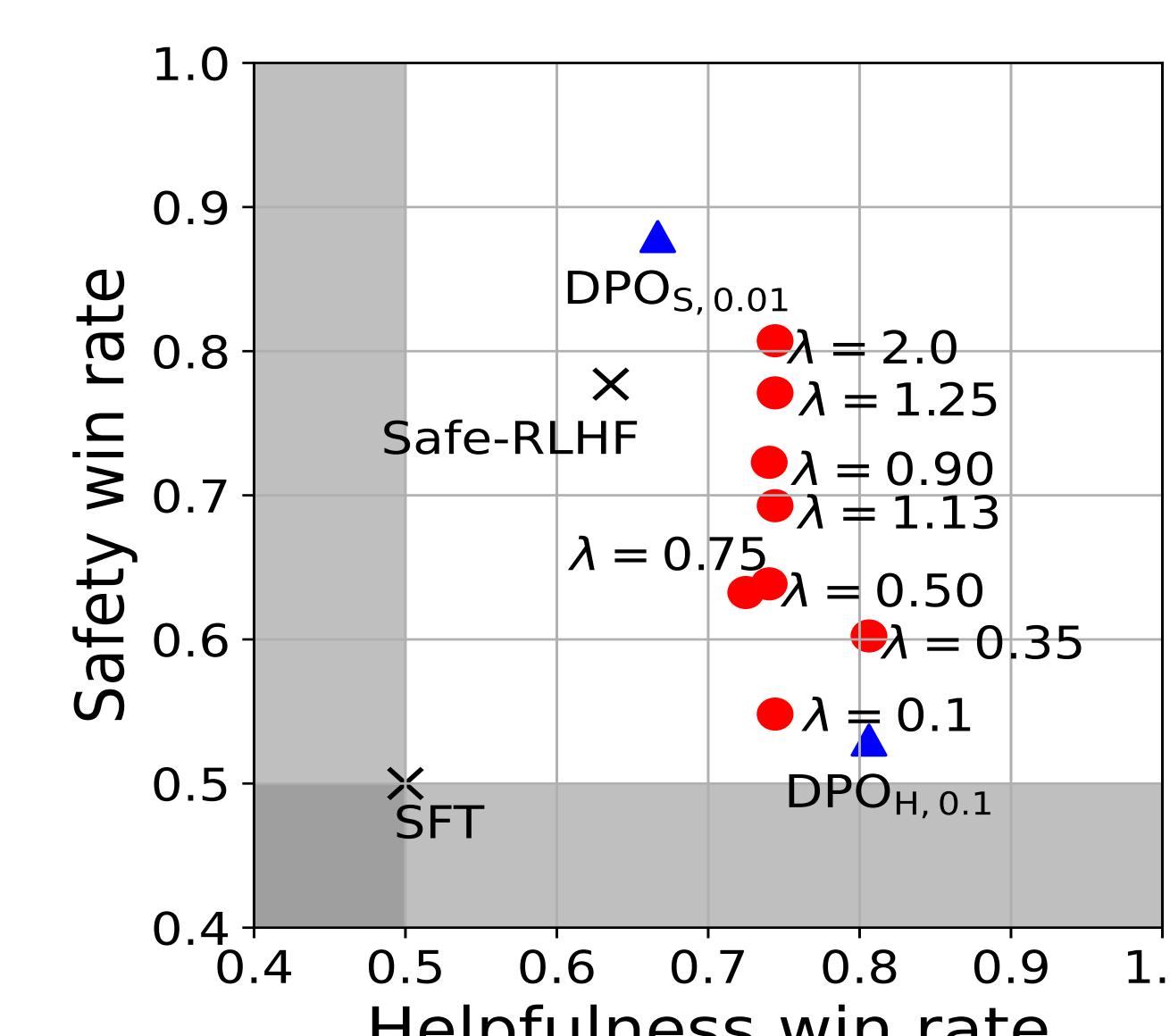
1. collect **offline data**  $(r(x, y), g(x, y))$ -pairs; estimate  $h(x, y)$
2. find the optimal dual  $\lambda^*$  using **model-based**  $D(\lambda)$
3. update LM w/ **pseudo preference** from  $r + (\lambda^*)^\top g$



### Preference-based CAN (PeCAN)

1. obtain unconstrained **pre-aligned models**  $(\pi_{\theta_r}, \pi_{\theta_g})$
2. collect **offline**  $(\ln \pi_{\text{ref}}(y | x), \ln \pi_{\theta_r}(y | x), \ln \pi_{\theta_g}(y | x))$ -tuples
3. estimate **KL terms**  $\text{KL}(\pi_{\text{ref}} \| \pi_{\theta_{g_j}})$ ,  $j = 1, \dots, m$
4. find the optimal dual  $\lambda^*$  using **preference-based**  $D(\lambda)$
5. update LM w/ **pseudo preference** from  $\beta \ln \frac{\pi_{\theta_r}}{\pi_{\text{ref}}} + \beta (\lambda^*)^\top \ln \frac{\pi_{\theta_g}}{\pi_{\text{ref}}}$

### Safety / helpfulness tradeoff (L: MoCAN, R: PeCAN)



### Key takeaways

- efficient dual optimization for safety improvement
- empirically optimal dual variable quickly stabilizes
- **MoCAN** finds the optimal safe LM in one-shot
- **PeCAN** performs similarly if pre-aligned models are accurate