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EMA Policy Gradient: Taming Reinforcement Learning for LLMs with EMA Anchor and Top-k KL

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Abstract

Reinforcement Learning (RL) has enabled Large Language Models (LLMs) to acquire increasingly complex reasoning and agentic behaviors. In this work, we propose two simple techniques to improve policy gradient algorithms for LLMs. First, we replace the fixed anchor policy during RL with an Exponential Moving Average (EMA), similar to a target network in deep Q-learning. Second, we introduce Top-k KL estimator, which allows for flexible interpolation between exact KL and sampled KL. We derive the stability conditions for using EMA anchor; moreover, we show that our Top-k KL estimator yields both unbiased KL values and unbiased gradients at any k, while bringing the benefits of exact KL. When combined with GRPO, the two techniques (**EMA-PG**) lead to a significant performance boost. On math reasoning, it allows R1-distilled Qwen-1.5B to reach 53.9% on OlympiadBench compared to 50.8% by GRPO. On agentic RL domains, with Qwen-3B base, EMA-PG improves GRPO by an average of 35.6% across 7 datasets of Q&A with search engines, including 29.7% $\rightarrow$ 45.8% on HotpotQA, 27.4% $\rightarrow$ 40.5% on 2WikiMultiHopQA. Overall, we show that EMA-PG is a simple, principled, and powerful approach to scaling RL for LLMs. Code: github.com/LunjunZhang/ema-pg.

1. Introduction

As the pre-training paradigm began to show diminishing returns for large-language models (LLMs), reinforcement learning (RL) has re-emerged as a powerful mechanism for LLMs to continually self-improve based on self-generated experience. While RL was initially only used for alignment within the RL from Human Feedback (RLHF) framework (Christiano et al., 2017; Ouyang et al., 2022; Bai et al., 2022a;b), it has since then been applied to reasoning models such as o1 (Jaech et al., 2024) and R1 (Guo et al., 2025). Perhaps surprisingly, the predominant RL algorithm for LLMs today is still REINFORCE (Williams, 1992; Sutton et al., 1999) and its modern off-policy variants like PPO (Schulman et al., 2017b), GRPO (Shao et al., 2024), and CISPO (Chen et al., 2025). This motivates us to study the foundational building blocks of policy gradient algorithms, so that such advancements can be broadly applied to LLMs.

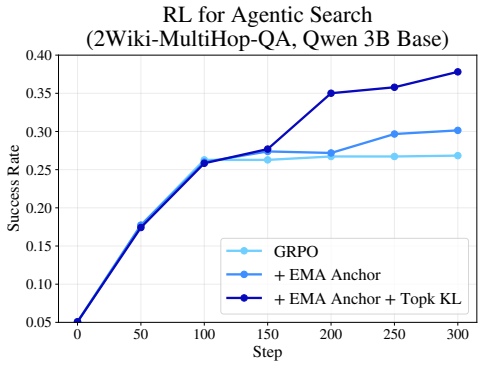


Figure 1. Using EMA anchor policy and Top-k KL estimator significantly improves the performance of RL algorithms like GRPO.

The use of a target network has been the common practice since the dawn of deep Q-learning (Mnih et al., 2015). A target network uses an Exponential Moving Average (EMA) to update its knowledge while producing stable supervision targets. Using EMA has seen success in self-supervised learning as well (Grill et al., 2020b). In RLHF, the idea of an EMA anchor policy has been explored in TR-DPO (Gorbatovski et al., 2024) and WARP (Ramé et al., 2024). A crucial difference between our work and theirs is how the EMA anchor is used: prior work optimizes sequence-level KL, but we optimize token-level KL, which we show makes a crucial difference in reasoning and agentic settings.

KL regularization is a key component of policy optimization. Initially, it was a way to enforce trust-region (Schulman et al., 2015) and ensure training stability. In LLM alignment, it mitigates reward hacking (Gao et al., 2023). In LLM reasoning, it helps preserve base model capabilities (Liu et al., 2025a). However, what KL estimator to use for LLM has long been a curious question. InstructGPT (Ouyang et al., 2022) adds a sequence-level sampled KL to the reward; GRPO (Shao et al., 2024) uses token-level sampled KL; the two objectives are different (Tang &

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Table 1. **Token-level KL Estimators**. For brevity, we omit the conditioning of π_θ and π_{ref} on past tokens. Notations: sg is stop-gradient, $p \sim \pi_\theta(\cdot)$ is the sampled token, $r = \pi_\theta(p)/\text{sg}(\pi_\theta(p))$, $w = \pi_{\text{ref}}(p)/\pi_\theta(p)$; $\mathcal{V}$ is the vocabulary, $\widehat{w}(j) = \pi_{\text{ref}}(j)/\pi_\theta(j), \forall j \in \mathcal{V}$. The estimators being highlighted in blue are the KL estimators that provide both unbiased KL values and unbiased KL gradients.

$\mathbb{E}_{\pi_\theta}[\hat{D}_f(\pi_\theta, \pi_{\text{ref}})]$	Expression	Value	Unbiased?	Gradient	Unbiased?	Memory	Overall
Reverse KL: exact	$\sum_{j\in\mathcal{V}} \pi_\theta(j)[-\log \widehat{w}(j)]$	$\text{KL}(\pi_\theta, \pi_{\text{ref}})$	✓	$\nabla_\theta \text{KL}(\pi_\theta, \pi_{\text{ref}})$	✓	$O(\lvert\mathcal{V}\rvert)$	×
K1	$-\log w$	$\text{KL}(\pi_\theta, \pi_{\text{ref}})$	✓	$\nabla_\theta 0$	×	$O(1)$	×
K2	$(\log w)^2/2$	$\mathbb{E}_{\pi_\theta}[(\log w)^2/2]$	×	$\nabla_\theta \text{KL}(\pi_\theta, \pi_{\text{ref}})$	✓	$O(1)$	×
K3	$-\log w + w - 1$	$\text{KL}(\pi_\theta, \pi_{\text{ref}})$	✓	$\nabla_\theta \text{KL}(\pi_{\text{ref}}, \pi_\theta)$	×	$O(1)$	×
K3^{++}	$r \cdot (-\log w + w - 1)$	$\text{KL}(\pi_\theta, \pi_{\text{ref}})$	✓	$\nabla_\theta \text{KL}(\pi_\theta, \pi_{\text{ref}})$	✓	$O(1)$	✓
K4	$r \cdot \text{sg}(-\log w)$	$\text{KL}(\pi_\theta, \pi_{\text{ref}})$	✓	$\nabla_\theta \text{KL}(\pi_\theta, \pi_{\text{ref}})$	✓	$O(1)$	✓
Topk**Reverse**KL	Alg 1	$\text{KL}(\pi_\theta, \pi_{\text{ref}})$	✓	$\nabla_\theta \text{KL}(\pi_\theta, \pi_{\text{ref}})$	✓	$O(k)$	✓
Forward KL: exact	$\sum_{j\in\mathcal{V}} \pi_{\text{ref}}(j)[\log \widehat{w}(j)]$	$\text{KL}(\pi_{\text{ref}}, \pi_\theta)$	✓	$\nabla_\theta \text{KL}(\pi_{\text{ref}}, \pi_\theta)$	✓	$O(\lvert\mathcal{V}\rvert)$	×
K5	$\text{sg}(w) \log w + \log r$	$\text{KL}(\pi_{\text{ref}}, \pi_\theta)$	✓	$\nabla_\theta \text{KL}(\pi_{\text{ref}}, \pi_\theta)$	✓	$O(1)$	✓
Topk**Forward**KL	Alg 2	$\text{KL}(\pi_{\text{ref}}, \pi_\theta)$	✓	$\nabla_\theta \text{KL}(\pi_{\text{ref}}, \pi_\theta)$	✓	$O(k)$	✓

Algorithm 1 Topk**Reverse**KL$(\pi_\theta, \pi_{\text{ref}}, \pi_{\text{sampling}}, q)$

Require: Policy π_θ, Anchor π_{ref} for $\text{KL}(\pi_\theta, \pi_{\text{ref}})$
Require: Top-k indices q of sampling policy π_{sampling}
$\text{KL}_{\text{trun}} = \sum_{j\in q} \pi_\theta(j)[\log \pi_\theta(j) - \log \pi_{\text{ref}}(j)]$
$\Delta = \sum_{j\in q}[\pi_\theta(j) - \text{sg}(\pi_\theta(j))]$
Draw tail token $z \sim \mu$, $\mu(j) \propto \pi_{\text{sampling}}(j)\, \mathbb{1}(j \notin q)$
$r_\theta = \pi_\theta(z)/\text{sg}(\pi_\theta(z))$, $w_\theta = \pi_{\text{ref}}(z)/\pi_\theta(z)$
$\widehat{\text{KL}}_{\text{sampled}} = r_\theta \cdot \text{sg}(-\log w_\theta)$
$s = \text{sg}(\pi_\theta(z)/\mu(z))$ {importance weight}
return $\text{KL}_{\text{trun}} - \Delta + s\, \widehat{\text{KL}}_{\text{sampled}}$

Algorithm 2 Topk**Forward**KL$(\pi_\theta, \pi_{\text{ref}}, q)$

Require: Policy π_θ, Anchor π_{ref} for $\text{KL}(\pi_{\text{ref}}, \pi_\theta)$
Require: Top-k indices q of anchor policy π_{ref}
$\text{FKL}_{\text{trun}} = \sum_{j\in q} \pi_{\text{ref}}(j)[\log \pi_{\text{ref}}(j) - \log \pi_\theta(j)]$
$\Delta = \sum_{j\in q}[\pi_\theta(j) - \text{sg}(\pi_\theta(j))]$
Draw tail token $z \sim \mu$, $\mu(j) \propto \pi_{\text{ref}}(j)\, \mathbb{1}(j \notin q)$
$r_\theta = \pi_\theta(z)/\text{sg}(\pi_\theta(z))$, $w_\theta = \pi_{\text{ref}}(z)/\pi_\theta(z)$
$\widehat{\text{FKL}}_{\text{sampled}} = \text{sg}(w_\theta) \log w_\theta + \log r_\theta$
$s = \text{sg}(\pi_\theta(z)/\mu(z))$ {importance weight}
return $\text{FKL}_{\text{trun}} + \Delta + s\, \widehat{\text{FKL}}_{\text{sampled}}$

Munos, 2025). Moreover, knowledge distillation (Hinton et al., 2015) shows that leveraging logits in KL computation can significantly facilitate learning. We analyze the trade-offs between sequence-level KL vs token-level KL, sampled KL vs exact KL, to identify the best practices in Top-k KL.

We propose **two very simple changes** to policy gradients. Given an RL update for LLM π_θ on prompt x:

$$\theta \leftarrow \theta + \alpha(\underbrace{A(x,y)\nabla_\theta \log \pi_\theta(y|x)}_{\text{Any policy gradient algorithm}} - \beta \underbrace{\nabla_\theta \widehat{\text{KL}}}_{\text{What we change}})$$

where y is the LLM response of length L, and $A(x,y)$ is the advantage function. We only change ***what*** the KL is regularizing against and ***how*** the KL is computed:

$$\widehat{\text{KL}} = \sum_{n=0}^{L-1} \text{TopkKL}(\pi_\theta(\cdot|x, y_{0:n-1}), \pi_{\theta_{\text{ema}}}(\cdot|x, y_{0:n-1}))$$

where TopkKL is an unbiased token-level KL estimator that computes exact KL on the top-k indices of logits and a sampled KL on the rest; θ_{ema} is an EMA target network:

$$\theta_{\text{ema}} \leftarrow \eta \cdot \theta_{\text{ema}} + (1-\eta) \cdot \theta$$

The two changes make a significant difference on RL training of reasoning and agentic models. On math, it allows R1-distilled Qwen-1.5B to reach 53.9% on OlympiadBench (text-only) (He et al., 2024) compared to 50.8% by GRPO. In agentic settings, with Qwen-3B base, EMA-PG improves GRPO by 35.6% across 7 datasets of Q&A with search engine, including 29.7% → 45.8% on HotpotQA (Yang et al., 2018), 27.4% → 40.5% on 2WikiMultiHopQA (Ho et al., 2020b), 12.8% → 34.7% on Bamboogle (Press et al., 2023).

The rest of the paper is organized as the following. **(1)** We derive the stability condition for using an EMA anchor (§4). **(2)** We explain why token-level KL is more suited for reasoning models than sequence-level KL (§5.1). **(3)** For token-level KL, common KL estimators such as K1, K2, K3 are unable to yield unbiased KL estimates and unbiased gradients at the same time, so we construct estimators K3^{++}, K4, and K5 that can (§5.2). **(4)** We propose Top-k KL estimators, which extract dense supervision from logits with low memory footprint (§5.3). Overall, EMA anchor and Top-k KL result in notable sample efficiency gain for RL.

2. Related Work

Improving RL for LLMs Leveraging verifiable domains such as math and coding, lots of effort has gone into scaling RL for reasoning (Jaech et al., 2024; Guo et al., 2025; Chen et al., 2025) and agentic tasks (Kimi et al., 2025a; Comanici et al., 2025). The predominant algorithm for RL in reasoning, GRPO (Shao et al., 2024), has gained widespread

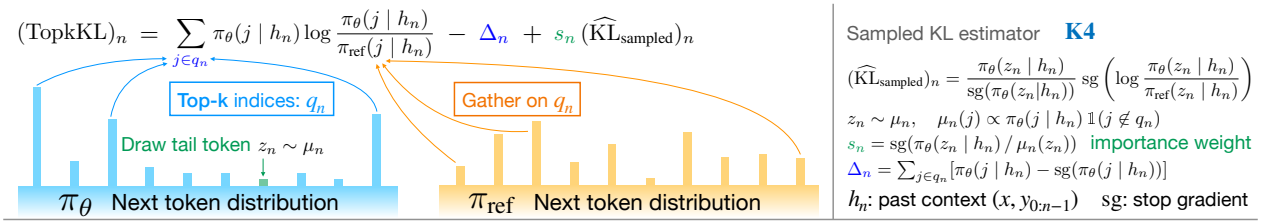


Figure 2. Top-k reverse KL (Alg 1) computes exact KL on the top-k indices, and adds a sampled KL on a tail token, with a zero-valued correction Δ_n, to keep the gradient estimator *unbiased*.

adoption due to its effectiveness. Many works have tried to further improve it, which include removing bias in policy gradient (Liu et al., 2025b), better importance weight clipping (Yu et al., 2025), using sequence-level objective (Zheng et al., 2025), asynchronous data generation (Piché et al., 2025), better scaling practices (Khatri et al., 2025). Since we exclusively focus on the KL component in RL, our work is largely orthogonal to those techniques above.

KL Estimators for LLMs KL estimation for LLMs is challenging due to autoregressive action space and large vocabulary size. Early work on RLHF adds a sequence-level KL penalty to the sequence-level reward (Ouyang et al., 2022; Bai et al., 2022a). As reasoning models begin to scale the sequence length of thinking traces, token-level KL regularization becomes popular (Guo et al., 2025). Token-level sampled KL estimators are typically K1, K2, and K3 (Schulman, 2020); K3 was used in GRPO. Since then, many works have pointed out that K3 gradients are forward KL gradients (Tang & Munos, 2025; Zhang et al., 2025; Shah et al., 2025). Sampled KL ignores the fact that we have white-box access to logits and next-token distributions; knowledge distillation has shown that such information is very useful to learning (Hinton et al., 2015; Kim & Rush, 2016; Agarwal et al., 2024; Zhou et al., 2024). When the vocabulary is large, storing full logits is too memory-intensive; our insight is to reduce the memory usage of logits via Top-k truncation.

EMA in Deep Learning Deep Q-learning almost universally uses an EMA network to produce stable learning targets (Mnih et al., 2015; Lillicrap et al., 2015; Haarnoja et al., 2018). Self-supervised learning has also used EMA for stable bootstrapping (He et al., 2020; Grill et al., 2020b; Busbridge et al., 2023). EMA has been shown to improve generalization in deep learning (Nichol et al., 2018; Zhang et al., 2019). In the diffusion model literature, EMA is often used to produce the final model (Ho et al., 2020a). For RL on LLMs, prior work has also suggested using an EMA anchor for alignment (Gorbatovski et al., 2024; Ramé et al., 2024); our work differs in how the KL is computed. Elastic reset (Noukhovitch et al., 2023) also keeps an EMA copy during RL, but does not use it for reference policy. The effectiveness of EMA can be partially explained by Linear Mode Connectivity (Frankle et al., 2020) and Monotonic Linear Interpolation (Goodfellow et al., 2014; Lucas et al., 2021) between neural networks that share the same initialization.

3. Background

Reinforcement Learning (RL) Given a pre-trained LLM, RL trains the model to maximize a reward function while remaining close to the original model. Concretely, let π_θ denote a policy (language model) parameterized by $\theta \in \mathbb{R}^d$, and let $R(x, y)$ be a reward function scoring response y to prompt x. The standard objective is to maximize:

$$\mathbb{E}_x\{\mathbb{E}_{\pi_\theta(y|x)}\big[R(x,y)\big] - \beta \text{KL}(\pi_\theta(\cdot \mid x) \| \pi_{\text{ref}}(\cdot \mid x))\} \quad (1)$$

where $x \sim \mathcal{D}$ is a sampled prompt, π_{ref} is the reference policy (also called the **anchor** policy), β controls how much π_θ is allowed to deviate from the anchor. The term $\text{KL}(\pi_\theta \| \pi_{\text{ref}}) = \mathbb{E}_x \mathbb{E}_{y\sim\pi_\theta(\cdot|x)}[\log(\pi_\theta(y|x)/\pi_{\text{ref}}(y|x))]$ is the reverse KL divergence for the policy π_θ.

Exponential Moving Average (EMA) EMA is a technique for maintaining a smoothed version of an iteratively updated quantity. Given a sequence $\{\theta_t\}_{t=0}^\infty$ and coefficient $\eta \in (0, 1)$, the EMA sequence $\{\theta_{\text{ema},\, t}\}$ is:

$$\theta_{\text{ema},\, 0} = \theta_0 \qquad \theta_{\text{ema},\, t+1} = \eta\, \theta_{\text{ema},\, t} + (1-\eta)\, \theta_t \quad (2)$$

which is widely used in deep Q-learning as *target network*.

Local Quadratic Approximation of KL The Fisher information matrix of a policy π_θ is defined as:

$$F_\theta \triangleq \mathbb{E}_{x\sim\mathcal{D}} \mathbb{E}_{y\sim\pi_\theta(\cdot|x)} \big[(\nabla_\theta \log \pi_\theta(y|x))(\nabla_\theta \log \pi_\theta(y|x))^\top\big]$$

which captures the local sensitivity of a policy's output distribution to parameter changes. The natural gradient $F_\theta^{-1} g$ is the steepest-ascent direction under a local KL trust-region constraint. For $\theta' = \theta + \delta$ with $\|\delta\| \to 0$,

$$\text{KL}(\pi_\theta \| \pi_{\theta+\delta}) = \delta^\top F_\theta \delta / 2 + O(\|\delta\|^3), \quad (3)$$

and the gradient w.r.t θ is: $\nabla_\theta \text{KL}(\pi_\theta \| \pi_{\theta'}) \approx F_\theta(\theta - \theta')$.

4. Training Dynamics of the EMA Anchor

Consider the policy gradient $g_t = (R\, \nabla_\theta \log \pi_\theta)|_{\theta=\theta_t}$ at t:

$$\theta_{t+1} = \theta_t + \alpha[g_t - \beta\, \nabla_\theta \text{KL}(\pi_\theta \| \pi_{\theta_{\text{ema},\, t}})|_{\theta=\theta_t}]$$
$$\theta_{\text{ema},\, t+1} = \eta\, \theta_{\text{ema},\, t} + (1-\eta)\, \theta_t$$

We define the *lag* between current and EMA weights as:

$$\delta_t := \theta_t - \theta_{\text{ema},\, t} \quad (4)$$

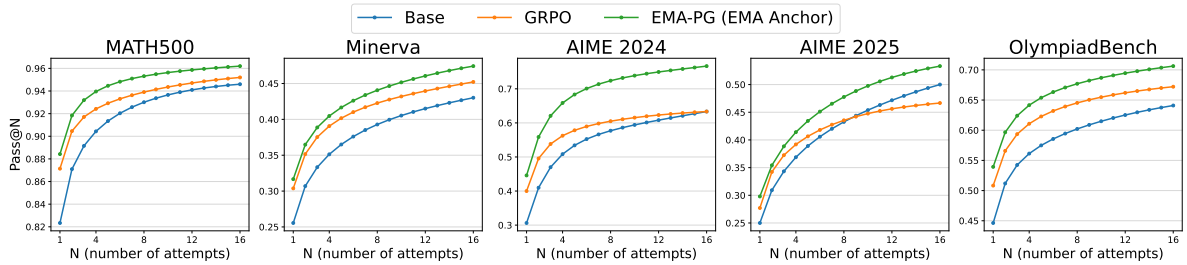


Figure 3. **On math reasoning datasets, using EMA Anchor improves not only Pass@1 but Pass@N as well compared to GRPO**. Results obtained on a 1.5B model DeepSeek-R1-Distill-Qwen-1.5B (Guo et al., 2025).

Using the local approximation (3), with $F_t = F_{\theta_t}$

$$\theta_{t+1} = \theta_t + \alpha g_t - \alpha\beta F_t \delta_t \tag{5}$$

The joint dynamics of θ_t and δ_t becomes:

$$\begin{bmatrix}\theta_{t+1}\\ \delta_{t+1}\end{bmatrix} = \begin{bmatrix} I & -\alpha\beta F_t \\ 0 & \eta I - \alpha\beta F_t\end{bmatrix}\begin{bmatrix}\theta_t\\ \delta_t\end{bmatrix} + \begin{bmatrix}\alpha I\\ \alpha I\end{bmatrix} g_t \tag{6}$$

Lemma 4.1. *Quasi-steady state: If we assume that the gradient and the Fisher matrix change extremely slowly over k steps, meaning that for $\Delta = 0 \cdots k-1$:*

$$g_{t+\Delta} \approx g, \qquad F_{t+\Delta} \approx F \tag{7}$$

then, under the following definitions of matrices D, S_k, M_k:

$$D = \eta I - \alpha\beta F \quad S_k = \sum_{\Delta=0}^{k-1} D^\Delta \quad M_k = \sum_{\Delta=0}^{k-1} S_\Delta$$

we have: firstly, $I - D$ is invertible and $S_k = (I - D^k)(I - D)^{-1}$, $M_k = (kI - S_k)(I - D)^{-1}$; secondly, we have a closed-form dynamics of EMA Policy Gradient:

$$\begin{bmatrix}\theta_{t+k}\\ \delta_{t+k}\\ g\end{bmatrix} = \begin{bmatrix} I & -\alpha\beta F S_k & \alpha k I - \alpha^2\beta F M_k \\ 0 & D^k & \alpha S_k \\ 0 & 0 & I\end{bmatrix}\begin{bmatrix}\theta_t\\ \delta_t\\ g\end{bmatrix}$$

Lemma 4.2. *Stability Condition: Let $\{v_i\}_{i=0}^{d-1}$ be the eigenbasis of the Fisher matrix F, and $\{\lambda_i\}_{i=0}^{d-1}$ be its corresponding eigenvalues (with $\lambda_{\max}$ being the largest eigenvalue). The dynamics of the lag δ_t in the eigenbasis of the Fisher, where $\delta_t^{(i)} := \delta_t{}^\top v_i$ and $g^{(i)} := g^\top v_i$, can be written as:*

$$\delta_{t+k}^{(i)} = \underbrace{(\chi_i)^k \delta_t^{(i)}}_{\textit{transient}} + \underbrace{\alpha \tfrac{1-(\chi_i)^k}{1-\chi_i} g^{(i)}}_{\textit{particular solution}} \qquad \chi_i = \eta - \alpha\beta\lambda_i \tag{8}$$

Thus, the stability condition of δ is:

$$\boxed{\alpha\beta\lambda_{\max} < 1 + \eta} \tag{9}$$

Summary of Stability / Oscillation Conditions:

1. $0 \le \alpha\beta\lambda_{\max} \le \eta$: stable, non-oscillatory.
2. $\eta < \alpha\beta\lambda_{\max} < 1 + \eta$: stable, oscillatory.
3. $\alpha\beta\lambda_{\max} \ge 1 + \eta$: unstable.

Which characterizes the exact conditions for stability in EMA-PG's training dynamics under mild assumptions (7).

5. KL Estimators: Which and Why

5.1. Sequence-level KL or Token-level KL?

Because LLMs have an autoregressive action space, it is worth discussing whether we should apply sequence-level KL or token-level KL. For a language model, the KL component in (1) can be rewritten as the loss:

$$\widehat{\mathrm{KL}}_{\text{seq}} \triangleq \log(\pi_\theta(y|x)/\pi_{\text{ref}}(y|x)) \tag{10}$$

$$\nabla_\theta L_{\text{KL}}^{\text{seq}} \triangleq \mathbb{E}_{\pi_\theta(y|x)}[\text{sg}(\widehat{\mathrm{KL}}_{\text{seq}})\nabla_\theta \log \pi_\theta(y|x)] \tag{11}$$

where $\text{sg}(\cdot)$ denotes the stop gradient operator. Note that this is an unbiased **sequence-level KL** estimator:

$$\nabla_\theta \mathrm{KL}(\pi_\theta(\cdot \mid x) \| \pi_{\text{ref}}(\cdot \mid x)) = \nabla_\theta L_{\text{KL}}^{\text{seq}}(\theta) \tag{12}$$

This KL regularizer was used in both InstructGPT (Ouyang et al., 2022) and WARP (Ramé et al., 2024). It is simple to implement: just adding a scalar sequence logprob difference to the scalar sequence-level reward would suffice. DPO (Rafailov et al., 2023) also uses sequence-level KL.

In contrast, **token-level KL** regularization, as popularized by GRPO (Shao et al., 2024; Guo et al., 2025; Liu et al., 2025a), implements the following:

$$\widehat{\mathrm{KL}}_n \approx \mathrm{KL}(\pi_\theta(\cdot \mid x, y_{0:n-1}) \| \pi_{\text{ref}}(\cdot \mid x, y_{0:n-1})) \tag{13}$$

$$\nabla_\theta L_{\text{KL}}^{\text{token}} \triangleq \mathbb{E}_{\pi_\theta(y|x)}\left[\sum_{n=0}^{L-1} \nabla_\theta \widehat{\mathrm{KL}}_n\right] \tag{14}$$

where the KL estimator is a design choice (See Tab 1). We assume the use of exact KL rather than sampled KL in our analysis of token-level KL. Token-level KL was traditionally seen as a surrogate objective for sequence-level KL; here we analyze their differences. Rewrite sequence-level KL as:

$$\rho_n \triangleq \log(\pi_\theta(y_n|x, y_{0:n-1})/\pi_{\text{ref}}(y_n|x, y_{0:n-1}))$$

$$\omega_n \triangleq \nabla_\theta \log \pi_\theta(y_n|x, y_{0:n-1})$$

It can be shown that (§C):

$$\nabla_\theta L_{\text{KL}}^{\text{seq}} = \mathbb{E}_{\pi_\theta(y|x)}\left[\sum_n \left(\sum_{m \ge n} \rho_m\right)\omega_n\right] \tag{15}$$

$$\nabla_\theta L_{\text{KL}}^{\text{token}} = \mathbb{E}_{\pi_\theta(y|x)}\left[\sum_n (\rho_n)\,\omega_n\right] \tag{16}$$

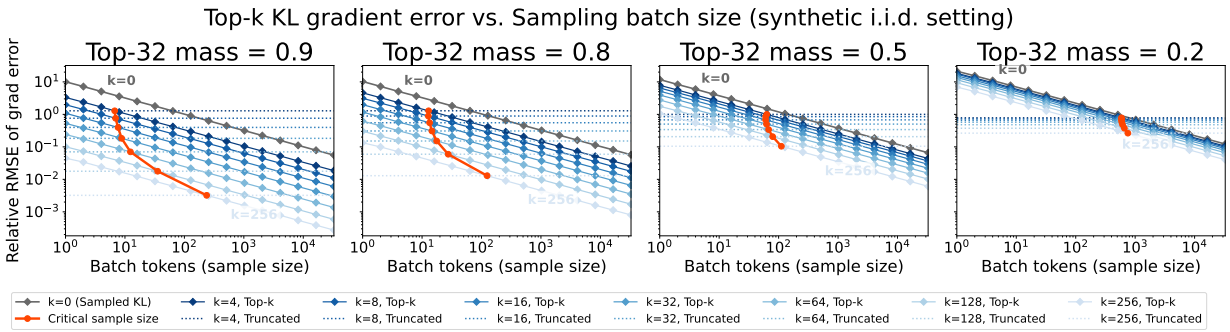


Figure 4. **Bias-variance tradeoff in Top-k KL estimator:** Top-k KL (unbiased) has lower gradient error than sampled KL (unbiased) in all regimes, but only outperforms Truncated KL (biased) beyond a certain *critical sample size*; we illustrate this bias-variance tradeoff in a synthetic setting (§F). Rule of thumb: when using a small k, add the tail term (25) (default); for a large k, consider Truncated KL.

The difference is clear: **sequence-level KL punishes each current token for the divergence of all its future tokens until the end of sequence**, while token-level KL does not.

We find that in reasoning and agentic settings, since the sequence lengths of thinking traces are long and the rewards are reliable, sequence-level KL does not help; **token-level KL should be used instead**. In other words, during RL training for reasoning, KL should be token-wise in the loss, not added to the outcome reward, even though sequence-level KL may seem more "correct" (12) for objective (1).

5.2. Exact KL or Sampled KL?

For token-level KL estimation, one can technically implement **exact KL**, which is unbiased and low-variance, but at the cost of memory. We use the following notations:

$$h_n \triangleq (x, y_{0:n-1}), \quad \mathbb{E}_n[\cdot] \triangleq \mathbb{E}_{y_n \sim \pi_\theta(\cdot|h_n)}[\cdot] \tag{17}$$

In the case of reverse KL, for each token $y_n \sim \pi_\theta(\cdot \mid h_n)$:

$$\mathrm{KL}_n \triangleq \sum\nolimits_{j \in \mathcal{V}} \pi_\theta(j \mid h_n) \log \frac{\pi_\theta(j \mid h_n)}{\pi_{\text{ref}}(j \mid h_n)} \tag{18}$$

Since this is the ground-truth definition of reverse KL, it naturally yields exact values and exact gradients. The problem with exact KL is that it requires storing full logits for every position in each sequence both for current policy π_θ and reference policy π_{ref}, costing a memory of $O(|\mathcal{V}|)$ per token. The alternative, which has negligible memory footprint $O(1)$, is **sampled KL**. For the n-th position in y, let

$$y_n \sim \pi_\theta(\cdot \mid h_n) \quad w_n \triangleq \pi_{\text{ref}}(y_n \mid h_n)/\pi_\theta(y_n \mid h_n) \tag{19}$$

The K1, K2, K3 estimators (Schulman, 2020) are given by:

$$(\mathrm{K1})_n \triangleq -\log w_n \quad (\mathrm{K2})_n \triangleq (1/2)(\log w_n)^2$$
$$(\mathrm{K3})_n \triangleq -\log w_n + w_n - 1$$

None of the existing sampled KL estimators simultaneously gives both unbiased value and unbiased gradient on the token level. Ideally, we would like a KL estimator $\widehat{\mathrm{KL}}_n$ to satisfy both conditions (with notations from (17)):

$$\mathbb{E}_n[\widehat{\mathrm{KL}}_n] = \mathrm{KL}_n \quad \mathbb{E}_n[\nabla_\theta \widehat{\mathrm{KL}}_n] = \nabla_\theta \mathrm{KL}_n \tag{20}$$

K1 and K3 give the correct values but wrong gradients; K2 gives the correct gradients but wrong values (see Tab 1). We show that K1 and K3 can be fixed with a simple trick. Let

$$r_n \triangleq \pi_\theta(y_n \mid h_n)/\mathrm{sg}(\pi_\theta(y_n \mid h_n)) \tag{21}$$

where sg means stop gradient. We construct the following unbiased sampled KL estimators to satisfy (20):

$$\boxed{(\textbf{K3}^{++})_n \triangleq r_n(-\log w_n + w_n - 1)} \tag{22}$$

$$\boxed{(\textbf{K4})_n \triangleq r_n \cdot \mathrm{sg}(-\log w_n)} \tag{23}$$

Eq (22) is named **K3**$^{++}$ because of its resemblance to the modified K3 in (Liu et al., 2025a), but here we disentangle generic off-policy correction (which can be applied to any sampled KL estimator, not just K3; moreover, importance weights should be applied with $\mathrm{sg}(\cdot)$ on themselves) from an actual change in KL direction:

- **K3**$^{++}$ is obtained by multiplying existing K3 by r_n in (21). **This simple change alone converts the gradient from forward KL to reverse KL.**
- **K4** is obtained by first doing stop gradient on K1 and then multiplying it by r_n in (21). It is simpler, and it is unbiased as well.

K3^{++} and **K4** satisfy the conditions in (20): they yield both unbiased value and unbiased gradient for reverse KL.

In addition, the success of K3's forward KL gradients raises the interesting question of whether forward KL is just as effective as reverse KL in regularizing RL training dynamics. We propose a **forward KL estimator K5**, which produces unbiased forward KL values and unbiased forward KL gradients under $\mathbb{E}_n[\cdot]$ (17) when sampling from (19):

$$\boxed{(\textbf{K5})_n \triangleq \mathrm{sg}(w_n) \log w_n + \log r_n} \tag{24}$$

When sampling is off-policy ($\pi_{\text{sampling}} \neq \pi_\theta$), any sampled KL estimator $\widehat{\mathrm{KL}}_n$ above simply needs to multiply the (stop-gradient) importance weight $\mathrm{sg}(\frac{\pi_\theta}{\pi_{\text{sampling}}})$ to remain unbiased.

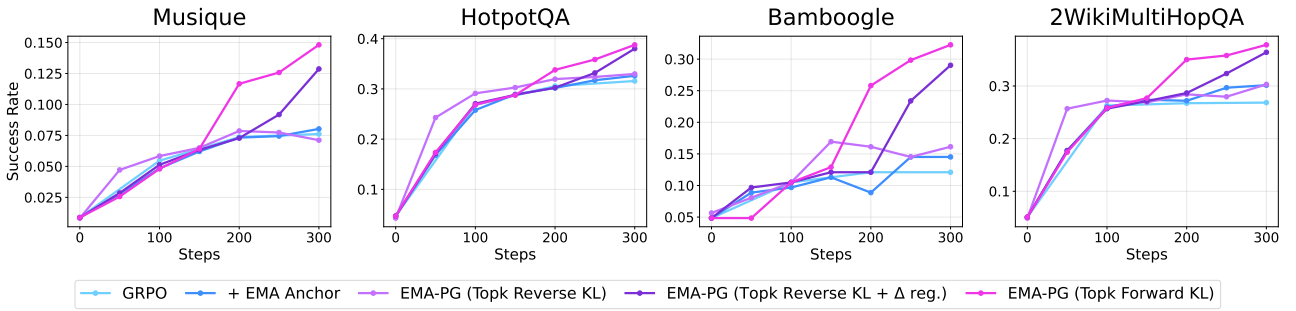


Figure 5. **EMA-PG not only learns faster but reaches higher asymptotic performance** on agentic tasks of Q&A with search engine. Both Topk Forward KL and Topk Reverse KL with Δ reg. (28) significantly outperform GRPO (and GRPO with EMA Anchor). This shows that the combination of EMA Anchor and Top-k KL is highly effective.

Concretely, when $y_n \sim \pi_{\text{sampling}}$, any previously unbiased $\widehat{\text{KL}}_n$ under $y_n \sim \pi_\theta$ will require an off-policy correction $\text{KL}_n = \mathbb{E}_{y_n}[s_n \widehat{\text{KL}}_n]$ with importance weight (IW) s_n:

$$y_n \sim \pi_{\text{sampling}}(\cdot|h_n) \quad s_n \triangleq \text{sg}(\pi_\theta(y_n|h_n)/\pi_{\text{sampling}}(y_n|h_n))$$

On the other hand, exact KL is always on-policy (but memory-intensive, with $O(|\mathcal{V}|)$ rather than $O(1)$ memory footprint), and thus does not require off-policy correction.

5.3. Top-k KL Estimator

We now aim to combine the best of both worlds of exact KL and sampled KL. We start from the observation that for modern LLMs, the probability mass tends to concentrate on a small number of top tokens at each generation step; it was for this reason that top-k sampling (Fan et al., 2018) and nucleus sampling (Holtzman et al., 2019) were effective. The vocabulary size for modern LMs is very large (typically 130k–260k), so most of the logit indices in $\mathcal{V}$ contribute very minimally to the KL value or KL gradients.

Key insight. We only partially compute exact KL on the top-k logit indices of the policy under which the expectation is taken (which is current policy for reverse KL, reference policy for forward KL), and then use a separate sampled KL for the rest of the indices, so that we arrive at an unbiased estimator for KL values and gradients, with lower variance than sampled KL under the same sampling distribution.

First, we consider Reverse KL. Let q_n be the set of top-k logit indices from $\pi_\theta(\cdot \mid h_n)$ at sequence position n,

$$q_n \leftarrow \text{Topk}(\pi_\theta(\cdot \mid h_n)) \qquad q_n \subseteq \mathcal{V} \qquad |q_n| = k$$

we can rewrite reverse KL by partitioning the vocabulary:

$$\underbrace{\sum_{j \in q_n} \pi_\theta(j|h_n) \log \frac{\pi_\theta(j|h_n)}{\pi_{\text{ref}}(j|h_n)}}_{\text{'Truncated' KL: } (\text{KL}_{\text{trun}})_n} + \underbrace{\sum_{j \notin q_n} \pi_\theta(j|h_n) \log \frac{\pi_\theta(j|h_n)}{\pi_{\text{ref}}(j|h_n)}}_{\text{'Tail' term: } (\text{KL}_{\text{tail}})_n}$$

The first term is computed exactly. The second term is a sum over the non-top-k indices, which we estimate with a separate sampled KL: we draw one *tail token* z_n from the non-top-k part of the distribution, and evaluate K4 on it,

$$\begin{aligned} z_n &\sim \mu_n \qquad \mu_n(j) \propto \pi_\theta(j \mid h_n)\, \mathbb{1}(j \notin q_n) \\ s_n &= \text{sg}\big(\pi_\theta(z_n \mid h_n) \,/\, \mu_n(z_n)\big) \\ (\widehat{\text{KL}}_{\text{tail}})_n &= s_n\, (\textbf{K4})_n\big|_{y_n = z_n} \end{aligned} \tag{25}$$

where $(\textbf{K4})_n|_{y_n=z_n}$ is K4 with z_n in place of the sampled token y_n, and s_n is the importance weight of z_n under its proposal μ_n (§5.2). Since this μ_n is π_θ itself renormalized on the non-top-k indices, s_n is always the probability mass of the non-top-k indices. The tail token is drawn separately from the rollout token y_n. The same tail term can also be estimated with y_n itself,

$$(\widehat{\text{KL}}_{\text{high-var. tail}})_n = \mathbb{1}(y_n \notin q_n)\, (\textbf{K4})_n \tag{26}$$

but an additional tail token adds almost no overhead with an efficient GPU kernel, and results in provably lower variance (§K.2), since y_n falls outside q_n only with the probability of the non-top-k indices. We therefore opt for (25).

The vanilla form has a gradient bias. The vanilla estimator is $\widehat{\text{KL}}_n = (\text{KL}_{\text{trun}})_n + (\widehat{\text{KL}}_{\text{tail}})_n$. Its *value* is unbiased, but its *gradient* is biased by one term:

$$\mathbb{E}_{z_n}\big[\nabla_\theta \widehat{\text{KL}}_n\big] = \nabla_\theta \text{KL}_n + \sum\nolimits_{j \in q_n} \nabla_\theta \pi_\theta(j \mid h_n) \tag{27}$$

where the expectation is over $z_n \sim \mu_n$, and the last term is the gradient of the probability mass of the top-k indices. The reason is that our sampled KL estimators are gradient-unbiased only over the full vocabulary, since they rely on $\sum_j \nabla_\theta \pi_\theta(j \mid h_n) = 0$, which holds only over all of $\mathcal{V}$: the stop-gradient in K4 drops this term from the exact gradient. In the vanilla form, the tail term drops its share $\sum_{j \notin q_n} \nabla_\theta \pi_\theta(j \mid h_n)$, while the truncated term keeps its share $\sum_{j \in q_n} \nabla_\theta \pi_\theta(j \mid h_n)$, so they no longer cancel.

A gradient correction term. We remove this bias with:

$$\Delta_n \triangleq \sum\nolimits_{j \in q_n} \big[\pi_\theta(j \mid h_n) - \text{sg}(\pi_\theta(j \mid h_n))\big] \tag{28}$$

which is zero in value, has gradient $\sum_{j\in q_n}\nabla_\theta\pi_\theta(j\mid h_n)$, and costs $O(k)$ since the top-k probabilities are already computed. The Top-k reverse KL estimator is:

$$\boxed{(\text{Topk}\mathbf{Reverse}\text{KL})_n = (\text{KL}_{\text{trun}})_n - \Delta_n + (\widehat{\text{KL}}_{\text{tail}})_n} \quad (29)$$

Similarly, we split forward KL into a truncated exact KL and a separate sampled tail term, with the top-k indices and the tail token now taken from the reference policy:

$$q_n \leftarrow \text{Topk}(\pi_{\text{ref}}(\cdot|h_n)) \qquad \mu_n(j) \propto \pi_{\text{ref}}(j\mid h_n)\,\mathbb{1}(j\notin q_n)$$
$$(\text{FKL}_{\text{trun}})_n = \sum\nolimits_{j\in q_n}\pi_{\text{ref}}(j\mid h_n)\log\frac{\pi_{\text{ref}}(j\mid h_n)}{\pi_\theta(j\mid h_n)}$$
$$(\widehat{\text{FKL}}_{\text{tail}})_n = s_n\,(\mathbf{K5})_n\big|_{y_n=z_n} \qquad z_n\sim\mu_n$$

with s_n as in (25). The vanilla estimator is the sum of the two terms, $\widehat{\text{FKL}}_n = (\text{FKL}_{\text{trun}})_n + (\widehat{\text{FKL}}_{\text{tail}})_n$. Its *value* is unbiased, but its *gradient* is biased by one term:

$$\mathbb{E}_{z_n}\left[\nabla_\theta\widehat{\text{FKL}}_n\right] = \nabla_\theta\text{FKL}_n - \sum\nolimits_{j\in q_n}\nabla_\theta\pi_\theta(j\mid h_n) \quad (30)$$

where FKL_n is the forward KL at position n, and the last term is the gradient of the policy's probability mass on the top-k indices, as in (27) with the opposite sign. The reason is the baseline $\log r_n$ in K5: its gradient has zero mean only over the full vocabulary, while the tail term covers only the non-top-k indices, which leaves the last term of (30). We remove this bias by adding the zero-valued correction term Δ_n (28), whose gradient is $\sum_{j\in q_n}\nabla_\theta\pi_\theta(j\mid h_n)$. The Top-k forward KL estimator is therefore:

$$\boxed{(\text{Topk}\mathbf{Forward}\text{KL})_n = (\text{FKL}_{\text{trun}})_n + \Delta_n + (\widehat{\text{FKL}}_{\text{tail}})_n} \quad (31)$$

Proposition 5.1. *Unbiased values and gradients: For any index set q_n, Top-k reverse KL (29) and Top-k forward KL (31) have unbiased values and unbiased gradients: they satisfy both conditions in (20), for KL_n and FKL_n respectively, with the expectation taken over $z_n\sim\mu_n$, where μ_n is any distribution over $\mathcal{V}$ with $\mu_n(j)>0$ iff $j\notin q_n$.*

We prove this in §K.1. Top-k KL estimators are thus unbiased regardless of whether the chosen logit indices are top-k or not, and regardless of how the rollout was sampled. In practice, reverse KL (Alg 1) takes q_n and μ_n from the sampling policy before any truncation such as nucleus sampling, while forward KL (Alg 2) takes them from the reference policy. Moreover, Top-k KL renders both exact KL ($k=|\mathcal{V}|$) and sampled KL ($k=0$) as special cases. Top-k KL allows for flexible interpolation between the two, remains unbiased at any k, and only requires $O(k)$ memory. We generalize our estimator to any f-divergence in §G.

The bias as a regularizer. The bias in (27) is not noise: it is the gradient of the top-k probability mass. The vanilla reverse form therefore minimizes $\text{KL}_n+\sum_{j\in q_n}\pi_\theta(j\mid h_n)$: it moves probability from the top-k indices to the tail. Since Δ_n isolates this effect, we can also keep it on purpose, as a form of entropy regularization.

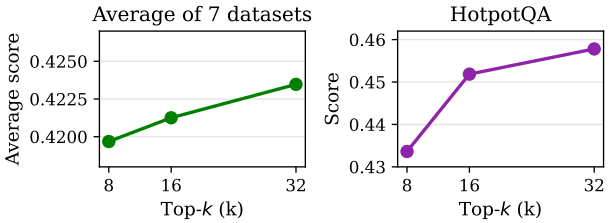


Figure 6. Ablation on k of Top-k (forward) KL in EMA-PG.

6. Experiments

We evaluate the efficacy of EMA Policy Gradients in reasoning RL and agentic RL. The base algorithm we use is GRPO (Shao et al., 2024) with clip-higher (Yu et al., 2025), a popular default for LLMs. To show that the two techniques we have introduced (EMA anchor and Topk KL) can benefit the base RL algorithm, we focus on the following tasks:

Math Reasoning. We follow the DeepScaleR setting (Luo et al., 2025) and train DeepSeek-R1-Distill-Qwen-1.5B (Guo et al., 2025) on an RL dataset of 40k question-answer pairs that comprise of: AIME problems from 1984-2023, Omni-MATH dataset (Gao et al., 2024), AMC problems prior to 2023, Still datasets (Jiang et al., 2024; Min et al., 2024). We then evaluate on the datasets of: MATH500 (Hendrycks et al., 2021), Minerva (Lewkowycz et al., 2022), AIME 2024 / 2025, and OlympiadBench (He et al., 2024).

Agentic RL for Search. We follow the Search-R1 setting (Jin et al., 2025) and train a Qwen-2.5 3B (Yang et al., 2024) to use the search engine with RL. GRPO being used here applies the RL loss only on CoT and action tokens, not on environment observation tokens that interleave with CoTs. RL uses the combined training sets of Natural Questions (NQ) (Kwiatkowski et al., 2019) and HotpotQA (Yang et al., 2018). After RL, we run the eval on both General QA and Multi-Hop QA. For General QA, we use the test set of NQ, TriviaQA (Joshi et al., 2017), PopQA (Mallen et al., 2023). For Multi-Hop QA, we use the test set of HotpotQA, 2WikiMultiHopQA (2wiki) (Ho et al., 2020b), Musique (Trivedi et al., 2022), and Bamboogle (Press et al., 2023).

Effect of EMA anchor We empirically demonstrate the benefits of using an EMA target network instead of a fixed anchor for RL on LLMs. Note that using EMA does not require storing an additional set of weights during training, since the anchor (reference) policy weights already need to be stored for standard KL-regularized policy gradients.

First of all, we empirically find that keeping the KL with a

Method	General QA			Multi-Hop QA				
	NQ	TriviaQA	PopQA	HotpotQA	2wiki	Musique	Bamboogle	Avg.
Qwen2.5-**3B-Instruct** (Prompting)								
CoT (no search) (Wei et al., 2022)	0.106	0.288	0.108	0.149	0.244	0.020	0.024	0.134
Search-o1 (Li et al., 2025)	0.238	0.472	0.262	0.221	0.218	0.054	0.320	0.255
RAG (Lewis et al., 2020)	0.348	0.544	0.387	0.255	0.226	0.047	0.080	0.270
Qwen2.5-**7B-Instruct** (Prompting)								
RAG	0.349	0.585	0.392	0.299	0.235	0.058	0.208	0.304
Qwen2.5-**3B-Base** (RL)								
before RL	0.060	0.122	0.076	0.047	0.051	0.009	0.048	0.059
WARP	0.114	0.197	0.116	0.103	0.140	0.014	0.056	0.106
PPO	0.406	0.587	0.435	0.284	0.273	0.049	0.088	0.303
GRPO	0.421	0.583	0.413	0.297	0.274	0.066	0.128	0.312
EMA-PG: *w/* EMA Anchor	0.468	0.624	0.445	0.345	0.277	0.084	0.194	0.348
Topk Reverse KL	0.484	0.627	0.463	0.360	0.325	0.085	0.202	0.364
Topk Reverse KL + Δ reg.	0.486	**0.635**	**0.467**	0.456	**0.414**	0.162	0.355	**0.425**
Topk Forward KL	**0.493**	0.627	0.464	**0.458**	0.405	0.171	0.347	0.423
Topk Forward KL + Δ reg.	0.492	0.630	0.464	0.448	0.395	**0.177**	**0.363**	0.424
Improvement over GRPO	17.1% ↑	7.5% ↑	12.3% ↑	54.2% ↑	47.8% ↑	159.1% ↑	171.1% ↑	35.6% ↑

Table 2. **EMA-PG excels at agentic RL tasks that require using a search engine inside CoTs to reason about questions.** 'Δ reg.' adds Δ_n (28) as a regularizer.

R1-Distill-Qwen-1.5B	Base	GRPO	EMA-PG	Δ (Rel)
MATH500	0.823	0.871	**0.884**	27% ↑
AMC 2024	0.499	0.656	**0.686**	19% ↑
Minerva	0.256	0.304	**0.317**	27% ↑
AIME 2024	0.306	0.400	**0.446**	49% ↑
AIME 2025	0.250	0.277	**0.298**	77% ↑
OlympiadBench (text)	0.446	0.508	**0.539**	50% ↑
Average	0.430	0.503	**0.528**	34% ↑

Table 3. Pass@1 comparison across six math reasoning datasets. Relative Improvement = (EMA-PG − GRPO)/(GRPO − Base).

small $\beta > 0$ is necessary for preventing training collapse when doing full-finetuning (no LoRA). This is corroborated by the common practice of still using KL in large-scale RL training runs (Liu et al., 2025a; Kimi et al., 2025a).

Secondly, we find that in math reasoning, using an EMA anchor ($\eta < 1$) improves GRPO across all evaluated datasets, as shown in Tab 3. For instance, using the EMA anchor gives us a boost of 50.8% → 53.9% on OlympiadBench. In addition, using an EMA anchor improves not just Pass@1 but Pass@16 as well, as shown in Fig 3; this suggests that target networks can effectively mitigate Pass@N collapse that is common in reasoning RL (Yue et al., 2025).

Using token-level KL instead of sequence-level KL is crucial for good performance. On agentic search, we compare against WARP (Ramé et al., 2024), which uses sequence-level KL (12) and EMA anchor; we find that WARP performs a lot worse than vanilla GRPO (10.6% vs 31.2%). When using token-level KL + EMA anchor, we see a gain from 31.2% → 34.8%. This validates our analysis in §5.1.

Effect of Top-k KL We find that the use of Top-k KL can make a substantial difference in RL performance; both Topk Forward KL (Alg 2) and Topk Reverse KL (Alg 1) with Δ reg. (28) simultaneously improve sample efficiency and asymptotic performance of RL. It is shown in Fig 5 that, compared to sampled KL, Top-k KL enables the learning process to rapidly take off and avoid premature convergence. This is because Top-k KL works like knowledge distillation: it enforces KL on the logit level rather than just on the level of a single token sample, which provides dense supervision and lower gradient variance. In terms of the final performance (Tab 2), when used with EMA anchor, Top-k forward KL obtains a 34.8% → 42.3% gain over K3.

We also find that **forward KL generally works better than reverse KL** in the absence of additional entropy regularization: on its own, Topk Reverse KL obtains 36.4% against 42.3% for Topk Forward KL, and it only catches up with the Δ regularizer of §5.3 (42.5%), which makes little difference to forward KL (42.4%). Forward KL is more mode-covering while reverse KL is more mode-seeking: Fig 9 shows that forward KL keeps a higher policy entropy than reverse KL for most of training.

The benefits of Top-k KL only appear when $k > 0$, but to save memory we need to keep k small. In general, the larger the k the better (with the limit being exact KL), but

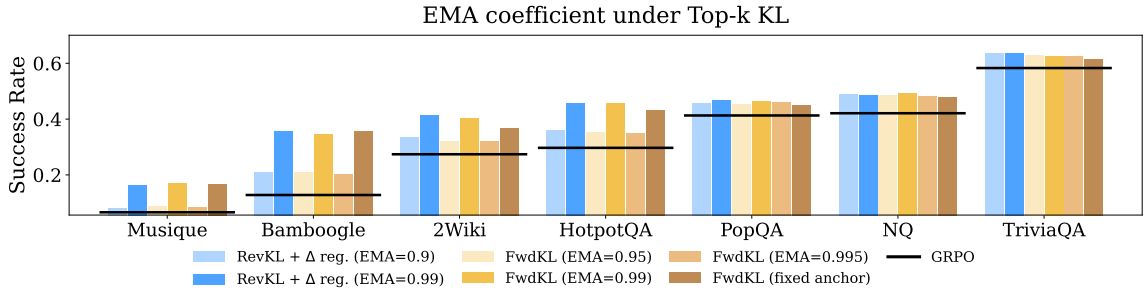


Figure 7. **Effect of the EMA coefficient and KL direction under Top-k KL** (with $k = 32$). Both Topk Forward KL and Topk Reverse KL with Δ reg. (28) perform best at EMA $\eta = 0.99$ (updated every 10 steps), which is the value we recommend.

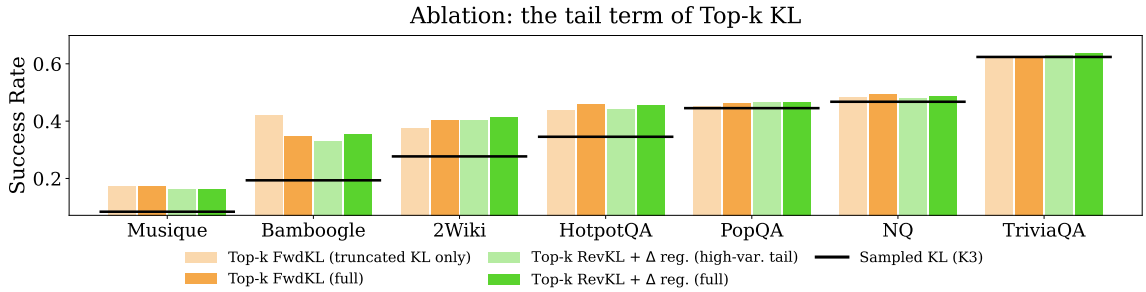


Figure 8. **Truncated KL alone already performs well**. With $k = 32$, Topk Forward KL without the tail term (truncated KL only) performs close to the full estimator on average, and both outperform sampled KL (K3). For Topk Reverse KL with Δ reg., 'high-var. tail' is a high-variance estimator of the tail term by re-using the rollout token (26) (§K.2).

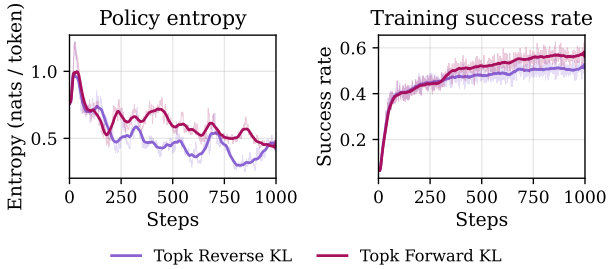


Figure 9. **Under Top-k KL, forward KL keeps a higher policy entropy than reverse KL for most of training.** Token-level policy entropy and training success rate, for Topk Reverse KL and Topk Forward KL of Tab 2 (moving average over 50 steps). Topk Reverse KL plateaus at a lower training success rate.

when k is large, the tail term ($\widehat{\mathrm{KL}}_{\mathrm{tail}}$ and $\widehat{\mathrm{FKL}}_{\mathrm{tail}}$) does not necessarily help, meaning that truncated KL alone might perform better. We illustrate this *bias-variance tradeoff* in a synthetic setting in Fig 4. For RL at scale, we empirically validate that increasing k from $8 \to 16 \to 32$ does lead to slightly improved performance (Fig 6). Moreover, Fig 8 shows that with $k = 32$, truncated KL alone performs close to the full Top-k KL (42.2% vs 42.3% on average). This suggests that at this k the tail term can be dropped; we keep it by default, since it makes the estimator unbiased at almost no extra cost. The high-variance tail (26) also works in practice (41.6%).

We also study what EMA coefficients are effective when using Top-k KL. In Fig 7, we find that $\eta = 0.99$ performs best along with $k = 32$ for Top-k KL, for both Topk Forward KL (42.3%) and Topk Reverse KL with Δ reg. (42.5%); $\eta = 0.9$, 0.95 and 0.995 all perform worse (36.0–36.7%), and Topk Forward KL with a fixed anchor obtains 40.9%. The Top-k rows of Tab 2 use $\eta = 0.99$.

7. Conclusion

In this work, we introduced two simple changes to policy gradients on LLMs: EMA anchor, which changes what KL is regularizing against, and Top-k KL, which changes how KL gradients are computed. We showed that the two changes are highly effective. Future work includes further investigation into Top-k f-divergence estimators (§G.2) beyond just KL, the application of Top-k KL to both offline and on-policy knowledge distillation of LLMs, and the application of our sampled KL (and more broadly, f-divergence) estimators to the policy gradient operator itself (§I– §J).

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Appendix Contents

- A Algorithm Box for EMA Policy Gradient 15
- B Derivations for EMA Policy Gradient Dynamics
  - B.1 Policy Gradient Dynamics under Local Quadratic KL Approximation . . . 17
  - B.2 Quasi-steady state analysis over a k-step window (Proof of Lemma 4.1) . . . 18
  - B.3 Eigen-decomposition of Fisher and mode-wise dynamics (Proof of Lemma 4.2) . . . 19
  - B.4 Stability and oscillations . . . 20
  - B.5 Steady-state lag and bounds . . . 20
- C Sequence-level KL vs. Token-level KL
  - C.1 Sequence-level KL gradients . . . 22
  - C.2 Analysis of sequence-level KL gradients . . . 22
  - C.3 Token-level KL gradients . . . 23
- D Derivation of Sampled Reverse KL Estimator
  - D.1 Sampled KL estimators (K1 / K2 / K3) and their expected values . . . 24
  - D.2 Gradients of K1 / K2 / K3 under autodiff $\mathbb{E}_p[\nabla_\theta(\cdot)]$ . . . 24
  - D.3 The $\boldsymbol{r}$-trick restores $\nabla_\theta \mathbb{E}_p[\cdot]$ from $\mathbb{E}_p[\nabla_\theta(\cdot)]$. . . . 25
  - D.4 **K3**$^{++}$ yields unbiased reverse-KL values and gradients . . . 25
  - D.5 **K4** yields unbiased reverse-KL values and gradients . . . 26
- E Derivation of Sampled Forward KL Estimator
  - E.1 Forward KL and its gradient . . . 27
  - E.2 The **K5** estimator has unbiased value . . . 27
  - E.3 The **K5** estimator has unbiased gradient . . . 28
  - E.4 Variance reduction in **K5** gradients . . . 28
- F Bias-Variance Tradeoff in Top-k KL: An Illustrative Synthetic Setup 29
- G Top-k $\boldsymbol{f}$-Divergence Estimator
  - G.1 f-divergence and its gradients . . . 31
  - G.2 A generic, unbiased, sampled f-divergence estimator . . . 32
  - G.3 Top-k f-divergence estimator: A generalization of Top-k KL estimator . . . 32
- H Optimal Policies under Forward vs Reverse KL Regularization
  - H.1 Reward transformation for equivalent optima between forward KL and reverse KL . . . 35
  - H.2 Reward transformation for equivalent optima across f-divergences . . . 36
- I Policy Gradient Methods can be Derived from Sampled KL Estimators
  - I.1 K1 estimator leads to on-policy PPO / GRPO loss . . . 38
  - I.2 K2 estimator leads to APA / Kimi loss . . . 39
  - I.3 K5 estimator leads to RWR / MPO loss . . . 40
  - I.4 K3 / K3^{++} / K4 estimators lead to the same losses . . . 40
- J Policy Gradient as $\boldsymbol{f}$-Divergence Minimization 42
- K Top-k KL: Unbiasedness and Variance
  - K.1 Unbiased values and gradients (Proof of Proposition 5.1) . . . 45
  - K.2 Tail token versus rollout token . . . 45
  - K.3 Top-k KL versus sampled KL . . . 46

A. Algorithm Box for EMA Policy Gradient

Algorithm 3 **EMA** Policy Gradient with TopkKL

Require: Prompt set $\mathcal{D}(x)$, LLM $\pi_\theta(y|x)$, reward $R(x, y)$.
Require: Anchor policy $\pi_{\theta_{\text{ema}}}(y|x)$.

$\theta_{\text{ema}} \leftarrow \theta$
for iteration $t = 1, 2, \ldots$ **do**
  Sample task prompt $x \sim \mathcal{D}$
  $\theta_{\text{old}} \leftarrow \theta$ for sampling
  Sample $y \sim \pi_{\theta_{\text{old}}}(\cdot \mid x)$; let L be the length of y
  Compute $\log \pi_{\theta_{\text{old}}}(y_n \mid x, y_{0:n-1})$ for $n = 0, \ldots, L-1$
  if using *reverse* KL **then**
    Compute $[q_0, \ldots, q_{L-1}]$, where q_n is the top-k logit indices from $\pi_{\theta_{\text{old}}}(\cdot \mid x, y_{0:n-1})$ {In *reverse* KL, the expectation is taken under π_θ}
  else
    Compute $[q_0, \ldots, q_{L-1}]$, where q_n is the top-k logit indices from $\pi_{\theta_{\text{ema}}}(\cdot \mid x, y_{0:n-1})$ {In *forward* KL, the expectation is taken under $\pi_{\theta_{\text{ema}}}$}
  end if
  Use $R(x, y)$ to compute advantage function A
  for $\upsilon = 1, \ldots, \Lambda$ **do**
    Compute $\log \pi_\theta(y_n \mid x, y_{0:n-1})$ for $n = 0, \ldots, L-1$
    Let $s_n = \text{sg}(\pi_\theta(y_n \mid x, y_{0:n-1}) / \pi_{\theta_{\text{old}}}(y_n \mid x, y_{0:n-1}))$
    $\mathcal{J}(\theta) = \sum_{n=0}^{L-1} s_n \, A \, \log \pi_\theta(y_n \mid x, y_{0:n-1})$, clip $\mathcal{J}(\theta)$ in PPO-style
    if using *reverse* KL **then**
      $\widehat{\text{KL}} = \sum_{n=0}^{L-1} \text{Topk}\textbf{Reverse}\text{KL}(\pi_\theta(\cdot|x, y_{0:n-1}), \pi_{\theta_{\text{ema}}}(\cdot|x, y_{0:n-1}), \pi_{\theta_{\text{old}}}(\cdot|x, y_{0:n-1}), q_n)$ {Alg 1}
    else
      $\widehat{\text{KL}} = \sum_{n=0}^{L-1} \text{Topk}\textbf{Forward}\text{KL}(\pi_\theta(\cdot|x, y_{0:n-1}), \pi_{\theta_{\text{ema}}}(\cdot|x, y_{0:n-1}), q_n)$ {Alg 2}
    end if
    $L(\theta) = -\mathcal{J}(\theta) + \beta \widehat{\text{KL}}$
    $\theta \leftarrow \theta - \alpha \nabla_\theta L(\theta)$
  end for
  if $t \bmod T_{\text{ema}} = 0$ **then**
    $\theta_{\text{ema}} \leftarrow \eta \, \theta_{\text{ema}} + (1 - \eta) \, \theta$
  end if
end for

The changes required to modify any policy gradient method into EMA-PG (with **EMA anchor** and **Top-k KL**) are highlighted above.

Details of Top-k KL: For completeness, we write down the full expression of Top-k KL terms. Using common notations, with the anchor $\pi_{\text{ref}} = \pi_{\theta_{\text{ema}}}$:

$$h_n = (x, y_{0:n-1}) \qquad \Delta_n = \sum\nolimits_{j \in q_n} \left[\pi_\theta(j \mid h_n) - \text{sg}(\pi_\theta(j \mid h_n))\right] \qquad z_n \sim \mu_n$$

where q_n is the set of top-k indices, Δ_n is the correction term (28), and z_n is the tail token, drawn from a proposal μ_n over the non-top-k indices. The Top-k Reverse KL (29) can be written as:

$$q_n \leftarrow \text{Topk}(\pi_{\theta_{\text{old}}}(\cdot \mid h_n)) \qquad \mu_n(j) \propto \pi_{\theta_{\text{old}}}(j \mid h_n) \, \mathbb{1}(j \notin q_n)$$

$$(\widehat{\text{KL}}_{\text{sampled}})_n = \frac{\pi_\theta(z_n \mid h_n)}{\text{sg}(\pi_\theta(z_n \mid h_n))} \, \text{sg}\left(\log \frac{\pi_\theta(z_n \mid h_n)}{\pi_{\text{ref}}(z_n \mid h_n)} \right)$$

$$(\text{Topk}\textbf{Reverse}\text{KL})_n = \sum_{j \in q_n} \pi_\theta(j \mid h_n) \log \frac{\pi_\theta(j \mid h_n)}{\pi_{\text{ref}}(j \mid h_n)} - \Delta_n + \text{sg}\left(\frac{\pi_\theta(z_n \mid h_n)}{\mu_n(z_n)} \right) \cdot (\widehat{\text{KL}}_{\text{sampled}})_n$$

And the Top-k Forward KL (31) can be written as:

$$
\begin{aligned}
&q_n \leftarrow \mathrm{Topk}(\pi_{\text{ref}}(\cdot \mid h_n)) \qquad \mu_n(j) \propto \pi_{\text{ref}}(j \mid h_n)\, \mathbb{1}(j \notin q_n) \\
&(\widehat{\mathrm{FKL}}_{\text{sampled}})_n = \mathrm{sg}\left(\frac{\pi_{\text{ref}}(z_n \mid h_n)}{\pi_\theta(z_n \mid h_n)}\right) \log \frac{\pi_{\text{ref}}(z_n \mid h_n)}{\pi_\theta(z_n \mid h_n)} + \log \frac{\pi_\theta(z_n \mid h_n)}{\mathrm{sg}(\pi_\theta(z_n \mid h_n))} \\
&(\text{Topk}\textbf{Forward}\text{KL})_n = \sum_{j \in q_n} \pi_{\text{ref}}(j \mid h_n) \log \frac{\pi_{\text{ref}}(j \mid h_n)}{\pi_\theta(j \mid h_n)} + \Delta_n + \mathrm{sg}\left(\frac{\pi_\theta(z_n \mid h_n)}{\mu_n(z_n)}\right) \cdot (\widehat{\mathrm{FKL}}_{\text{sampled}})_n
\end{aligned}
$$

Then we sum up the token-wise KL along the sequence length:

$$
\widehat{\mathrm{KL}} = \sum\nolimits_{n=0}^{L-1} (\text{Topk}\textbf{Reverse}\text{KL})_n \qquad \widehat{\mathrm{FKL}} = \sum\nolimits_{n=0}^{L-1} (\text{Topk}\textbf{Forward}\text{KL})_n
$$

Details of the Base RL Algorithm We discuss some additional implementation details below.

- For the policy gradient loss function $\mathcal{J}(\theta)$, we use a standard version of GRPO: PPO-style clipping (Schulman et al., 2017b), Monte-Carlo estimation of advantages (Shao et al., 2024; Liu et al., 2025a), with clip-higher (Yu et al., 2025):

$$
\begin{aligned}
&y^{(i)} \sim \pi_{\theta_{\text{old}}}(\cdot \mid x), \quad i = 0, \ldots, N-1 \\
&V(x) = \tfrac{1}{N} \sum\nolimits_{i=0}^{N-1} R(x, y^{(i)}) \\
&A(x, y^{(i)}) = R(x, y^{(i)}) - V(x) \qquad \mathrm{std}(x) = \sqrt{\tfrac{1}{N-1} \sum\nolimits_{i=0}^{N-1} \left(R(x, y^{(i)}) - V(x)\right)^2} \\
&s_n^{(i)} = \mathrm{sg}\left(\frac{\pi_\theta(y_n^{(i)} \mid x, y_{0:n-1}^{(i)})}{\pi_{\theta_{\text{old}}}(y_n^{(i)} \mid x, y_{0:n-1}^{(i)})}\right) \qquad M_n^{(i)} = \begin{cases} 0 & \text{if } A(x, y^{(i)}) > 0 \text{ and } s_n^{(i)} > 1 + \epsilon_{\text{high}}, \\ 0 & \text{if } A(x, y^{(i)}) < 0 \text{ and } s_n^{(i)} < 1 - \epsilon_{\text{low}}, \\ 1 & \text{otherwise.} \end{cases} \\
&\mathcal{J}^{\text{clip}}(x) = \tfrac{1}{N} \sum\nolimits_{i=0}^{N-1} \tfrac{1}{L^{(i)}} \left(\sum\nolimits_{n=0}^{L^{(i)}-1} s_n^{(i)}\, M_n^{(i)}\, \log \pi_\theta(y_n^{(i)} \mid x, y_{0:n-1}^{(i)})\right) A(x, y^{(i)}) \\
&\mathcal{J}(\theta) = \mathbb{E}_{x \sim \mathcal{D}}\left[\mathcal{J}^{\text{clip}}(x) \,/\, \mathrm{std}(x)\right]
\end{aligned}
$$

  where $L^{(i)}$ is the length of $y^{(i)}$, $\epsilon_{\text{high}} = 0.28$ and $\epsilon_{\text{low}} = 0.2$ (on agentic search, the average is over all the tokens of a batch instead of per rollout). $\mathcal{J}^{\text{clip}}$ applies the PPO-clip objective written in an equivalent form using binary masks (Wang et al., 2020; Chen et al., 2025). Note that the two techniques of EMA-PG are orthogonal to how we compute $\mathcal{J}(\theta)$; we can in principle also choose to use CISPO (Chen et al., 2025) or GSPO (Zheng et al., 2025) as the base algorithm.

- For the optimizer, we use Adam (Kingma, 2014) with decoupled weight decay (Loshchilov & Hutter, 2017), with a learning rate of 1e-6 for *full finetuning* (5e-7 for Topk Forward KL on agentic search). Since the focus of our study is to devise a better algorithm for full-scale post-training, we do not use any low-rank adaptation (LoRA) (Hu et al., 2022) in our experiments.

- $\beta = 0.001$ for KL regularization.

- $T_{\text{ema}} = 10$, following prior empirical practice among practitioners of Deep Q-learning that target networks (even though under EMA soft update) still only get updated every T_{ema} iterations; (Zhang et al., 2021) set the value to 10 (see `target_update_freq` $= 10$ in their implementation).

B. Derivations for EMA Policy Gradient Dynamics

Fisher matrix The Fisher information matrix of a policy π_θ is:

$$F_\theta \triangleq \mathbb{E}_{x\sim\mathcal{D}}\mathbb{E}_{y\sim\pi_\theta(\cdot|x)}\left[(\nabla_\theta \log \pi_\theta(y|x))(\nabla_\theta \log \pi_\theta(y|x))^\top\right]$$

The Fisher matrix is positive semidefinite (PSD), so all eigenvalues satisfy $\lambda_i \geq 0$. Consequently,

$$\lambda_{\max}(F_\theta) \leq \mathrm{tr}(F_\theta) = \mathbb{E}_{\substack{x\sim\mathcal{D}\\ y\sim\pi_\theta(\cdot|x)}}\left[\|\nabla_\theta \log \pi_\theta(y|x)\|_2^2\right] \tag{32}$$

giving us a practical way of estimating an upper bound on the largest Fisher eigenvalue of a policy under $\mathcal{D}$.

Setup. Let $J(\theta) \coloneqq R(\pi_\theta)$ denote the (expected) RL objective. Define the EMA parameters and the *lag*

$$\theta_{\text{ema},t+1} = \eta\,\theta_{\text{ema},t} + (1-\eta)\,\theta_t, \qquad \eta \in [0,1),$$
$$\delta_t \coloneqq \theta_t - \theta_{\text{ema},t}.$$

Let $g_t \coloneqq \nabla_\theta J(\theta)|_{\theta=\theta_t}$ be the policy-gradient (or any ascent direction). We consider the update

$$\theta_{t+1} = \theta_t + \alpha\Big[g_t - \beta\,\nabla_\theta \mathrm{KL}(\pi_\theta \,\|\, \pi_{\theta_{\text{ema},t}})\Big]_{\theta=\theta_t}, \tag{33}$$

with step size $\alpha > 0$ and regularization coefficient $\beta \geq 0$.

B.1. Policy Gradient Dynamics under Local Quadratic KL Approximation

We assume a local quadratic approximation of the KL around θ_t:

$$\mathrm{KL}(\pi_{\theta_t} \,\|\, \pi_{\theta_{\text{ema},t}}) \;\approx\; \frac{1}{2}(\theta_t - \theta_{\text{ema},t})^\top F_t(\theta_t - \theta_{\text{ema},t}) \;=\; \frac{1}{2}\delta_t^\top F_t \delta_t, \tag{34}$$

where $F_t \coloneqq F_{\theta_t}$ is the (empirical) Fisher information matrix at θ_t. Differentiating the RHS of (34) w.r.t. θ_t yields

$$\nabla_{\theta_t}\,\mathrm{KL}(\pi_{\theta_t} \,\|\, \pi_{\theta_{\text{ema},t}}) \;\approx\; \nabla_{\theta_t}\left(\tfrac{1}{2}\delta_t^\top F_t \delta_t\right) \;=\; F_t\delta_t, \tag{35}$$

where we treat F_t as locally constant under this approximation. Substituting (35) into (33) gives

$$\theta_{t+1} = \theta_t + \alpha g_t - \alpha\beta F_t \delta_t. \tag{36}$$

Lemma B.1 (Lag dynamics)**.** *Under* (36) *and the EMA recursion, the lag obeys*

$$\delta_{t+1} = (\eta I - \alpha\beta F_t)\,\delta_t + \alpha g_t. \tag{37}$$

Proof. By definition $\delta_{t+1} = \theta_{t+1} - \theta_{\text{ema},t+1}$, and by the EMA update,

$$\theta_{\text{ema},t+1} = \eta\theta_{\text{ema},t} + (1-\eta)\theta_t \;\Rightarrow\; \theta_t - \theta_{\text{ema},t+1} = \theta_t - \eta\theta_{\text{ema},t} - (1-\eta)\theta_t = \eta(\theta_t - \theta_{\text{ema},t}) = \eta\,\delta_t. \tag{38}$$

Therefore,

$$\delta_{t+1} = (\theta_{t+1} - \theta_t) + (\theta_t - \theta_{\text{ema},t+1}) = (\theta_{t+1} - \theta_t) + \eta\,\delta_t. \tag{39}$$

Using (36), $\theta_{t+1} - \theta_t = \alpha g_t - \alpha\beta F_t\delta_t$, so

$$\delta_{t+1} = \eta\delta_t + \alpha g_t - \alpha\beta F_t\delta_t = (\eta I - \alpha\beta F_t)\delta_t + \alpha g_t. \tag{40}$$

□

Define the (time-varying) linear operator

$$D_t \coloneqq \eta I - \alpha\beta F_t. \tag{41}$$

Collecting (36) and (37) gives the affine joint update

$$\begin{bmatrix}\theta_{t+1}\\ \delta_{t+1}\end{bmatrix} = \begin{bmatrix} I & -\alpha\beta F_t \\ 0 & \eta I - \alpha\beta F_t\end{bmatrix}\begin{bmatrix}\theta_t\\ \delta_t\end{bmatrix} + \begin{bmatrix}\alpha I\\ \alpha I\end{bmatrix} g_t. \tag{42}$$

B.2. Quasi-steady state analysis over a k-step window (Proof of Lemma 4.1)

Assumption (frozen gradient and Fisher). Fix an integer $k \geq 1$ and assume that over the window $\{t, \dots, t+k-1\}$,

$$g_{t+j} \approx g, \qquad F_{t+j} \approx F \qquad \text{for } j = 0, \dots, k-1, \tag{43}$$

for some constant vectors/matrices g, F. Define the corresponding constant operator

$$D \coloneqq \eta I - \alpha\beta F. \tag{44}$$

B.2.1. Closed form for δ_{t+k}

Unrolling (37) with constant D and g yields

$$\begin{aligned}
\delta_{t+1} &= D\delta_t + \alpha g, \\
\delta_{t+2} &= D\delta_{t+1} + \alpha g = D^2\delta_t + \alpha(D+I)g, \\
&\vdots \\
\delta_{t+k} &= D^k\delta_t + \alpha \sum_{j=0}^{k-1} D^j g.
\end{aligned} \tag{45}$$

Define the geometric-series matrix

$$S_k \coloneqq \sum_{j=0}^{k-1} D^j. \tag{46}$$

Then (45) becomes

$$\delta_{t+k} = D^k\delta_t + \alpha S_k\, g. \tag{47}$$

B.2.2. Invertibility of $I - D$ and closed form for S_k

Let v_i be an eigenvector of F, and λ_i be its corresponding eigenvalue. Using $D = \eta I - \alpha\beta F$,

$$Dv_i = (\eta I - \alpha\beta F)v_i = (\eta - \alpha\beta\lambda_i)v_i. \tag{48}$$

Define

$$\chi_i \coloneqq \eta - \alpha\beta\lambda_i. \tag{49}$$

Then $Dv_i = \chi_i v_i$. Since $\lambda_i \geq 0$ ($F \succeq 0$), $\eta < 1$, and $\beta, \alpha \geq 0$, we have

$$\chi_i \leq \eta < 1. \tag{50}$$

Hence $1 - \chi_i > 0$ for all i, so $I - D$ is invertible. Consequently,

$$S_k = \sum_{j=0}^{k-1} D^j = (I - D^k)(I - D)^{-1}. \tag{51}$$

B.2.3. Closed form for θ_{t+k} and the M_k matrix

From (36) with frozen F, g,

$$\theta_{t+1} = \theta_t + \alpha g - \alpha\beta F\delta_t, \tag{52}$$

$$\theta_{t+k} = \theta_t + \sum_{j=0}^{k-1} \big(\alpha g - \alpha\beta F\delta_{t+j}\big) = \theta_t + \alpha k\, g - \alpha\beta F \sum_{j=0}^{k-1} \delta_{t+j}. \tag{53}$$

Using (47) at times $t+j$,

$$\delta_{t+j} = D^j \delta_t + \alpha S_j g, \tag{54}$$

so

$$\sum_{j=0}^{k-1} \delta_{t+j} = \sum_{j=0}^{k-1} D^j \delta_t + \alpha \sum_{j=0}^{k-1} S_j g = S_k \delta_t + \alpha \Big(\sum_{j=0}^{k-1} S_j \Big) g. \tag{55}$$

Define

$$M_k \coloneqq \sum_{j=0}^{k-1} S_j. \tag{56}$$

Then

$$\theta_{t+k} = \theta_t + \alpha k\, g - \alpha\beta F S_k \delta_t - \alpha^2 \beta F M_k\, g. \tag{57}$$

Closed form for M_k. Using $S_j = (I - D^j)(I - D)^{-1}$ from (51),

$$M_k = \sum_{j=0}^{k-1} (I - D^j)(I - D)^{-1} = \Big(kI - \sum_{j=0}^{k-1} D^j \Big) (I - D)^{-1} = (kI - S_k)(I - D)^{-1}. \tag{58}$$

Collecting (57) and (47), one may write the dynamics as a homogeneous linear map in (θ, δ, g):

$$\begin{bmatrix} \theta_{t+k} \\ \delta_{t+k} \\ g \end{bmatrix} = \begin{bmatrix} I & -\alpha\beta F S_k & \alpha k I - \alpha^2 \beta F M_k \\ 0 & D^k & \alpha S_k \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} \theta_t \\ \delta_t \\ g \end{bmatrix}$$

B.3. Eigen-decomposition of Fisher and mode-wise dynamics (Proof of Lemma 4.2)

Since F is a Fisher information matrix (or symmetric empirical approximation), we assume F is symmetric PSD:

$$F \succeq 0.$$

Therefore, there exists an orthonormal eigenbasis $\{v_i\}_{i=0}^{d-1}$ and eigenvalues $\lambda_i \geq 0$ such that

$$F v_i = \lambda_i v_i, \qquad \lambda_i \geq 0.$$

We refer to v_i as the i-th Fisher eigenvector (eigen-direction). "High curvature" corresponds to large λ_i. Previously we have already shown that

$$\chi_i \coloneqq \eta - \alpha\beta\lambda_i \qquad \chi_i \leq \eta < 1,$$

and χ_i may be negative if $\alpha\beta\lambda_i > \eta$. Now we define the scalar projections

$$\delta_t^{(i)} \coloneqq v_i^\top \delta_t, \qquad g^{(i)} \coloneqq v_i^\top g. \tag{59}$$

Projecting (47) onto v_i yields

$$\delta_{t+k}^{(i)} = v_i^\top D^k \delta_t + \alpha\, v_i^\top S_k g = \chi_i^k \delta_t^{(i)} + \alpha \sum_{j=0}^{k-1} \chi_i^j\, g^{(i)} \tag{60}$$

$$= \chi_i^k \delta_t^{(i)} + \alpha\, \frac{1 - \chi_i^k}{1 - \chi_i}\, g^{(i)}. \tag{61}$$

This yields the decomposition into a transient term and a particular solution.

B.4. Stability and oscillations

B.4.1. Stability condition

The transient part of the lag dynamics is $\delta_{t+1} = D\delta_t$. Stability (transient $\to 0$) requires $\rho(D) < 1$, equivalently

$$\max_i |\chi_i| < 1. \tag{62}$$

Since $\chi_i \le \eta < 1$, the inequality $|\chi_i| < 1$ is only violated if $\chi_i \le -1$ for some i. The most negative eigenvalue occurs at $\lambda_{\max} \coloneqq \max_i \lambda_i$, so stability is equivalent to

$$\eta - \alpha\beta\lambda_{\max} > -1 \quad \iff \quad \alpha\beta\lambda_{\max} < 1 + \eta. \tag{63}$$

This proves (9).

B.4.2. Non-oscillatory vs. oscillatory transients

From (61), the sign of the transient in mode i is governed by χ_i^k. If $\chi_i \in (0, 1)$, the transient decays monotonically. If $\chi_i \in (-1, 0)$, the transient alternates sign each step (damped overshoot/undershoot), which we call "oscillatory". Thus:

- **Non-oscillatory in all modes** iff $\chi_i \ge 0$ for all i, i.e.

$$\eta - \alpha\beta\lambda_{\max} \ge 0 \quad \iff \quad \alpha\beta\lambda_{\max} \le \eta. \tag{64}$$

- **Oscillatory in some high-curvature directions** if there exists i with $\chi_i < 0$, which can occur when $\alpha\beta\lambda_{\max} > \eta$.

Combined with stability (63) yields the three regimes summarized in the main text:

- If $0 \le \alpha\beta\lambda_{\max} \le \eta$, then $\chi_i \in [0, \eta] \subset [0, 1)$ for all i, so the dynamics is stable and all transients decay monotonically (non-oscillatory).
- If $\eta < \alpha\beta\lambda_{\max} < 1 + \eta$, then stability holds ($|\chi_i| < 1$ for all i) but there exist high-curvature directions with $\chi_i < 0$, producing damped sign-flipping transients (oscillations).
- If $\alpha\beta\lambda_{\max} \ge 1 + \eta$, then $\chi_{\max} \le -1$ for the top-curvature direction, so $\max_i |\chi_i| \ge 1$ and the lag dynamics is unstable.

B.5. Steady-state lag and bounds

Assume stability (63), $D^k \to 0$ as $k \to \infty$. Taking $k \to \infty$ in (47) gives the steady lag

$$\delta_* = \lim_{k\to\infty} \delta_{t+k} = \alpha\Big(\sum_{j=0}^{\infty} D^j\Big) g = \alpha(I - D)^{-1} g. \tag{65}$$

Using $I - D = I - (\eta I - \alpha\beta F) = (1 - \eta)I + \alpha\beta F$, we obtain

$$\delta_* = \alpha\big((1 - \eta)I + \alpha\beta F\big)^{-1} g. \tag{66}$$

In each eigen-direction,

$$\delta_*^{(i)} = \frac{\alpha}{(1 - \eta) + \alpha\beta\lambda_i}\, g^{(i)}. \tag{67}$$

B.5.1. Euclidean norm upper bound

Since $F \succeq 0$, we have the PSD ordering

$$(1 - \eta)I + \alpha\beta F \ \succeq \ (1 - \eta)I.$$

For positive definite matrices, PSD ordering reverses under inversion, hence

$$\big((1-\eta)I + \alpha\beta F\big)^{-1} \;\preceq\; \frac{1}{1-\eta} I.$$

Therefore,

$$\|\delta_*\|_2 = \alpha \Big\| \big((1-\eta)I + \alpha\beta F\big)^{-1} g \Big\|_2 \le \alpha \Big\| \big((1-\eta)I + \alpha\beta F\big)^{-1} \Big\|_2 \|g\|_2 \;\le\; \alpha \cdot \frac{1}{1-\eta} \|g\|_2. \tag{68}$$

B.5.2. QUASI-STEADY KL MAGNITUDE

Under the quadratic KL approximation (34), the quasi-steady KL is

$$\widehat{\mathrm{KL}}_* \;\approx\; \frac{1}{2} \delta_*^\top F \delta_*. \tag{69}$$

Expanding in the eigenbasis, $F = \sum_i \lambda_i v_i v_i^\top$ and $\delta_* = \sum_i \delta_*^{(i)} v_i$, gives

$$\delta_*^\top F \delta_* = \sum_{i=0}^{d-1} \lambda_i \big(\delta_*^{(i)}\big)^2. \tag{70}$$

Substituting (67) yields

$$\widehat{\mathrm{KL}}_* \;\approx\; \frac{\alpha^2}{2} \sum_{i=0}^{d-1} \frac{\lambda_i \big(g^{(i)}\big)^2}{\big((1-\eta) + \alpha\beta\lambda_i\big)^2}. \tag{71}$$

Thus, within the quasi-steady model, increasing η increases $\widehat{\mathrm{KL}}_*$ unless β is increased or α is decreased.

C. Sequence-level KL vs. Token-level KL

Notation and setup For prompt x, consider the conditional distribution over output sequence $y = (y_0, \dots, y_{L-1})$.

$$\pi_\theta(y \mid x) = \prod_{n=0}^{L-1} \pi_\theta(y_n \mid x, y_{0:n-1}).$$

For each position n, define the prefix (history)

$$h_n \triangleq (x, y_{0:n-1}),$$

and the per-token log-ratio and score term

$$\rho_n \triangleq \log \frac{\pi_\theta(y_n \mid h_n)}{\pi_{\mathrm{ref}}(y_n \mid h_n)}, \qquad \omega_n \triangleq \nabla_\theta \log \pi_\theta(y_n \mid h_n).$$

Note that $\log \frac{\pi_\theta(y|x)}{\pi_{\mathrm{ref}}(y|x)} = \sum_{n=0}^{L-1} \rho_n$ and $\nabla_\theta \log \pi_\theta(y \mid x) = \sum_{n=0}^{L-1} \omega_n$.

C.1. Sequence-level KL gradients

Define the (sequence-level) conditional KL:

$$\mathrm{KL}\big(\pi_\theta(\cdot \mid x) \,\|\, \pi_{\mathrm{ref}}(\cdot \mid x)\big) \triangleq \mathbb{E}_{y \sim \pi_\theta(\cdot|x)} \left[\log \frac{\pi_\theta(y \mid x)}{\pi_{\mathrm{ref}}(y \mid x)} \right].$$

Differentiate it:

$$\begin{aligned} \nabla_\theta \mathrm{KL} &= \nabla_\theta \int \pi_\theta(y \mid x)\, \log \frac{\pi_\theta(y \mid x)}{\pi_{\mathrm{ref}}(y \mid x)}\, dy \\ &= \int \nabla_\theta \pi_\theta(y \mid x)\, \log \frac{\pi_\theta(y \mid x)}{\pi_{\mathrm{ref}}(y \mid x)}\, dy + \int \pi_\theta(y \mid x)\, \nabla_\theta \log \pi_\theta(y \mid x)\, dy. \end{aligned}$$

Using $\nabla_\theta \pi_\theta = \pi_\theta \nabla_\theta \log \pi_\theta$ and $\int \pi_\theta \nabla_\theta \log \pi_\theta \, dy = \mathbb{E}_{\pi_\theta}[\nabla_\theta \log \pi_\theta] = 0$, we obtain the standard score-function form:

$$\nabla_\theta \mathrm{KL}\big(\pi_\theta(\cdot \mid x) \,\|\, \pi_{\mathrm{ref}}(\cdot \mid x)\big) = \mathbb{E}_{y \sim \pi_\theta(\cdot|x)} \left[\log \frac{\pi_\theta(y \mid x)}{\pi_{\mathrm{ref}}(y \mid x)}\, \nabla_\theta \log \pi_\theta(y \mid x) \right]. \tag{72}$$

C.2. Analysis of sequence-level KL gradients

Substitute the autoregressive decompositions:

$$\nabla_\theta \mathrm{KL}\big(\pi_\theta(\cdot \mid x) \,\|\, \pi_{\mathrm{ref}}(\cdot \mid x)\big) = \mathbb{E}_{y \sim \pi_\theta(\cdot|x)} \left[\left(\sum_{m=0}^{L-1} \rho_m \right) \left(\sum_{n=0}^{L-1} \omega_n \right) \right] = \mathbb{E}_{y \sim \pi_\theta(\cdot|x)} \left[\sum_{n=0}^{L-1} \sum_{m=0}^{L-1} \rho_m \omega_n \right]. \tag{73}$$

Split the inner sum into "future" and "past" relative to n:

$$\sum_{m=0}^{L-1} \rho_m \omega_n = \left(\sum_{m \geq n} \rho_m \right) \omega_n + \left(\sum_{m < n} \rho_m \right) \omega_n. \tag{74}$$

Why the "past" terms vanish Recall the conditional expectation notation

$$\mathbb{E}_n[\cdot] \triangleq \mathbb{E}_{y_n \sim \pi_\theta(\cdot|h_n)}[\cdot], \qquad h_n \triangleq (x, y_{0:n-1}).$$

We will use the standard Law of total expectation in the following explicit form: for any random variable $Z = Z(x, y_{0:n})$,

$$\mathbb{E}_{y \sim \pi_\theta(\cdot|x)}[Z] = \mathbb{E}_{y_{0:n-1} \sim \pi_\theta(\cdot|x)} \Big[\mathbb{E}_{y_n \sim \pi_\theta(\cdot|x, y_{0:n-1})}[Z] \Big] = \mathbb{E}_{y_{0:n-1} \sim \pi_\theta(\cdot|x)} \big[\mathbb{E}_n[Z] \big]. \tag{75}$$

Step 1: the score has zero mean. Conditioning on a fixed prefix h_n, we have

$$\mathbb{E}_n[\omega_n] = \sum_a \pi_\theta(a \mid h_n)\, \nabla_\theta \log \pi_\theta(a \mid h_n) = \sum_a \nabla_\theta \pi_\theta(a \mid h_n) = \nabla_\theta \sum_a \pi_\theta(a \mid h_n) = \nabla_\theta 1 = 0.$$

Step 2: past log-ratios are constant under $\mathbb{E}_n[\cdot]$. Since $\sum_{m<n} \rho_m$ depends only on the prefix $h_n = (x, y_{0:n-1})$, it does not depend on y_n and can be pulled out of $\mathbb{E}_n[\cdot]$:

$$\mathbb{E}_n\left[\left(\sum_{m<n} \rho_m\right) \omega_n\right] = \left(\sum_{m<n} \rho_m\right) \mathbb{E}_n[\omega_n] = 0.$$

Step 3: unconditional past terms also vanish. Apply (75) with $Z = \left(\sum_{m<n} \rho_m\right) \omega_n$:

$$\mathbb{E}_{y\sim\pi_\theta(\cdot|x)}\left[\left(\sum_{m<n} \rho_m\right) \omega_n\right] = \mathbb{E}_{y_{0:n-1}\sim\pi_\theta(\cdot|x)}\left[\mathbb{E}_n\left[\left(\sum_{m<n} \rho_m\right) \omega_n\right]\right] = 0, \tag{76}$$

which justifies dropping the "past tokens" contribution in the main derivation.

C.3. Token-level KL gradients

Define the token-level conditional KL at position n:

$$\mathrm{KL}_n \triangleq \mathrm{KL}\big(\pi_\theta(\cdot \mid h_n) \,\|\, \pi_{\mathrm{ref}}(\cdot \mid h_n)\big) = \mathbb{E}_{y_n\sim\pi_\theta(\cdot|h_n)}\left[\log \frac{\pi_\theta(y_n \mid h_n)}{\pi_{\mathrm{ref}}(y_n \mid h_n)}\right].$$

By the same argument as (72), its gradient can be written as

$$\nabla_\theta \mathrm{KL}_n = \mathbb{E}_{y_n\sim\pi_\theta(\cdot|h_n)}\left[\log \frac{\pi_\theta(y_n \mid h_n)}{\pi_{\mathrm{ref}}(y_n \mid h_n)}\, \nabla_\theta \log \pi_\theta(y_n \mid h_n)\right] = \mathbb{E}_{y_n\sim\pi_\theta(\cdot|h_n)}[\rho_n\, \omega_n]. \tag{77}$$

Hence the token-level KL objective yields the per-token weighting:

$$\nabla_\theta L_{\mathrm{KL}}^{\text{token}} = \mathbb{E}_{y\sim\pi_\theta(\cdot|x)}\left[\sum_{n=0}^{L-1} \nabla_\theta \mathrm{KL}_n\right] = \mathbb{E}_{y\sim\pi_\theta(\cdot|x)}\left[\sum_{n=0}^{L-1} \rho_n \omega_n\right]. \tag{78}$$

Comparison Sequence-level KL weights token n by the cumulative *future* log-ratio $\sum_{m\geq n} \rho_m$, while token-level KL weights token n only by the *local* log-ratio ρ_n.

$$\nabla_\theta L_{\mathrm{KL}}^{\text{seq}} = \mathbb{E}_{\pi_\theta(y|x)}\Big[\sum_n \Big(\sum_{m\geq n} \rho_m\Big)\, \omega_n\Big] \qquad \nabla_\theta L_{\mathrm{KL}}^{\text{token}} = \mathbb{E}_{\pi_\theta(y|x)}\Big[\sum_n \big(\rho_n\big)\, \omega_n\Big]$$

In other words, **sequence-level KL punishes each current token for the divergence of all its future tokens**; token-level KL is only concerned with the current token.

D. Derivation of Sampled Reverse KL Estimator

We focus on a fixed token position n with prefix $h_n = (x, y_{0:n-1})$. Let $p \sim \pi_\theta(\cdot \mid h_n)$ be the sampled token, and define

$$w(p) \triangleq \frac{\pi_{\text{ref}}(p \mid h_n)}{\pi_\theta(p \mid h_n)}, \qquad \ell(p) \triangleq -\log w(p) = \log \frac{\pi_\theta(p \mid h_n)}{\pi_{\text{ref}}(p \mid h_n)}.$$

To avoid ambiguity, throughout this section we use the shorthand

$$\mathbb{E}_p\big[\,\cdot\,\big] \;\triangleq\; \mathbb{E}_{p\sim\pi_\theta(\cdot|h_n)}\big[\,\cdot\,\big]$$

Reverse KL at a fixed prefix. The token-level reverse KL at history h_n is (with $\mathcal{V}$ being the vocabulary):

$$\mathrm{KL}_n(\theta) \;\triangleq\; \mathrm{KL}\big(\pi_\theta(\cdot \mid h_n) \,\|\, \pi_{\text{ref}}(\cdot \mid h_n)\big) = \sum_{j\in\mathcal{V}} \pi_\theta(j \mid h_n) \log \frac{\pi_\theta(j \mid h_n)}{\pi_{\text{ref}}(j \mid h_n)} = \mathbb{E}_p\big[\ell(p)\big].$$

Exact reverse-KL gradient.

$$\nabla_\theta \mathrm{KL}_n(\theta) = \sum_{j\in\mathcal{V}} \pi_\theta(j) \log \frac{\pi_\theta(j)}{\pi_{\text{ref}}(j)} \nabla_\theta \log \pi_\theta(j) = \mathbb{E}_{p\sim\pi_\theta(\cdot|h_n)}\Big[\ell(p)\, \nabla_\theta \log \pi_\theta(p \mid h_n)\Big].$$

$\mathbb{E}_p[\nabla_\theta(\cdot)]$ **versus** $\nabla_\theta \mathbb{E}_p[\cdot]$ Since $\pi_\theta(\cdot \mid h_n)$ depends on θ, $\mathbb{E}_{p\sim\pi_\theta(\cdot|h_n)}[\cdot]$ is itself a function of θ; we write it as $\mathbb{E}_p[\cdot]$. For any scalar function $f(p, \theta)$, the gradient $\nabla_\theta \mathbb{E}_p[\cdot]$ is:

$$\mathbb{E}_p\big[f(p,\theta)\big] = \sum_{j\in\mathcal{V}} \pi_\theta(j \mid h_n)\, f(j,\theta) \qquad \nabla_\theta \mathbb{E}_p\big[f(p,\theta)\big] = \mathbb{E}_p\Big[f(p,\theta)\, \nabla_\theta \log \pi_\theta(p \mid h_n) + \nabla_\theta f(p,\theta)\Big]. \tag{79}$$

In contrast, $\mathbb{E}_p[\nabla_\theta f(p, \theta)]$ alone is in general not equal to $\nabla_\theta \mathbb{E}_p[f]$, as it has only one of the two terms in the full gradient.

D.1. Sampled KL estimators (K1 / K2 / K3) and their expected values

Define the single-sample estimators

$$(\mathrm{K1})_n \triangleq \ell(p), \qquad (\mathrm{K2})_n \triangleq \frac{1}{2}\,\ell(p)^2, \qquad (\mathrm{K3})_n \triangleq \ell(p) + w(p) - 1. \tag{80}$$

Then

$$\mathbb{E}_p\big[(\mathrm{K1})_n\big] = \mathbb{E}_p\big[\ell(p)\big] = \mathrm{KL}_n(\theta), \tag{81}$$

$$\mathbb{E}_p\big[w(p)\big] = \sum_{j\in\mathcal{V}} \pi_\theta(j \mid h_n) \frac{\pi_{\text{ref}}(j \mid h_n)}{\pi_\theta(j \mid h_n)} = \sum_{j\in\mathcal{V}} \pi_{\text{ref}}(j \mid h_n) = 1, \tag{82}$$

$$\mathbb{E}_p\big[(\mathrm{K3})_n\big] = \mathbb{E}_p\big[\ell(p)\big] + \mathbb{E}_p\big[w(p)\big] - 1 = \mathrm{KL}_n(\theta), \tag{83}$$

while in general $\mathbb{E}_p\big[(\mathrm{K2})_n\big] = \frac{1}{2}\mathbb{E}_p[\ell(p)^2] \neq \mathbb{E}_p[\ell(p)]$, so K2 has incorrect expected values.

D.2. Gradients of K1 / K2 / K3 under autodiff $\mathbb{E}_p[\nabla_\theta(\cdot)]$

Here $\nabla_\theta(\cdot)$ denotes the autodiff gradient of the sampled scalar while treating the sampled token p as fixed.

K1: correct value but wrong gradient. Since $(\mathrm{K1})_n = \ell(p) = \log \pi_\theta(p \mid h_n) - \log \pi_{\text{ref}}(p \mid h_n)$ and π_{ref} is fixed,

$$\nabla_\theta (\mathrm{K1})_n = \nabla_\theta \log \pi_\theta(p \mid h_n).$$

Averaging over $p \sim \pi_\theta(\cdot \mid h_n)$ gives

$$\mathbb{E}_p\big[\nabla_\theta (\mathrm{K1})_n\big] = \sum_{j\in\mathcal{V}} \pi_\theta(j \mid h_n) \nabla_\theta \log \pi_\theta(j \mid h_n) = \sum_{j\in\mathcal{V}} \nabla_\theta \pi_\theta(j \mid h_n) = \nabla_\theta 1 = 0,$$

which is zero.

K2: correct reverse-KL gradient but wrong value. We have $(\mathrm{K2})_n = \frac{1}{2}\ell(p)^2$, so

$$\nabla_\theta(\mathrm{K2})_n = \ell(p)\,\nabla_\theta\ell(p) = \ell(p)\,\nabla_\theta \log \pi_\theta(p \mid h_n).$$

Therefore,

$$\mathbb{E}_p\big[\nabla_\theta(\mathrm{K2})_n\big] = \mathbb{E}_p\Big[\ell(p)\,\nabla_\theta \log \pi_\theta(p \mid h_n)\Big]. \tag{84}$$

K3: yields the forward-KL gradient under $\mathbb{E}_p[\nabla_\theta(\cdot)]$. Since $(\mathrm{K3})_n = \ell(p) + w(p) - 1$ and,

$$w(p) = \pi_{\mathrm{ref}}(p \mid h_n)/\pi_\theta(p \mid h_n) \quad \nabla_\theta w(p) = -w(p)\,\nabla_\theta \log \pi_\theta(p \mid h_n),$$
$$\nabla_\theta(\mathrm{K3})_n = \nabla_\theta\ell(p) + \nabla_\theta w(p) = \big(1 - w(p)\big)\,\nabla_\theta \log \pi_\theta(p \mid h_n).$$

Averaging over $p \sim \pi_\theta(\cdot \mid h_n)$ gives

$$\begin{aligned}
\mathbb{E}_p\big[\nabla_\theta(\mathrm{K3})_n\big] &= \mathbb{E}_p\big[\nabla_\theta \log \pi_\theta(p \mid h_n)\big] - \mathbb{E}_p\big[w(p)\,\nabla_\theta \log \pi_\theta(p \mid h_n)\big] \\
&= 0 - \sum_{j\in\mathcal{V}} \pi_\theta(j \mid h_n)\frac{\pi_{\mathrm{ref}}(j \mid h_n)}{\pi_\theta(j \mid h_n)}\nabla_\theta \log \pi_\theta(j \mid h_n) \\
&= -\sum_{j\in\mathcal{V}} \pi_{\mathrm{ref}}(j \mid h_n)\,\nabla_\theta \log \pi_\theta(j \mid h_n) = \nabla_\theta \mathrm{KL}\big(\pi_{\mathrm{ref}}(\cdot \mid h_n) \,\|\, \pi_\theta(\cdot \mid h_n)\big),
\end{aligned} \tag{85}$$

which is the forward-KL gradient, not the reverse-KL gradient.

D.3. The r-trick restores $\nabla_\theta\mathbb{E}_p[\cdot]$ from $\mathbb{E}_p[\nabla_\theta(\cdot)]$.

Define $r(\cdot)$ as:

$$r(p,\theta) \triangleq \frac{\pi_\theta(p \mid h_n)}{\mathrm{sg}\big(\pi_\theta(p \mid h_n)\big)}. \tag{86}$$

In the forward pass $r(p,\theta) = 1$, but in backpropagation the denominator is treated as constant, hence

$$\nabla_\theta r(p,\theta) = r(p,\theta)\,\nabla_\theta \log \pi_\theta(p \mid h_n) = \nabla_\theta \log \pi_\theta(p \mid h_n).$$

For any scalar $f(p,\theta)$, differentiating $r(p,\theta)f(p,\theta)$ gives

$$\nabla_\theta\big(rf\big) = f\,\nabla_\theta r + r\,\nabla_\theta f = f(p,\theta)\,\nabla_\theta \log \pi_\theta(p \mid h_n) + \nabla_\theta f(p,\theta),$$

where we used $r = 1$ in the forward pass so $r\,\nabla_\theta f = \nabla_\theta f$. Taking $\mathbb{E}_p[\cdot]$ on both sides and comparing with (79) yields

$$\mathbb{E}_p\big[\nabla_\theta\big(r(p,\theta)f(p,\theta)\big)\big] = \nabla_\theta\mathbb{E}_p\big[f(p,\theta)\big]. \tag{87}$$

This identity holds even when f depends on θ (via the $\nabla_\theta f$ term).

D.4. K3^{++} yields unbiased reverse-KL values and gradients

Define

$$(\mathrm{K3}^{++})_n \triangleq r(p,\theta)\,(\mathrm{K3})_n = r(p,\theta)\big(\ell(p) + w(p) - 1\big). \tag{88}$$

Value: since $r = 1$ in the forward pass,

$$\mathbb{E}_p\big[(\mathrm{K3}^{++})_n\big] = \mathbb{E}_p\big[(\mathrm{K3})_n\big] = \mathrm{KL}_n(\theta) \quad \text{by (83)}. \tag{89}$$

Gradient: by (87) with $f = (\mathrm{K3})_n$,

$$\mathbb{E}_p\big[\nabla_\theta(\mathrm{K3}^{++})_n\big] = \nabla_\theta\mathbb{E}_p\big[(\mathrm{K3})_n\big] = \nabla_\theta\mathrm{KL}_n(\theta), \tag{90}$$

because $\mathbb{E}_p[(\mathrm{K3})_n] = \mathrm{KL}_n(\theta)$.

D.4.1. ALTERNATIVE PROOF

Alternatively, we compute the $\mathrm{K3}^{++}$ gradients in a brute force manner by directly differentiating using the product rule:

$$\nabla_\theta(\mathrm{K3}^{++})_n = \big(\ell + w - 1\big)\,\nabla_\theta r + r\big(\nabla_\theta \ell + \nabla_\theta w\big). \tag{91}$$

Now compute each piece (all conditioned on the sampled p and fixed h_n):

$$\nabla_\theta r = \nabla_\theta \log \pi_\theta(p \mid h_n), \tag{92}$$
$$\nabla_\theta \ell = \nabla_\theta \log \pi_\theta(p \mid h_n), \tag{93}$$
$$\nabla_\theta w = \nabla_\theta \left(\frac{\pi_{\mathrm{ref}}(p \mid h_n)}{\pi_\theta(p \mid h_n)} \right) = -w\,\nabla_\theta \log \pi_\theta(p \mid h_n). \tag{94}$$

Substitute (92)–(94) into (91). Using that $r = 1$ in the forward pass,

$$\nabla_\theta(\mathrm{K3}^{++})_n = \big(\ell + w - 1\big)\,\nabla_\theta \log \pi_\theta(p \mid h_n) + \big(1 - w\big)\,\nabla_\theta \log \pi_\theta(p \mid h_n) = \ell(p)\,\nabla_\theta \log \pi_\theta(p \mid h_n) \tag{95}$$

Taking expectation over the sampled token $p \sim \pi_\theta(\cdot \mid h_n)$ on both sides of (95) yields

$$\mathbb{E}_{p\sim\pi_\theta(\cdot|h_n)}\big[\nabla_\theta(\mathrm{K3}^{++})_n\big] = \mathbb{E}_{p\sim\pi_\theta(\cdot|h_n)}\Big[\ell(p)\,\nabla_\theta \log \pi_\theta(p \mid h_n)\Big] = \nabla_\theta \mathrm{KL}_n(\theta).$$

D.5. K4 yields unbiased reverse-KL values and gradients

Define

$$(\mathrm{K4})_n \triangleq r(p,\theta) \cdot \mathrm{sg}\big((\mathrm{K1})_n\big) = r(p,\theta) \cdot \mathrm{sg}\big(\ell(p)\big). \tag{96}$$

Value: since $r = 1$ in the forward pass,

$$\mathbb{E}_p\big[(\mathrm{K4})_n\big] = \mathbb{E}_p\big[\ell(p)\big] = \mathrm{KL}_n(\theta). \tag{97}$$

Gradient: $\mathrm{sg}(\ell(p))$ is treated as constant in backprop, so differentiating yields

$$\nabla_\theta(\mathrm{K4})_n = \mathrm{sg}\big(\ell(p)\big)\,\nabla_\theta r(p,\theta) = \mathrm{sg}\big(\ell(p)\big)\,\nabla_\theta \log \pi_\theta(p \mid h_n). \tag{98}$$

Taking expectation over $p \sim \pi_\theta(\cdot \mid h_n)$ gives

$$\mathbb{E}_p\big[\nabla_\theta(\mathrm{K4})_n\big] = \mathbb{E}_p\Big[\ell(p)\,\nabla_\theta \log \pi_\theta(p \mid h_n)\Big] = \nabla_\theta \mathrm{KL}_n(\theta). \tag{99}$$

E. Derivation of Sampled Forward KL Estimator

Similar to before, we focus on a fixed token position n with prefix $h_n = (x, y_{0:n-1})$. For brevity, write

$$\pi_\theta(j) \triangleq \pi_\theta(j \mid h_n), \qquad \pi_{\text{ref}}(j) \triangleq \pi_{\text{ref}}(j \mid h_n).$$

At this position we sample a token

$$p \sim \pi_\theta(\cdot \mid h_n),$$

and define the importance ratio and stop-gradient ratio

$$w(p) \triangleq \frac{\pi_{\text{ref}}(p)}{\pi_\theta(p)}, \qquad r(p,\theta) \triangleq \frac{\pi_\theta(p)}{\text{sg}(\pi_\theta(p))}.$$

The expectation over p is also same as before:

$$\mathbb{E}_p\big[\,\cdot\,\big] \triangleq \mathbb{E}_{p\sim\pi_\theta(\cdot|h_n)}\big[\,\cdot\,\big]$$

E.1. Forward KL and its gradient

The token-wise forward KL is

$$\text{FKL}_n(\theta) \triangleq \text{KL}\big(\pi_{\text{ref}}(\cdot \mid h_n) \,\|\, \pi_\theta(\cdot \mid h_n)\big) = \sum_{j\in\mathcal{V}} \pi_{\text{ref}}(j) \log \frac{\pi_{\text{ref}}(j)}{\pi_\theta(j)}.$$

Differentiating w.r.t. θ (note π_{ref} does not depend on θ),

$$\nabla_\theta \text{FKL}_n(\theta) = \sum_{j\in\mathcal{V}} \pi_{\text{ref}}(j)\, \nabla_\theta(\log \pi_{\text{ref}}(j) - \log \pi_\theta(j)) = -\sum_{j\in\mathcal{V}} \pi_{\text{ref}}(j)\, \nabla_\theta \log \pi_\theta(j). \tag{100}$$

We can rewrite (100) as an expectation over $p \sim \pi_\theta(\cdot \mid h_n)$ using $w(p)$:

$$-\sum_{j\in\mathcal{V}} \pi_{\text{ref}}(j)\, \nabla_\theta \log \pi_\theta(j) = -\sum_{j\in\mathcal{V}} \pi_\theta(j) \frac{\pi_{\text{ref}}(j)}{\pi_\theta(j)}\, \nabla_\theta \log \pi_\theta(j) = -\mathbb{E}_p\Big[w(p)\, \nabla_\theta \log \pi_\theta(p)\Big]. \tag{101}$$

Finally, we use the score-mean identity $\mathbb{E}_p[\nabla_\theta \log \pi_\theta(p)] = 0$ to obtain an equivalent form:

$$\nabla_\theta \text{FKL}_n(\theta) = -\mathbb{E}_p\Big[w(p)\, \nabla_\theta \log \pi_\theta(p)\Big] = \mathbb{E}_p\Big[(1 - w(p))\, \nabla_\theta \log \pi_\theta(p)\Big]. \tag{102}$$

E.2. The K5 estimator has unbiased value

We propose the forward-KL estimator

$$(\mathbf{K5})_n \triangleq \text{sg}(w(p)) \log w(p) + \log r(p,\theta). \tag{103}$$

For the KL value estimation, note that $r(p,\theta) = 1$ in the forward pass, so $\log r(p,\theta) = 0$ in value. Therefore

$$\begin{aligned}\mathbb{E}_p\big[(\mathbf{K5})_n\big] &= \mathbb{E}_p\big[w(p) \log w(p)\big] = \sum_{j\in\mathcal{V}} \pi_\theta(j) \frac{\pi_{\text{ref}}(j)}{\pi_\theta(j)} \log \frac{\pi_{\text{ref}}(j)}{\pi_\theta(j)} \\ &= \sum_{j\in\mathcal{V}} \pi_{\text{ref}}(j) \log \frac{\pi_{\text{ref}}(j)}{\pi_\theta(j)} = \text{FKL}_n(\theta),\end{aligned} \tag{104}$$

which is the token-wise forward KL.

E.3. The K5 estimator has unbiased gradient

We next show that $\mathbb{E}_p[\nabla_\theta(\mathbf{K5})_n] = \nabla_\theta \mathrm{FKL}_n(\theta)$.

First, compute the gradient of each term in (103). Since $\mathrm{sg}(w(p))$ is treated as a constant in backprop,

$$\nabla_\theta\big(\mathrm{sg}(w(p))\log w(p)\big) = \mathrm{sg}(w(p))\,\nabla_\theta \log w(p).$$

Because $\log w(p) = \log \pi_{\mathrm{ref}}(p) - \log \pi_\theta(p)$ and π_{ref} is fixed,

$$\nabla_\theta \log w(p) = -\nabla_\theta \log \pi_\theta(p) \qquad \nabla_\theta \log r(p,\theta) = \nabla_\theta \log \pi_\theta(p).$$

Combining them yields the per-sample gradient

$$\nabla_\theta(\mathbf{K5})_n = -\mathrm{sg}(w(p))\,\nabla_\theta \log \pi_\theta(p) + \nabla_\theta \log \pi_\theta(p) = (1 - w(p))\,\nabla_\theta \log \pi_\theta(p). \tag{105}$$

Taking expectation over $p \sim \pi_\theta(\cdot \mid h_n)$ gives

$$\mathbb{E}_p\big[\nabla_\theta(\mathbf{K5})_n\big] = \mathbb{E}_p\Big[(1 - w(p))\,\nabla_\theta \log \pi_\theta(p)\Big] = \nabla_\theta \mathrm{FKL}_n(\theta), \tag{106}$$

where the last equality follows from (102).

E.4. Variance reduction in K5 gradients

We start from the exact forward-KL gradient written in the importance-weighted form (Eq. (101)):

$$\nabla_\theta \mathrm{FKL}_n(\theta) = -\mathbb{E}_{p\sim\pi_\theta(\cdot|h_n)}\Big[w(p)\,\nabla_\theta \log \pi_\theta(p \mid h_n)\Big], \qquad w(p) = \frac{\pi_{\mathrm{ref}}(p \mid h_n)}{\pi_\theta(p \mid h_n)}.$$

A key observation is that under the same sampling distribution $p \sim \pi_\theta(\cdot \mid h_n)$, the weight $w(p)$ has mean 1:

$$\mathbb{E}_{p\sim\pi_\theta(\cdot|h_n)}[w(p)] = \sum_{j\in\mathcal{V}} \pi_\theta(j \mid h_n)\frac{\pi_{\mathrm{ref}}(j \mid h_n)}{\pi_\theta(j \mid h_n)} = \sum_{j\in\mathcal{V}} \pi_{\mathrm{ref}}(j \mid h_n) = 1.$$

Therefore, we can subtract this constant baseline from $w(p)$ without changing the expectation of the gradient estimator. Indeed, using the score-mean identity $\mathbb{E}_{p\sim\pi_\theta(\cdot|h_n)}[\nabla_\theta \log \pi_\theta(p \mid h_n)] = 0$, we have

$$\begin{aligned}
-\mathbb{E}_p\Big[w(p)\,\nabla_\theta \log \pi_\theta(p \mid h_n)\Big] &= -\mathbb{E}_p\Big[(w(p) - 1)\,\nabla_\theta \log \pi_\theta(p \mid h_n)\Big] - \underbrace{\mathbb{E}_p\Big[1 \cdot \nabla_\theta \log \pi_\theta(p \mid h_n)\Big]}_{=0} \\
&= \mathbb{E}_p\Big[(1 - w(p))\,\nabla_\theta \log \pi_\theta(p \mid h_n)\Big].
\end{aligned}$$

Thus, replacing $-w(p)$ with $(1 - w(p))$ centered around 0 preserves an unbiased gradient while typically reducing variance, known as the use of a *baseline* in policy gradient methods.

F. Bias-Variance Tradeoff in Top-k KL: An Illustrative Synthetic Setup

This appendix specifies the synthetic setting used to produce Fig. 4. The goal is to isolate the *bias–variance* behavior of the **Top-k Reverse KL** estimator in a controlled regime that reflects how KL penalties are applied to LLM policies, while removing confounders such as long-horizon autoregressive dependencies.

F.1. Token-wise i.i.d. simplification

Let $\pi_\theta(\cdot \mid h_n)$ be an LLM policy over the vocabulary $\mathcal{V}$ at token position n given history $h_n = (x, y_{0:n-1})$, and let $\pi_{\text{ref}}(\cdot \mid h_n)$ be the reference policy. The token-level reverse KL is:

$$\mathrm{KL}\big(\pi_\theta(\cdot \mid h_n) \,\|\, \pi_{\text{ref}}(\cdot \mid h_n)\big) = \sum_{j \in \mathcal{V}} \pi_\theta(j \mid h_n) \log \frac{\pi_\theta(j \mid h_n)}{\pi_{\text{ref}}(j \mid h_n)}. \tag{107}$$

To focus purely on the estimator (rather than the dynamics that produce h_n), we adopt the following simplification:

> **(i.i.d. token-position assumption)** Each token position contributes an i.i.d. draw from a common distribution over (π, π_{ref}), and we analyze a representative position whose ground-truth objective is the reverse KL in (107). In other words, we ignore autoregressive coupling across positions when constructing synthetic tasks.

F.2. Synthetic task and metric

Under this assumption, each token position is treated as a draw of a single-step categorical policy pair (π, π_{ref}) over a fixed vocabulary $\mathcal{V}$. We fix $|\mathcal{V}| = 32000$ and sample

$$\pi_{\text{ref}} = \mathrm{softmax}(\tilde{z}_{\text{ref}}), \qquad \tilde{z}_{\text{ref}} \sim \mathcal{N}(0, I_V), \tag{108}$$

$$\pi = \mathrm{softmax}(s \cdot \tilde{z}), \qquad \tilde{z} \sim \mathcal{N}(0, I_V),\ s > 0. \tag{109}$$

Controlling concentration via top-32 mass. Define the top-32 probability mass

$$M_{32}(\pi) \triangleq \sum_{j \in \mathrm{Topk}(\pi, 32)} \pi(j). \tag{110}$$

We tune the logit scale s so that $M_{32}(\pi)$ matches one of the target values

$$M_{32}(\pi) \approx m, \qquad m \in \{0.2,\ 0.5,\ 0.8,\ 0.9\}, \tag{111}$$

thereby probing a range of entropy regimes from diffuse to highly concentrated policies.

Estimators and error metric. We compare three per-token gradient estimators for the reverse-KL penalty: (i) *sampled-only* reverse KL (K4 on every batch token; fully Monte Carlo), (ii) *truncated-only* (the exact top-k head $(\mathrm{KL}_{\text{trun}})_n - \Delta_n$ without the tail term; biased), and (iii) *Top-k* reverse KL (29) (the same head plus one tail token per batch token (25); unbiased). We sweep

$$k \in \{4, 8, 16, 32, 64, 128, 256\}, \qquad B \in \{1, 2, 4, 8, 16, 32, 64, 128, 256, 512, 1024, 2048, 4096, 8192, 16384, 32768\},$$

where B denotes the number of "batch tokens": sampled KL uses B i.i.d. samples drawn from π, and Top-k KL draws one tail token for each of them. For each estimator, we measure the relative root-mean-squared error (RMSE) of the per-token gradient:

$$\mathrm{RelRMSE} \triangleq \frac{\sqrt{\mathbb{E}\big[\|\hat{g} - g_{\text{true}}\|_2^2\big]}}{\|g_{\text{true}}\|_2}, \tag{112}$$

where g_{true} is the exact gradient of (107) with respect to the token logits at that position, and $\hat{g}$ is the corresponding estimator. The expectation in (112) is approximated by Monte Carlo sampling and averaging over many independently generated synthetic tasks.

Critical sample size. For each k, the truncated-only estimator induces a bias floor (its error does not vanish with more samples since it omits the tail). The Top-k estimator is unbiased but has sampling variance from the tail term. We define the *critical sample size* as the smallest B beyond which Top-k KL achieves lower gradient error than Truncated KL, i.e., the intersection point between the Top-k RMSE curve and the truncated-only bias floor.

G. Top-k f-Divergence Estimator

We generalize the Top-k "truncated exact term + sampled tail" construction from KL to a broad class of f-divergences, while retaining (i) unbiased value estimates and (ii) unbiased gradients under the convention $\mathbb{E}[\nabla_\theta(\cdot)]$ (i.e., the expectation of autodiff gradients of sampled scalars).

Setup and notation. Fix a token position n and prefix $h_n = (x, y_{0:n-1})$. Let the current policy at this position be

$$P_\theta(j) \triangleq \pi_\theta(j \mid h_n), \qquad j \in \mathcal{V},$$

and let the reference policy be

$$Q(j) \triangleq \pi_{\mathrm{ref}}(j \mid h_n),$$

which is treated as independent of θ. We use an explicit expectation shorthand:

$$\mathbb{E}_p\big[\,\cdot\,\big] \triangleq \mathbb{E}_{p\sim P_\theta(\cdot)}\big[\,\cdot\,\big]$$

G.1. f-divergence and its gradients

Let $f : \mathbb{R}_+ \to \mathbb{R}$ be convex with $f(1) = 0$. The (discrete) f-divergence is

$$D_f(P_\theta\|Q) \triangleq \sum_{j\in\mathcal{V}} Q(j)\, f\!\left(\frac{P_\theta(j)}{Q(j)}\right). \tag{113}$$

Define the likelihood ratio and its inverse

$$t(j) \triangleq \frac{P_\theta(j)}{Q(j)}, \qquad w(j) \triangleq \frac{Q(j)}{P_\theta(j)} = \frac{1}{t(j)}. \tag{114}$$

Eq. (113) can be written as an expectation under Q:

$$D_f(P_\theta\|Q) = \mathbb{E}_{j\sim Q}\big[f(t(j))\big]. \tag{115}$$

It also admits an equivalent importance-weighted expectation under P_θ. Define

$$g_f(w) \triangleq w\, f(1/w). \tag{116}$$

Then

$$\begin{aligned} D_f(P_\theta\|Q) &= \sum_{j\in\mathcal{V}} Q(j)\, f\!\left(\frac{P_\theta(j)}{Q(j)}\right) = \sum_{j\in\mathcal{V}} P_\theta(j)\,\frac{Q(j)}{P_\theta(j)}\, f\!\left(\frac{P_\theta(j)}{Q(j)}\right) \\ &= \sum_{j\in\mathcal{V}} P_\theta(j)\, g_f(w(j)) = \mathbb{E}_p\big[g_f(w(p))\big], \end{aligned} \tag{117}$$

where $p \sim P_\theta(\cdot)$ and $w(p) = Q(p)/P_\theta(p)$.

G.1.1. Exact gradient w.r.t. θ (reference policy fixed)

Since Q is fixed, differentiating (113) yields

$$\begin{aligned} \nabla_\theta D_f(P_\theta\|Q) &= \sum_{j\in\mathcal{V}} Q(j)\, f'(t(j))\, \nabla_\theta\!\left(\frac{P_\theta(j)}{Q(j)}\right) = \sum_{j\in\mathcal{V}} f'(t(j))\, \nabla_\theta P_\theta(j) \\ &= \sum_{j\in\mathcal{V}} P_\theta(j)\, f'(t(j))\, \nabla_\theta \log P_\theta(j) = \mathbb{E}_p\Big[f'(t(p))\, \nabla_\theta \log P_\theta(p)\Big]. \end{aligned} \tag{118}$$

Eq. (118) is the policy-gradient-shaped form used throughout this appendix.

Table 4. Sampled f-divergence estimators $\mathbf{K}f^{++}$ (120), the tail term of the Top-k f-divergence estimator.
Let $P_\theta(j) = \pi_\theta(j|h_n),\ Q(j) = \pi_{\text{ref}}(j|h_n),\ t_j = P_\theta(j)/Q(j)$.
Sample $p \sim P_\theta(\cdot)$. We compute $r = P_\theta(p)/\text{sg}(P_\theta(p)), \quad w = Q(p)/P_\theta(p)$. Note that $\text{sg}(w)/w = r$.

	$\boldsymbol{f(t)}$ (so $D_f = \sum_j Q(j)\, f(t_j)$)	**Sampled f-divergence estimator** $= \text{sg}(w)\, f(1/w)$
Forward KL	$-\log t$	$\text{sg}(w) \cdot \log w$
Reverse KL	$t \log t$	$r \cdot (-\log w)$
Pearson χ^2	$(t-1)^2$	$r \cdot \frac{(1-w)^2}{w}$
Neyman χ^2	$\frac{(t-1)^2}{t}$	$r \cdot (1-w)^2$
Squared Hellinger	$(\sqrt{t}-1)^2$	$r \cdot (1-\sqrt{w})^2$
Jensen–Shannon (JS)	$\frac{1}{2}\left(t \log t - (t+1)\log\left(\frac{t+1}{2}\right)\right)$	$r \cdot \frac{1}{2}\left[-\log w - (1+w)\log\left(\frac{1+w}{2w}\right)\right]$
Total variation (TV)	$\frac{1}{2}\lvert t-1\rvert$	$r \cdot \frac{1}{2}\lvert 1-w\rvert$
α-divergence	$\frac{4}{1-\alpha^2}\left(1 - t^{\frac{1+\alpha}{2}}\right),\ \alpha \neq \pm 1$	$r \cdot \frac{4}{1-\alpha^2}\left(w - w^{\frac{1-\alpha}{2}}\right)$

G.2. A generic, unbiased, sampled f-divergence estimator

We define the following quantities as before:

$$r(p) \triangleq \frac{P_\theta(p)}{\text{sg}\big(P_\theta(p)\big)} \qquad g_f(w(p)) \triangleq w(p)\, f(1/w(p)) \qquad w(p) = \frac{Q(p)}{P_\theta(p)}$$

Then we have our sampled f-divergence estimator, $\mathbf{K}f^{++}$:

$$(\mathbf{K}f^{++})_n \triangleq r(p)\, g_f(w(p)), \qquad p \sim P_\theta(\cdot). \tag{119}$$

Which in effect becomes:

$$\boxed{(\mathbf{K}f^{++})_n = \text{sg}\left(\frac{Q(p)}{P_\theta(p)}\right) f\left(\frac{P_\theta(p)}{Q(p)}\right) = \text{sg}(w)\, f(1/w)} \tag{120}$$

Another way to write this expression is $(\mathbf{K}f^{++})_n = \text{sg}\left(\frac{\pi_{\text{ref}}(p|h_n)}{\pi_\theta(p|h_n)}\right) f\left(\frac{\pi_\theta(p|h_n)}{\pi_{\text{ref}}(p|h_n)}\right)$.

Unbiased value. Since $r = 1$ in the forward pass, from (117) we have

$$\mathbb{E}_p\big[(\mathbf{K}f^{++})_n\big] = \mathbb{E}_p\big[g_f(w(p))\big] = D_f(P_\theta \| Q). \tag{121}$$

Unbiased gradient under $\mathbb{E}[\nabla_\theta(\cdot)]$. Differentiate (119) using product rule:

$$\nabla_\theta(\mathbf{K}f^{++})_n = g_f(w(p))\, \nabla_\theta r(p) + r(p)\, \nabla_\theta g_f(w(p)) = g_f(w(p))\, \nabla_\theta \log P_\theta(p) + \nabla_\theta g_f(w(p)) \tag{122}$$

Taking expectation over $p \sim P_\theta(\cdot)$ gives

$$\mathbb{E}_p\big[\nabla_\theta(\mathbf{K}f^{++})_n\big] = \nabla_\theta \mathbb{E}_p\big[g_f(w(p))\big] = \nabla_\theta D_f(P_\theta \| Q), \tag{123}$$

where the last equality follows from (117). Thus $(\mathbf{K}f^{++})_n$ provides both unbiased values and unbiased gradients for any f-divergence.

G.3. Top-k f-divergence estimator: A generalization of Top-k KL estimator

Let $q_n \subseteq \mathcal{V}$ be any index set of size k (e.g., $q_n = \text{Topk}(P_\theta)$ or $q_n = \text{Topk}(Q)$). Being an unbiased estimator does not require q_n to be top-k; top-k is a variance/compute heuristic.

Truncated exact term. Define the truncated f-divergence (computed exactly given logits on q_n):

$$\boxed{(D_{f,\mathrm{trun}})_n \triangleq \sum_{j \in q_n} Q(j)\, f\!\left(\frac{P_\theta(j)}{Q(j)}\right)} \tag{124}$$

Sampled tail term. As in (25), draw one tail token $z_n \sim \mu_n$, where μ_n is any distribution over $\mathcal{V}$ with $\mu_n(j) > 0$ iff $j \notin q_n$, and let $s_n = \mathrm{sg}(P_\theta(z_n)/\mu_n(z_n))$ be its importance weight. Define the tail estimator

$$\boxed{(\widehat{D}_{f,\mathrm{tail}})_n \triangleq s_n\, (\mathbf{K} f^{++})_n\big|_{p=z_n}} = s_n\, r(z_n)\, g_f\!\left(\frac{Q(z_n)}{P_\theta(z_n)}\right) \tag{125}$$

Top-k f-divergence estimator. We define the Top-k f-divergence estimator

$$\boxed{(\text{Top-}k\text{-}D_f)_n \triangleq (D_{f,\mathrm{trun}})_n + (\widehat{D}_{f,\mathrm{tail}})_n} \tag{126}$$

Unbiased value. The weight s_n carries no gradient and $r = 1$ in the forward pass, so by the definition of g_f,

$$\mathbb{E}_{z_n}\big[(\widehat{D}_{f,\mathrm{tail}})_n\big] = \sum_{j \notin q_n} \mu_n(j)\, \frac{P_\theta(j)}{\mu_n(j)}\, g_f\!\left(\frac{Q(j)}{P_\theta(j)}\right) = \sum_{j \notin q_n} Q(j)\, f\!\left(\frac{P_\theta(j)}{Q(j)}\right), \tag{127}$$

so

$$\mathbb{E}_{z_n}\big[(\text{Top-}k\text{-}D_f)_n\big] = (D_{f,\mathrm{trun}})_n + \mathbb{E}_{z_n}\big[(\widehat{D}_{f,\mathrm{tail}})_n\big] = D_f(P_\theta \| Q). \tag{128}$$

Unbiased gradient. Since $(D_{f,\mathrm{trun}})_n$ is computed exactly on q_n, it has the correct gradient contribution from indices in q_n. For the tail term, the gradient of (120) at a token j is

$$\nabla_\theta (\mathbf{K} f^{++})_n\big|_{p=j} = \mathrm{sg}(w(j))\, f'(t(j))\, \nabla_\theta t(j) = f'(t(j))\, \nabla_\theta \log P_\theta(j), \tag{129}$$

which is the j-th term of the exact gradient (118), with no additional term. Hence

$$\mathbb{E}_{z_n}\big[\nabla_\theta (\widehat{D}_{f,\mathrm{tail}})_n\big] = \sum_{j \notin q_n} P_\theta(j)\, f'(t(j))\, \nabla_\theta \log P_\theta(j) = \nabla_\theta \sum_{j \notin q_n} Q(j)\, f\!\left(\frac{P_\theta(j)}{Q(j)}\right), \tag{130}$$

and therefore

$$\mathbb{E}_{z_n}\big[\nabla_\theta (\text{Top-}k\text{-}D_f)_n\big] = \nabla_\theta D_f(P_\theta \| Q). \tag{131}$$

The same holds with the rollout token in place of the tail token, i.e., with the tail term $\mathbb{1}(p \notin q_n)\, (\mathbf{K} f^{++})_n$ for $p \sim P_\theta(\cdot)$, at a higher variance (§K.2).

Adding a baseline. For any constant c, adding $c \log r(z_n)$ to the tail term and $c\,\Delta_n$ (28) to the truncated term keeps both the value and the gradient unbiased:

$$\boxed{(\text{Top-}k\text{-}D_f^{(c)})_n \triangleq (D_{f,\mathrm{trun}})_n + c\,\Delta_n + s_n\, \big[(\mathbf{K} f^{++})_n + c \log r\big]_{p=z_n}} \tag{132}$$

Both c-terms are zero in value, and their expected gradients cancel: $c \sum_{j \in q_n} \nabla_\theta P_\theta(j) + c \sum_{j \notin q_n} \nabla_\theta P_\theta(j) = 0$. A baseline on the tail term alone, without $c\,\Delta_n$, biases the gradient by $-c \sum_{j \in q_n} \nabla_\theta P_\theta(j)$. The estimator (126) is the case $c = 0$. Top-k reverse KL (29) is the case $f(t) = t \log t$ with $c = -1$, and Top-k forward KL (31) is the case $f(t) = -\log t$ with $c = +1$. In both, $c = -f'(1)$, for which the gradient of the tail term at a token, $(f'(t) - f'(1))\, \nabla_\theta \log P_\theta$, vanishes where $P_\theta = Q$.

A note on variance reduction in Forward and Reverse KL gradient estimators.

- The Forward KL estimator derived from the standard f-divergence formula in Eq (120) is $\mathrm{sg}(w)\log w$, which differs from our **K5** estimator $\mathrm{sg}(w)\log w + \log r$. This is explained in §E.4: the additional term $\log r$ is added as a *baseline* to reduce gradient variance, where the baseline is $\mathbb{E}[\mathrm{sg}(w)] = 1$.
- The Reverse KL estimator derived from Eq (120) is $r \cdot (-\log w)$; this also differs from our **K4** estimator $r \cdot \mathrm{sg}(-\log w)$. The reason is similar: the stop gradient on $(-\log w)$ removes the term $-\nabla_\theta \log w = \nabla_\theta \log P_\theta(p)$ from the gradient, so that **K4** equals $r \cdot (-\log w) - \log r$ in both value and gradient. Since $\mathbb{E}_p[\nabla_\theta \log P_\theta(p)] = 0$, this keeps the gradients unbiased while typically reducing variance.
- Both baselines are multiples of $\log r$, whose gradient has zero mean over the full vocabulary but not over the non-top-k indices alone: $\mathbb{E}_{z_n}[s_n \nabla_\theta \log r(z_n)] = \sum_{j \notin q_n} \nabla_\theta P_\theta(j) = -\sum_{j \in q_n} \nabla_\theta P_\theta(j)$. This is why, inside a Top-k estimator, they come with the term $c\,\Delta_n$ of (132): $-\Delta_n$ for Top-k reverse KL ($c = -1$) and $+\Delta_n$ for Top-k forward KL ($c = +1$).

H. Optimal Policies under Forward vs Reverse KL Regularization

We now study the optimal policies under different types of regularizers and see if the optimal policies are interchangeable.

The RL objectives under reverse and forward KL regularization are:

$$J = \mathbb{E}_{y\sim\pi_\theta(\cdot|x)}[R(x,y)] - \beta\,\mathrm{KL}(\pi_\theta(\cdot\mid x)\|\pi_{\text{ref}}(\cdot\mid x)) \tag{133}$$
$$J_{\text{fwd}} = \mathbb{E}_{y\sim\pi_\theta(\cdot|x)}[R(x,y)] - \beta\mathrm{KL}(\pi_{\text{ref}}(\cdot\mid x)\|\pi_\theta(\cdot\mid x)) \tag{134}$$

Optimal Policy under Reverse KL It is well known that the optimal policy for objective (133) is (Peters et al., 2010; Schulman et al., 2017a; Abdolmaleki et al., 2018):

$$\boxed{\pi^*(y|x) = \pi_{\text{ref}}(y|x)\,\frac{\exp(R(x,y)/\beta)}{Z(x)}} \qquad Z(x) = \sum\nolimits_y \pi_{\text{ref}}(y|x)\exp(R(x,y)/\beta) \tag{135}$$

Optimal Policy under Forward KL We derive the optimal policy for objective (134). Expanding the forward KL:

$$J_{\text{fwd}} = \sum\nolimits_y \pi_\theta(y|x)R(x,y) + \beta\sum\nolimits_y \pi_{\text{ref}}(y|x)\log\pi_\theta(y|x) + \text{const} \tag{136}$$

where the constant absorbs terms independent of π_θ. This objective decomposes into an RL term (first sum) and a behavioral cloning (BC) term (second sum). Forming the Lagrangian:

$$\mathcal{L} = \sum\nolimits_y \pi_\theta(y|x)R(x,y) + \beta\sum\nolimits_y \pi_{\text{ref}}(y|x)\log\pi_\theta(y|x) - \lambda\left(\sum\nolimits_y \pi_\theta(y|x) - 1\right)$$
$$\frac{\partial\mathcal{L}}{\partial\pi_\theta(y|x)} = R(x,y) + \beta\,\frac{\pi_{\text{ref}}(y|x)}{\pi_\theta(y|x)} - \lambda = 0$$
$$\pi_\theta(y\mid x) = \frac{\beta\,\pi_{\text{ref}}(y\mid x)}{\lambda - R(x,y)}$$

For this to be a valid probability distribution, we need $\lambda > \max_y R(x,y)$. Denote $Z^*(x) := \lambda$, we require $Z^*(x)$ to satisfy:

$$\sum\nolimits_y \frac{\pi_{\text{ref}}(y\mid x)}{Z^*(x) - R(x,y)} = \frac{1}{\beta} \tag{137}$$

Equation (137) implicitly defines $Z^*(x)$ as a function of the reward distribution as well. The optimal policy is:

$$\boxed{\pi^*_{\text{fwd}}(y\mid x) = \pi_{\text{ref}}(y\mid x)\,\frac{\beta}{Z^*(x) - R(x,y)}} \tag{138}$$

A similar result was obtained in (Grill et al., 2020a) under a different context.

H.1. Reward transformation for equivalent optima between forward KL and reverse KL

We now derive the reward transformation that makes the two objectives yield the same optimal policy.

$$\pi^*(y\mid x) = \pi^*_{\text{fwd}}(y\mid x) \qquad \frac{\pi_{\text{ref}}(y|x)\exp(\tilde{R}/\beta)}{Z(x)} = \frac{\beta\,\pi_{\text{ref}}(y\mid x)}{Z^*(x) - R(x,y)} \tag{139}$$

Therefore, the optimal policy under reward function R and forward KL regularizer is equivalent to the counterpart under reward function $\tilde{R}$ and reverse KL regularizer:

$$\text{Forward KL (with } R) \to \text{Reverse KL (with } \tilde{R}) \qquad \boxed{\tilde{R} = -\beta\log(Z^* - R) + \beta\log(\beta Z)} \tag{140}$$

Proposition H.1. *The function $\tilde{R} = -\beta\log(Z^* - R) + \text{const}$ is strictly monotonically increasing and strictly convex in R.*

Proof. Taking the derivative with respect to R (treating Z^* as constant): $\frac{\partial\tilde{R}}{\partial R} = -\beta\cdot\frac{-1}{Z^*-R} = \frac{\beta}{Z^*-R} > 0$. The last step was due to $Z^* > \max_y R(x,y)$ by construction. Thus $\tilde{R}$ is strictly monotonically increasing in R.

Taking the second derivative: $\frac{\partial^2\tilde{R}}{\partial R^2} = \frac{\partial}{\partial R}\left(\frac{\beta}{Z^*-R}\right) = \beta\cdot\frac{1}{(Z^*-R)^2} = \frac{\beta}{(Z^*-R)^2} > 0$. Thus $\tilde{R}$ is strictly convex in R. □

Inverse transformation: Given a reward R used in the reverse KL objective J, what reward R_{fwd} should be used in the forward KL objective J_{fwd} to obtain the same optimal policy?

Setting $\pi^*(y|x) = \pi^*_{\text{fwd}}(y|x)$, we have $\exp(R/\beta)/Z = \beta/(Z^* - R_{\text{fwd}})$, which simplifies to:

$$\text{Reverse KL (with } R) \to \text{Forward KL (with } R_{\text{fwd}}) \qquad \boxed{R_{\text{fwd}} = Z^* - \beta Z \exp(-R/\beta)} \tag{141}$$

Proposition H.2. *The function $R_{fwd} = Z^* - \beta Z \exp(-R/\beta)$ is strictly monotonically increasing and strictly concave in R.*

Proof. Taking first-order derivative $\frac{\partial R_{\text{fwd}}}{\partial R} = -\beta Z \cdot \left(-\frac{1}{\beta}\right) \exp(-R/\beta) = Z \exp(-R/\beta) > 0$; therefore, R_{fwd} is strictly monotonically increasing (preserving reward ordering).

The second-order derivative is $\frac{\partial^2 R_{\text{fwd}}}{\partial R^2} = Z \cdot \left(-\frac{1}{\beta}\right) \exp(-R/\beta) = -\frac{Z}{\beta} \exp(-R/\beta) < 0$; therefore, R_{fwd} is strictly concave (compressing high rewards). □

Direction	Transformation	Monotonic?	Curvature	Effect
Forward KL $\to$ Reverse KL	$-\beta \log(Z^* - R) + \text{const}$	Yes	Convex	Amplify high rewards
Reverse KL $\to$ Forward KL	$Z^* - \beta Z e^{-R/\beta}$	Yes	Concave	Compress high rewards

H.2. Reward transformation for equivalent optima across f-divergences

We now generalize beyond KL divergence to arbitrary f-divergence regularization. Consider the objective:

$$J_f = \mathbb{E}_{y \sim \pi_\theta(\cdot|x)}[R(x,y)] - \beta\, D_f(\pi_\theta(\cdot|x) \| \pi_{\text{ref}}(\cdot|x)) \tag{142}$$

where the f-divergence is defined as $D_f(P\|Q) = \sum_y Q(y)\, f\left(\frac{P(y)}{Q(y)}\right)$ where $f : \mathbb{R}^+ \to \mathbb{R}$ is a convex function with $f(1) = 0$. Standard KKT conditions yield the optimal policy:

$$\boxed{\pi^*_f(y \mid x) = \pi_{\text{ref}}(y \mid x) \cdot (f')^{-1}\left(\frac{R(x,y) - \lambda(x)}{\beta}\right)} \tag{143}$$

where $\lambda(x)$ is determined by the normalization constraint:

$$\sum_y \pi_{\text{ref}}(y \mid x) \cdot (f')^{-1}\left(\frac{R(x,y) - \lambda(x)}{\beta}\right) = 1 \tag{144}$$

which was previously derived in (Wang et al., 2023).

Given two f-divergences with f_1 and f_2, the optimal policies $\pi^*_{f_1}$ and $\pi^*_{f_2}$ coincide when:

$$(f_1')^{-1}\left(\frac{R_1 - \lambda_1}{\beta}\right) = (f_2')^{-1}\left(\frac{R_2 - \lambda_2}{\beta}\right) \tag{145}$$

This yields the general reward transformation:

$$\boxed{R_2 = \beta \cdot f_2'\left((f_1')^{-1}\left(\frac{R_1 - \lambda_1}{\beta}\right)\right) + \lambda_2} \tag{146}$$

The curvature of this transformation is determined by the composition $(f_2') \circ (f_1')^{-1}$.

Table 5. **Optimal Policy form** under each f-divergence regularization.

Divergence	$f(t)$	$f'(t)$	$(f')^{-1}(s)$	Optimal Policy Form
Reverse KL	$t\log t - t + 1$	$\log t$	e^s	$\pi_{\text{ref}} \cdot \exp\big((R-\lambda)/\beta\big)$
Forward KL	$-\log t + t - 1$	$1 - \frac{1}{t}$	$\frac{1}{1-s}$	$\pi_{\text{ref}} \cdot \frac{1}{1-(R-\lambda)/\beta}$
Jensen–Shannon	$\frac{1}{2}\Big[t\log t - (t+1)\log\Big(\frac{t+1}{2}\Big)\Big]$	$\frac{1}{2}\log\Big(\frac{2t}{t+1}\Big)$	$\frac{1}{2e^{-2s}-1}$	$\pi_{\text{ref}} \cdot \frac{\exp\big(2(R-\lambda)/\beta\big)}{2-\exp\big(2(R-\lambda)/\beta\big)}$
Squared Hellinger	$(\sqrt{t}-1)^2 = t - 2\sqrt{t} + 1$	$1 - \frac{1}{\sqrt{t}}$	$\frac{1}{(1-s)^2}$	$\pi_{\text{ref}} \cdot \frac{1}{\big(1-(R-\lambda)/\beta\big)^2}$
Pearson χ^2	$(t-1)^2$	$2(t-1)$	$1 + \frac{s}{2}$	$\pi_{\text{ref}} \cdot \Big(1 + \frac{R-\lambda}{2\beta}\Big)$
Neyman χ^2	$\frac{(t-1)^2}{t} = t - 2 + \frac{1}{t}$	$1 - \frac{1}{t^2}$	$\frac{1}{\sqrt{1-s}}$	$\pi_{\text{ref}} \cdot \frac{1}{\sqrt{1-(R-\lambda)/\beta}}$
α-divergence	$\frac{4}{1-\alpha^2}\Big(1 - t^{\frac{1+\alpha}{2}}\Big)$	$-\frac{2}{1-\alpha}\,t^{\frac{\alpha-1}{2}}$	$\big(-\frac{1-\alpha}{2}\,s\big)^{\frac{2}{\alpha-1}}$	$\pi_{\text{ref}} \cdot \Big(-\frac{1-\alpha}{2} \cdot \frac{R-\lambda}{\beta}\Big)^{\frac{2}{\alpha-1}}$

Table 6. **Reward transformations that produce the *same optimal policy* as each f-divergence under Reverse KL.** Let λ and $\widetilde{\lambda}$ be normalization constants enforcing $\sum_y \pi^*(y \mid x) = 1$ for the f-divergence and Reverse KL objectives, respectively. Then the equivalence is achieved by $\widetilde{R}(x,y) = \beta\log\big((f')^{-1}((R-\lambda)/\beta)\big) + \widetilde{\lambda}$, for each $f(\cdot)$ in f-divergence.

Divergence f (target)	$(f')^{-1}(s)$	**Reverse-KL reward transform** $\widetilde{R}(x,y)$	Ranges of $\lambda(x)$
Forward KL	$\dfrac{1}{1-s}$	$-\beta\log\Big(1 - \dfrac{R-\lambda}{\beta}\Big) + \widetilde{\lambda}$	$\lambda > R - \beta$
Jensen–Shannon	$\dfrac{1}{2e^{-2s}-1}$	$-\beta\log\Big(2\exp\big(-2\dfrac{R-\lambda}{\beta}\big) - 1\Big) + \widetilde{\lambda}$	$\lambda > R - \frac{\beta}{2}\log 2$
Squared Hellinger	$\dfrac{1}{(1-s)^2}$	$-2\beta\log\Big(1 - \dfrac{R-\lambda}{\beta}\Big) + \widetilde{\lambda}$	$\lambda > R - \beta$
Pearson χ^2	$1 + \dfrac{s}{2}$	$\beta\log\Big(1 + \dfrac{R-\lambda}{2\beta}\Big) + \widetilde{\lambda}$	$\lambda < R + 2\beta$
Neyman χ^2	$\dfrac{1}{\sqrt{1-s}}$	$-\dfrac{\beta}{2}\log\Big(1 - \dfrac{R-\lambda}{\beta}\Big) + \widetilde{\lambda}$	$\lambda > R - \beta$
α-divergence	$\Big(-\dfrac{1-\alpha}{2}\,s\Big)^{\frac{2}{\alpha-1}}$	$\dfrac{2\beta}{\alpha-1}\log\Big(-\dfrac{1-\alpha}{2}\cdot\dfrac{R-\lambda}{\beta}\Big) + \widetilde{\lambda}$	$-(1-\alpha)(R-\lambda) > 0$

I. Policy Gradient Methods can be Derived from Sampled KL Estimators

If RL optimization is simply written as closing the reverse KL between current policy π_θ and the reference policy distribution π_{ref} transformed by the return R (Peters & Schaal, 2007; Schulman et al., 2017a; Haarnoja et al., 2018), we have:

$$\min_\theta \mathrm{KL}\left(\pi_\theta(\cdot|x)\middle\|\frac{1}{Z(x)}\pi_{\text{ref}}(\cdot|x)\exp\Big(R(x,\cdot)\Big)\right) \tag{147}$$

to make the connection with sampled KL estimators clear, we define the ratio between the optimal policy π^* and current policy π_θ as w, same as before:

$$w = \frac{\pi_{\text{ref}}(y|x)\ \exp R(x,y)}{\pi_\theta(y|x)\, Z(x)} \tag{148}$$

where the partition function $Z(x)$ is approximated via a group of N trajectories per prompt $y^{(i)} \sim \pi_\theta(\cdot \mid x)$ for $i = 1, \ldots, N$:

$$\log Z(x) \triangleq \log \mathbb{E}_{\pi_{\text{ref}}(y|x)}[\exp R(x,y)] \approx \log \frac{1}{N}\sum_{i=1}^{N} \mathrm{sg}\left(\frac{\pi_{\text{ref}}(y^{(i)} \mid x)}{\pi_\theta(y^{(i)} \mid x)}\right)\exp\Big(R(x,y^{(i)})\Big) \tag{149}$$

$$\geq \frac{1}{N}\sum_{i=1}^{N}\left(R(x,y^{(i)}) - \mathrm{sg}\left(\log\frac{\pi_\theta(y^{(i)} \mid x)}{\pi_{\text{ref}}(y^{(i)} \mid x)}\right)\right) \tag{150}$$

where the last step uses Jensen's inequality. We split it into two terms, value function ($V(x)$) and aggregate KL ($\widehat{\mathrm{KL}}$):

$$V(x) \triangleq \frac{1}{N}\sum_{i=1}^{N} R(x,y^{(i)}) \qquad \widehat{\mathrm{KL}} \triangleq \frac{1}{N}\sum_{i=1}^{N}\mathrm{sg}\left(\log\frac{\pi_\theta(y^{(i)} \mid x)}{\pi_{\text{ref}}(y^{(i)} \mid x)}\right) \tag{151}$$

As a side note, *to sharpen or flatten the target distribution, we simply need to multiply all rewards by* $1/\beta$; as a result, we omit β in our derivation and let it be absorbed by $R(x,y)$.

Next, we show that **every sampled KL estimator in Tab 1 can be turned into a policy gradient algorithm**.

I.1. K1 estimator leads to on-policy PPO / GRPO loss

We start with $\mathbf{K1} = -\log w$. Its autodiff gradient has zero mean (§D.2), so we use its score-function gradient, $\nabla_\theta \log \pi_\theta(y|x) \cdot \mathrm{sg}(-\log w)$:

$$\text{K1:}\quad \min_\theta -\log w \qquad \nabla_\theta L_1 = -\nabla_\theta \log\pi_\theta(y|x)\left(R(x,y) - \log Z(x) - \mathrm{sg}\left(\log\frac{\pi_\theta(y \mid x)}{\pi_{\text{ref}}(y \mid x)}\right)\right)$$
$$\approx -\nabla_\theta \log\pi_\theta(y|x)\left(R(x,y) - V(x) + \widehat{\mathrm{KL}} - \mathrm{sg}\left(\log\frac{\pi_\theta(y \mid x)}{\pi_{\text{ref}}(y \mid x)}\right)\right)$$

Summing over all N rollouts, we get

$$\underbrace{-\sum_{j=1}^{N}\nabla_\theta \log\pi_\theta(y^{(j)} \mid x)\Big(R(x,y^{(j)}) - V(x)\Big)}_{\text{REINFORCE}} + \underbrace{\sum_{j=1}^{N}\nabla_\theta \log\pi_\theta(y^{(j)} \mid x)\left(\mathrm{sg}\left(\log\frac{\pi_\theta(y^{(j)} \mid x)}{\pi_{\text{ref}}(y^{(j)} \mid x)}\right) - \widehat{\mathrm{KL}}\right)}_{\text{The regularizer gradient}}$$

Lemma I.1. *The regularizer gradient is equivalent to the expected KL gradient: its expected value is* $(N-1)\,\nabla_\theta \mathrm{KL}(\pi_\theta \,\|\, \pi_{ref})$*, since*

$$\mathbb{E}_{\substack{y^{(j)}\sim\pi_\theta(\cdot|x)\\ j=1,\ldots,N}}\left[\sum_{j=1}^{N}\nabla_\theta \log\pi_\theta(y^{(j)} \mid x)\,\widehat{\mathrm{KL}}\right] = \mathbb{E}_{\substack{y^{(j)}\sim\pi_\theta(\cdot|x)\\ j=1,\ldots,N}}\left[\frac{1}{N}\sum_{j=1}^{N}\nabla_\theta \log\pi_\theta(y^{(j)} \mid x)\,\mathrm{sg}\left(\log\tfrac{\pi_\theta(y^{(j)}|x)}{\pi_{ref}(y^{(j)}|x)}\right)\right] \tag{152}$$
$$= \nabla_\theta \mathrm{KL}(\pi_\theta(\cdot \mid x) \,\|\, \pi_{ref}(\cdot \mid x))$$

Proof. Expanding the product of sums gives

$$\mathbb{E}_{\substack{y^{(j)}\sim\pi_\theta(\cdot|x)\\ j=1,\dots,N}}\left[\sum_{j=1}^{N}\nabla_\theta\log\pi_\theta(y^{(j)}\mid x)\,\widehat{\mathrm{KL}}\right]=\mathbb{E}_{\substack{y^{(j)}\sim\pi_\theta(\cdot|x)\\ j=1,\dots,N}}\left[\frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{N}\nabla_\theta\log\pi_\theta(y^{(j)}\mid x)\,\mathrm{sg}\left(\log\frac{\pi_\theta(y^{(i)}\mid x)}{\pi_{\text{ref}}(y^{(i)}\mid x)}\right)\right]$$

which can be written as two components:

$$\begin{aligned}&\frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{N}\nabla_\theta\log\pi_\theta(y^{(j)}\mid x)\,\mathrm{sg}\left(\log\frac{\pi_\theta(y^{(i)}\mid x)}{\pi_{\text{ref}}(y^{(i)}\mid x)}\right)\\ =&\underbrace{\frac{1}{N}\sum_{j=1}^{N}\nabla_\theta\log\pi_\theta(y^{(j)}\mid x)\,\mathrm{sg}\left(\log\frac{\pi_\theta(y^{(j)}\mid x)}{\pi_{\text{ref}}(y^{(j)}\mid x)}\right)}_{=\mathbb{E}_{y\sim\pi_\theta}\left[\nabla_\theta\log\pi_\theta(y\mid x)\,\mathrm{sg}\left(\log\frac{\pi_\theta(y|x)}{\pi_{\text{ref}}(y|x)}\right)\right]}+\underbrace{\frac{1}{N}\sum_{j=1}^{N}\sum_{i\neq j}\nabla_\theta\log\pi_\theta(y^{(j)}\mid x)\,\mathrm{sg}\left(\log\frac{\pi_\theta(y^{(i)}\mid x)}{\pi_{\text{ref}}(y^{(i)}\mid x)}\right)}_{\text{has an expected value }=0,\text{ since }\mathbb{E}_{y\sim\pi_\theta}[\nabla_\theta\log\pi_\theta(y\mid x)]=0}\end{aligned}$$

For $i\neq j$, independence of samples and the score-function identity $\mathbb{E}_{y\sim\pi_\theta}[\nabla_\theta\log\pi_\theta(y\mid x)]=0$ imply that these off-diagonal terms have zero expectation. The only non-vanishing contribution comes from the diagonal $i=j$, yielding

$$\mathbb{E}_{y\sim\pi_\theta}\left[\nabla_\theta\log\pi_\theta(y\mid x)\,\mathrm{sg}\left(\log\frac{\pi_\theta(y\mid x)}{\pi_{\text{ref}}(y\mid x)}\right)\right]=\nabla_\theta\mathrm{KL}(\pi_\theta(\cdot\mid x)\parallel\pi_{\text{ref}}(\cdot\mid x)).$$

The first part of the regularizer gradient is a sum of N such terms, with an expected value of $N\,\nabla_\theta\mathrm{KL}(\pi_\theta\parallel\pi_{\text{ref}})$, and its second part, with $\widehat{\mathrm{KL}}$, has an expected value of $\nabla_\theta\mathrm{KL}(\pi_\theta\parallel\pi_{\text{ref}})$. Thus, the regularizer gradient is equivalent to the common KL gradient. □

By the same argument, the REINFORCE term with the group baseline $V(x)$ has an expected value of $-(N-1)\,\nabla_\theta\mathbb{E}_{\pi_\theta(y|x)}[R(x,y)]$. Therefore, L_1 is simply a typical KL-regularized policy gradient objective:

$$\text{K1:}\quad\min_\theta-\log w\qquad\boxed{\nabla_\theta L_1=-\nabla_\theta\log\pi_\theta(y\mid x)\Big(R(x,y)-V(x)\Big)+\nabla_\theta\mathrm{KL}(\pi_\theta(\cdot\mid x)\parallel\pi_{\text{ref}}(\cdot\mid x))}\tag{153}$$

Which is what typical policy gradient algorithms like PPO (Schulman et al., 2017b) and GRPO (Shao et al., 2024) optimize in the on-policy case.

I.2. K2 estimator leads to APA / Kimi loss

Using the K2 estimator:

$$\text{K2:}\qquad\min_\theta\frac{1}{2}(\log w)^2\qquad\qquad\nabla_\theta L_2=\frac{1}{2}\nabla_\theta\left(\log\pi_\theta(y|x)-\log\pi_{\text{ref}}(y|x)-R(x,y)+\log Z(x)\right)^2$$

Expanding the partition function:

$$\begin{aligned}&\frac{1}{2}\nabla_\theta\left(\log\pi_\theta(y|x)-\log\pi_{\text{ref}}(y|x)-(R(x,y)-V(x))-\widehat{\mathrm{KL}}\right)^2\\ =&\underbrace{\frac{1}{2}\nabla_\theta\left(\log\pi_\theta(y|x)-\log\pi_{\text{ref}}(y|x)-(R(x,y)-V(x))\right)^2}_{\text{APA Loss}}-\underbrace{\nabla_\theta\log\pi_\theta(y\mid x)\,\widehat{\mathrm{KL}}}_{\substack{\text{Becomes }\nabla_\theta\mathrm{KL}(\pi_\theta(\cdot\mid x)\parallel\pi_{\text{ref}}(\cdot\mid x))\\ \text{when summed over }N\text{ trajectories (Lemma I.1)}}}\end{aligned}$$

The loss L_2 is the Advantage-induced Policy Alignment (**APA**) (Zhu et al., 2023), which was also used by Kimi models (Kimi et al., 2025b). The second term was often ignored, since prior works often approximate $\log Z(x)\approx V(x)$ rather than $\log Z(x)\approx V(x)-\widehat{\mathrm{KL}}$. The APA loss already incorporates the same KL term in expectation:

$$\begin{aligned}&\frac{1}{2}\nabla_\theta\Big(\log\pi_\theta(y|x)-\log\pi_{\text{ref}}(y|x)-(R(x,y)-V(x))\Big)^2\\ =&-\nabla_\theta\log\pi_\theta(y|x)\Big(R(x,y)-V(x)\Big)+\nabla_\theta\mathrm{KL}(\pi_\theta(\cdot\mid x)\|\pi_{\text{ref}}(\cdot\mid x))\end{aligned}$$

Which means that the additional $-\nabla_\theta \log \pi_\theta(y \mid x)\, \widehat{\mathrm{KL}}$ term just downweights the KL. Both APA and Kimi showed that this loss is effective in the off-policy regime without necessarily adding off-policy correction:

$$\text{K2:} \qquad \min_\theta \frac{1}{2}(\log w)^2 \qquad \boxed{\nabla_\theta L_2 = \frac{1}{2}\nabla_\theta \Big(\log \pi_\theta(y|x) - \log \pi_{\text{ref}}(y|x) - (R(x,y) - V(x)) \Big)^2} \tag{154}$$

I.3. K5 estimator leads to RWR / MPO loss

Under the K5 estimator, the divergence minimization in policy optimization becomes:

$$\text{K5:} \quad \min_\theta \mathrm{sg}(w) \log w + \log r \qquad \nabla_\theta L_5 = \nabla_\theta \log \pi_\theta(y|x) \left(1 - \frac{\pi_{\text{ref}}(y|x)\, \exp R(x,y)}{\pi_\theta(y|x)\, Z(x)} \right)$$

The constant 1 comes from $\log r$ (§E.4) and has zero mean, since $\mathbb{E}_{y\sim\pi_\theta}[\nabla_\theta \log \pi_\theta(y \mid x)] = 0$. Dropping it and averaging over all N rollouts per x to simplify the partition function:

$$\begin{aligned}
& -\frac{1}{N}\sum_{i=1}^N \nabla_\theta \log \pi_\theta(y^{(i)} \mid x) \left(\frac{\pi_{\text{ref}}(y^{(i)} \mid x)\, \exp R(x, y^{(i)})}{\pi_\theta(y^{(i)} \mid x)\, Z(x)} \right) \\
\approx & -\frac{1}{N}\sum_{i=1}^N \nabla_\theta \log \pi_\theta(y^{(i)} \mid x) \left(\frac{\mathrm{sg}\left(\frac{\pi_{\text{ref}}(y^{(i)}|x)}{\pi_\theta(y^{(i)}|x)}\right) \exp R(x, y^{(i)})}{\frac{1}{N}\sum_{j=1}^N \mathrm{sg}\left(\frac{\pi_{\text{ref}}(y^{(j)}|x)}{\pi_\theta(y^{(j)}|x)}\right) \exp R(x, y^{(j)})} \right) \\
= & -\sum_{i=1}^N \nabla_\theta \log \pi_\theta(y^{(i)} \mid x) \cdot \mathrm{sg} \underbrace{\left(\frac{\exp\left(R(x, y^{(i)}) - \log \frac{\pi_\theta(y^{(i)}|x)}{\pi_{\text{ref}}(y^{(i)}|x)}\right)}{\sum_{j=1}^N \exp\left(R(x, y^{(j)}) - \log \frac{\pi_\theta(y^{(j)}|x)}{\pi_{\text{ref}}(y^{(j)}|x)}\right)} \right)}_{\text{softmax over } [y^{(1)}, \ldots, y^{(N)}]}
\end{aligned}$$

Which can be written in a batched manner over a group of N rollouts per prompt $\boldsymbol{y} = [y^{(1)}, \ldots, y^{(N)}]$, where sum and softmax are taken along the axis of the group dimension $i = 1, \ldots, N$ (which we denote as sum_y and $\mathrm{softmax}_y$):

$$-\mathrm{sum}_y \left(\nabla_\theta \log \pi_\theta(\boldsymbol{y} \mid x) \cdot \mathrm{softmax}_y \left(R(x, \boldsymbol{y}) - \log \frac{\pi_\theta(\boldsymbol{y} \mid x)}{\pi_{\text{ref}}(\boldsymbol{y} \mid x)} \right) \right)$$

This loss closely resembles Reward-Weighted Regression (**RWR**) (Peters & Schaal, 2007) and Maximum a Posteriori Policy Optimisation (**MPO**) (Abdolmaleki et al., 2018).

$$\text{K5:} \quad \min_\theta \mathrm{sg}(w) \log w + \log r \qquad \boxed{\nabla_\theta L_5 = -\nabla_\theta \log \pi_\theta(y|x) \cdot \mathrm{softmax}_y \Big(R(x,y) - \log(\pi_\theta(y|x)/\pi_{\text{ref}}(y|x)) \Big)} \tag{155}$$

I.4. K3 / K3^{++} / K4 estimators lead to the same losses

The K3 estimator leads to L_5 (same as the RWR / MPO loss):

$$\begin{aligned}
& \text{K3:} \quad \min_\theta(-\log w + w - 1) \\
& \nabla_\theta L_3 = \underbrace{\nabla_\theta \log \pi_\theta(y|x)}_{\text{From } -\log w} - \underbrace{\Big(\nabla_\theta \log \pi_\theta(y|x)\Big) \left(\frac{\pi_{\text{ref}}(y|x)\, \exp R(x,y)}{\pi_\theta(y|x)\, Z(x)} \right)}_{\text{From } w-1} = \nabla_\theta L_5
\end{aligned} \tag{156}$$

The K3^{++} estimator leads to L_2 (same as the APA loss):

$$\begin{aligned}
& \text{K3}^{++}\text{:} \quad \min_\theta r \cdot (-\log w + w - 1) \qquad r = \frac{\pi_\theta(y|x)}{\mathrm{sg}(\pi_\theta(y|x))} \\
& \nabla_\theta L_{3++} = \Big(\nabla_\theta \log \pi_\theta(y|x)\Big) \Big(\log \pi_\theta(y|x) - \log \pi_{\text{ref}}(y|x) - R(x,y) + \log Z(x) \Big) = \nabla_\theta L_2
\end{aligned} \tag{157}$$

The K4 estimator leads to L_2 (same as the APA loss):

$$\text{K4:} \quad \min_\theta r \cdot \mathrm{sg}(-\log w)$$

$$\nabla_\theta L_4 = \Big(\nabla_\theta \log \pi_\theta(y|x)\Big)\left(\log \pi_\theta(y|x) - \log \pi_{\text{ref}}(y|x) - R(x,y) + \log Z(x)\right) = \nabla_\theta L_2 \tag{158}$$

A Note on Off-policy Correction Just like the off-policy correction for any sampled KL, any policy loss derived above can simply multiply a stop gradient version of the importance weight to remain unbiased when sampling is not on-policy:

$$y \sim \pi_{\text{sampling}}(\cdot \mid x) \qquad s = \mathrm{sg}\left(\frac{\pi_\theta(y \mid x)}{\pi_{\text{sampling}}(y \mid x)}\right)$$

With the option of using additional PPO-like binary masks on the loss

$$M(x,y) = \begin{cases} 0 & \text{if } R(x,y) - V(x) > 0 \text{ and } s > 1 + \epsilon_{\text{high}} \\ 0 & \text{if } R(x,y) - V(x) < 0 \text{ and } s < 1 - \epsilon_{\text{low}} \\ 1 & \text{otherwise} \end{cases}$$

Leading us to conclude that the off-policy gradient under any loss function L above is

$$\mathbb{E}_{y \sim \pi_{\text{sampling}}(\cdot|x)}[s(x,y)\, M(x,y)\, \nabla_\theta L(x,y)]$$

Though it is worth noting that many prior works find those losses to be effective in the absence of off-policy correction.

Summary of the Equivalence between Policy Gradient and Divergence Minimization We have shown that many existing policy gradient methods can be derived from sampled KL estimators. In other words, better techniques in sampled KL estimation may directly lead to better policy gradient algorithms under such an equivalence.

Estimator	Expression	Corresponding policy gradient	Prior literature?
K1	$-\log w$	$\nabla_\theta L_1 = -\nabla_\theta \log \pi_\theta(y\|x)\Big(R(x,y) - V(x)\Big) + \nabla_\theta \mathrm{KL}(\pi_\theta(\cdot\|x)\|\pi_{\text{ref}}(\cdot\|x))$	**PPO**, **GRPO**, etc
K2	$\frac{1}{2}(\log w)^2$	$\nabla_\theta L_2 = \frac{1}{2}\nabla_\theta\Big(\log \pi_\theta(y\|x) - \log \pi_{\text{ref}}(y\|x) - R(x,y) + V(x)\Big)^2$	**APA**, **Kimi**
K4	$r \cdot \mathrm{sg}(-\log w)$	$\nabla_\theta L_4 = \nabla_\theta L_2$	APA, Kimi
K5	$\mathrm{sg}(w)\log w + \log r$	$\nabla_\theta L_5 = -\nabla_\theta \log \pi_\theta(y\|x)\ \mathrm{softmax}_y\Big(R(x,y) - \log\big(\pi_\theta(y\|x)/\pi_{\text{ref}}(y\|x)\big)\Big)$	**RWR**, **MPO**
K3	$-\log w + w - 1$	$\nabla_\theta L_3 = \nabla_\theta L_5$	RWR, MPO
K3^{++}	$r(-\log w + w - 1)$	$\nabla_\theta L_{3++} = \nabla_\theta L_2$	APA, Kimi

Table 7. **Each KL estimator directly corresponds to a policy gradient loss** under the divergence minimization view of RL.

J. Policy Gradient as f-Divergence Minimization

Once a problem is framed as minimizing a KL, it can typically be recast into the general framework of f-divergence minimization, leading to a family of loss functions. We have seen this in a variety of other optimization problems: the generalization of GAN (Goodfellow et al., 2020) to f-GAN (Nowozin et al., 2016), GAIL (Ho & Ermon, 2016) to f-MAX (Ghasemipour et al., 2020) and f-VIM (Ke et al., 2020), DPO (Rafailov et al., 2023) to f-DPO (Wang et al., 2023). In this section, we still assume that the optimal policy takes the form of a Boltzmann policy (Ziebart et al., 2008; Schulman et al., 2017a) due to its partition function having an intuitive interpretation (which says that the log partition function is equivalent to the soft value function), but explore using a sampled f-divergence estimator for policy optimization.

We now extend the results in §I to generic f-divergence estimators. Let the optimal policy π^* be:

$$\pi^*(y|x) = \frac{1}{Z(x)}\pi_{\text{ref}}(y|x)\exp(R(x,y)) \qquad w = \frac{\pi^*(y|x)}{\pi_\theta(y|x)} = \frac{\pi_{\text{ref}}(y|x)\,\exp R(x,y)}{\pi_\theta(y|x)\,Z(x)}$$

Re-iterating the definition of f-divergence, with $f(\cdot)$ being convex and $f(1) = 0$:

$$D_f(p\|q) = \mathbb{E}_{y\sim q}\left[f\left(\frac{p(y)}{q(y)}\right)\right]$$

We now study two directions of f-divergence minimization: $D_f(\pi_\theta(\cdot|x)\|\pi^*(\cdot|x))$ and $D_f(\pi^*(\cdot|x)\|\pi_\theta(\cdot|x))$.

J.1. Minimizing $D_f(\pi_\theta\|\pi^*)$

If we define function $g_f(\cdot)$ as:

$$g_f(w) \triangleq w\, f\left(\frac{1}{w}\right) \tag{159}$$

Then, using the definition of f-divergence:

$$D_f(\pi_\theta(\cdot|x)\|\pi^*(\cdot|x)) = \mathbb{E}_{y\sim\pi^*(\cdot|x)}\left[f\left(\frac{1}{w}\right)\right] = \mathbb{E}_{y\sim\pi_\theta(\cdot|x)}\left[w\, f\left(\frac{1}{w}\right)\right] = \mathbb{E}_{y\sim\pi_\theta(\cdot|x)}\left[g_f(w(x,y))\right] \tag{160}$$

Note that $w(x,y)$ has the following properties:

$$\nabla_\theta \log w(x,y) = -\nabla_\theta \log \pi_\theta(y|x), \qquad \nabla_\theta w(x,y) = -w(x,y)\,\nabla_\theta \log \pi_\theta(y|x). \tag{161}$$

Therefore, using the score-function identity, we arrive at:

$$\begin{aligned}\nabla_\theta D_f(\pi_\theta\|\pi^*) = \nabla_\theta \mathbb{E}_{y\sim\pi_\theta(\cdot|x)}\left[g_f(w)\right] &= \mathbb{E}_{y\sim\pi_\theta(\cdot|x)}\Big[\nabla_\theta \log \pi_\theta(y|x)\, g_f(w) + \nabla_\theta g_f(w)\Big] \\ &= \mathbb{E}_{y\sim\pi_\theta(\cdot|x)}\Big[\nabla_\theta \log \pi_\theta(y|x)\,\big(g_f(w) - w\, g_f'(w)\big)\Big].\end{aligned} \tag{162}$$

Hence, minimizing $D_f(\pi_\theta\|\pi^*)$ is equivalent to a policy gradient update with scalar weight $-\phi_f(w)$ where $\phi_f(w)$ is

$$\phi_f(w) \triangleq g_f(w) - w\, g_f'(w) = f'(1/w). \tag{163}$$

J.2. Minimizing $D_f(\pi^*\|\pi_\theta)$

We now consider the reverse direction:

$$D_f(\pi^*(\cdot|x)\,\|\,\pi_\theta(\cdot|x)) = \mathbb{E}_{y\sim\pi_\theta(\cdot|x)}\left[f\left(\frac{\pi^*(y|x)}{\pi_\theta(y|x)}\right)\right] = \mathbb{E}_{y\sim\pi_\theta(\cdot|x)}\left[f(w(x,y))\right]. \tag{164}$$

By the same derivation as above,

$$\nabla_\theta D_f(\pi^*\|\pi_\theta) = \mathbb{E}_{y\sim\pi_\theta(\cdot|x)}\Big[\nabla_\theta \log \pi_\theta(y|x)\,\big(f(w) - w\, f'(w)\big)\Big]. \tag{165}$$

Thus the induced policy-gradient weight for the reverse direction is

$$\psi_f(w) \triangleq f(w) - w\, f'(w). \tag{166}$$

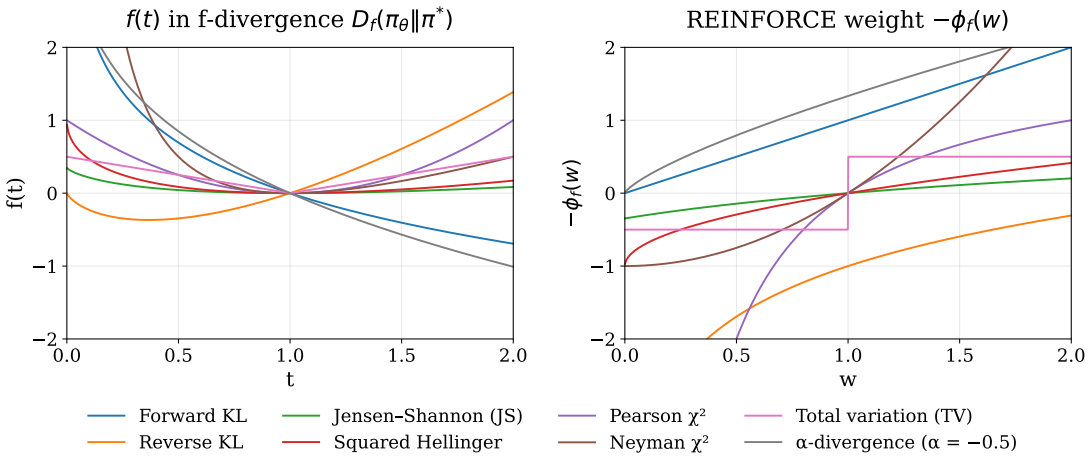


Figure 10. Policy gradient based on $\nabla_\theta D_f(\pi_\theta\|\pi^*)$, where the REINFORCE weight for $\nabla_\theta \log \pi_\theta(y|x)$ is $-\phi_f(w) = -f'(1/w)$.

Summary of f-divergence loss. The two directions of f-divergence minimization are reduced to the following:

$$\nabla_\theta D_f(\pi_\theta\|\pi^*) = \mathbb{E}_{y\sim\pi_\theta}\Big[\nabla_\theta \log \pi_\theta(y|x)\,\phi_f(w)\Big], \qquad \phi_f(w) = f'(1/w), \tag{167}$$

$$\nabla_\theta D_f(\pi^*\|\pi_\theta) = \mathbb{E}_{y\sim\pi_\theta}\Big[\nabla_\theta \log \pi_\theta(y|x)\,\psi_f(w)\Big], \qquad \psi_f(w) = f(w) - wf'(w). \tag{168}$$

The EM Algorithm The expectation-maximization (EM) process can be summarized as the following. For each prompt or task x, we sample N rollouts $[y^{(1)}, \ldots, y^{(N)}]$ from $\pi_\theta(\cdot \mid x)$ to estimate the partition function $Z(x)$ and the ratio w as:

$$\textbf{E-Step} \qquad Z(x) \approx \frac{1}{N}\sum_{i=1}^{N} \mathrm{sg}\left(\frac{\pi_{\text{ref}}(y^{(i)} \mid x)}{\pi_\theta(y^{(i)} \mid x)}\right) \exp\Big(R(x, y^{(i)})\Big) \qquad w = \frac{\pi_{\text{ref}}(y \mid x)}{\pi_\theta(y \mid x)} \cdot \frac{\exp R(x,y)}{Z(x)}$$

where the returns $R(x, y^{(i)})$ are (pre-) scaled by $1/\beta$ to control the regularization effect of the anchor π_{ref}. After the E-Step, M-Step performs gradient updates based on f-divergence minimization; the following two tables, Table 8 and Table 9, summarize what to minimize under each f-divergence (**M-Step**).

Table 8. **M-Step:** Minimizing $D_f(\pi_\theta\|\pi^*)$ results in the gradient update $\mathbb{E}_{y\sim\pi_\theta}[\nabla_\theta \log \pi_\theta(y|x)\,\phi_f(w)]$

f-**divergence**	$f(t)$	$\phi_f(w) = f'(1/w)$
Forward KL	$-\log t$	$-w$
Reverse KL	$t \log t$	$-\log w + 1$
Jensen–Shannon (JS)	$\frac{1}{2}\left(t\log t - (t+1)\log\left(\frac{t+1}{2}\right)\right)$	$\frac{1}{2}\log\left(\frac{2}{1+w}\right)$
Squared Hellinger	$(\sqrt{t}-1)^2$	$1-\sqrt{w}$
Pearson χ^2	$(t-1)^2$	$-2+2/w$
Neyman χ^2	$\frac{(t-1)^2}{t}$	$1-w^2$
Total variation (TV)	$\frac{1}{2}\lvert t-1\rvert$	$-\frac{1}{2}\,\mathrm{sgn}(w-1)$
α-divergence ($\alpha \neq \pm 1$)	$\frac{4}{1-\alpha^2}\left(1 - t^{\frac{1+\alpha}{2}}\right)$	$\frac{2}{\alpha-1}w^{\frac{1-\alpha}{2}}$

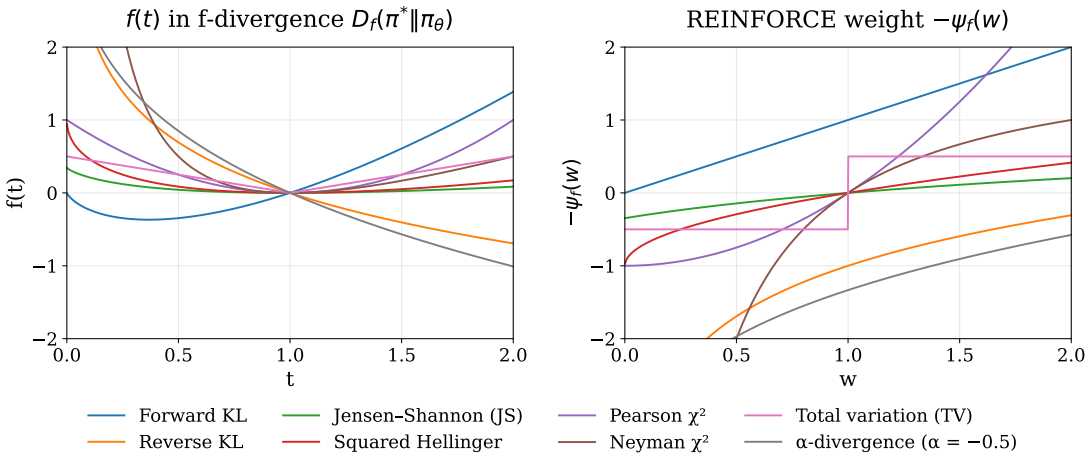


Figure 11. Policy gradient based on $\nabla_\theta D_f(\pi^*\|\pi_\theta)$, where the REINFORCE weight for $\nabla_\theta \log \pi_\theta(y|x)$ is $-\psi_f(w) = -f(w) + wf'(w)$.

Table 9. **M-Step:** Minimizing $D_f(\pi^*\|\pi_\theta)$ results in the gradient update $\mathbb{E}_{y\sim\pi_\theta}[\nabla_\theta \log \pi_\theta(y|x)\, \psi_f(w)]$

f**-divergence**	$f(t)$	$\psi_f(w) = f(w) - wf'(w)$
Forward KL	$t \log t$	$-w$
Reverse KL	$-\log t$	$-\log w + 1$
Jensen–Shannon (JS)	$\frac{1}{2}\left(t \log t - (t+1)\log\left(\frac{t+1}{2}\right)\right)$	$\frac{1}{2}\log\left(\frac{2}{1+w}\right)$
Squared Hellinger	$(\sqrt{t}-1)^2$	$1-\sqrt{w}$
Pearson χ^2	$(t-1)^2$	$1-w^2$
Neyman χ^2	$\frac{(t-1)^2}{t}$	$-2+2/w$
Total variation (TV)	$\frac{1}{2}\lvert t-1\rvert$	$-\frac{1}{2}\operatorname{sgn}(w-1)$
α-divergence ($\alpha \neq \pm 1$)	$\frac{4}{1-\alpha^2}\left(1 - t^{\frac{1+\alpha}{2}}\right)$	$-\frac{2}{\alpha+1}w^{\frac{\alpha+1}{2}} - \frac{4}{(\alpha-1)(\alpha+1)}$

K. Top-k KL: Unbiasedness and Variance

This appendix proves that the Top-k KL estimators of §5.3 have unbiased values and gradients (Proposition 5.1), compares their tail token with the rollout token, and compares their variance with that of sampled KL. We fix a position n with prefix h_n, and omit h_n from the notation.

K.1. Unbiased values and gradients (Proof of Proposition 5.1)

Let $\ell_n(j) \triangleq \log \pi_\theta(j) - \log \pi_{\text{ref}}(j)$ and $w_n(j) \triangleq \pi_{\text{ref}}(j)/\pi_\theta(j)$, so that $\mathrm{KL}_n = \sum_{j\in\mathcal{V}} \pi_\theta(j)\,\ell_n(j)$ and $\mathrm{FKL}_n = \sum_{j\in\mathcal{V}} \pi_\theta(j)\,w_n(j)\log w_n(j)$. At a tail token $z_n = j$, the two sampled estimators of §5.2 are

$$(\mathbf{K4})_n\big|_{y_n=j} = r_n(j)\,\mathrm{sg}(\ell_n(j)) \qquad (\mathbf{K5})_n\big|_{y_n=j} = \mathrm{sg}(w_n(j))\log w_n(j) + \log r_n(j)$$

where $r_n(j) = \pi_\theta(j)/\mathrm{sg}(\pi_\theta(j))$ equals 1 in value and has $\nabla_\theta r_n(j) = \nabla_\theta \log r_n(j) = \nabla_\theta \log \pi_\theta(j)$. Their gradients are therefore

$$\nabla_\theta(\mathbf{K4})_n\big|_{y_n=j} = \ell_n(j)\,\nabla_\theta \log \pi_\theta(j) \qquad \nabla_\theta(\mathbf{K5})_n\big|_{y_n=j} = (1 - w_n(j))\,\nabla_\theta \log \pi_\theta(j) \tag{169}$$

The index set q_n, the proposal μ_n and the importance weight $s_n = \mathrm{sg}(\pi_\theta(z_n)/\mu_n(z_n))$ carry no gradient, and $\mu_n(j) > 0$ for every $j \notin q_n$. Hence, for any function ϕ of the tail token,

$$\mathbb{E}_{z_n}\left[s_n\,\phi(z_n)\right] = \sum\nolimits_{j\notin q_n} \mu_n(j)\,\frac{\pi_\theta(j)}{\mu_n(j)}\,\phi(j) = \sum\nolimits_{j\notin q_n} \pi_\theta(j)\,\phi(j) \tag{170}$$

so the importance weight turns the tail draw into the sum over the non-top-k indices, whatever the proposal.

Proof of Proposition 5.1. Values. Δ_n and $\log r_n$ are zero in value, so by (170),

$$\mathbb{E}_{z_n}\left[(\widehat{\mathrm{KL}}_{\text{tail}})_n\right] = \sum\nolimits_{j\notin q_n} \pi_\theta(j)\,\ell_n(j)$$
$$\mathbb{E}_{z_n}\left[(\widehat{\mathrm{FKL}}_{\text{tail}})_n\right] = \sum\nolimits_{j\notin q_n} \pi_\theta(j)\,w_n(j)\log w_n(j) = \sum\nolimits_{j\notin q_n} \pi_{\text{ref}}(j)\log\frac{\pi_{\text{ref}}(j)}{\pi_\theta(j)}$$

These are the terms of KL_n and FKL_n that the truncated sums over q_n leave out, so both estimators have unbiased values.

Gradients, reverse KL. Since $\nabla_\theta[\pi_\theta(j)\,\ell_n(j)] = (\ell_n(j)+1)\,\nabla_\theta\pi_\theta(j)$ and $\nabla_\theta\Delta_n = \sum_{j\in q_n}\nabla_\theta\pi_\theta(j)$, and by (169) and (170),

$$\nabla_\theta\left[(\mathrm{KL}_{\text{trun}})_n - \Delta_n\right] = \sum\nolimits_{j\in q_n} \ell_n(j)\,\nabla_\theta\pi_\theta(j)$$
$$\mathbb{E}_{z_n}\left[\nabla_\theta(\widehat{\mathrm{KL}}_{\text{tail}})_n\right] = \sum\nolimits_{j\notin q_n} \pi_\theta(j)\,\ell_n(j)\,\nabla_\theta\log\pi_\theta(j) = \sum\nolimits_{j\notin q_n} \ell_n(j)\,\nabla_\theta\pi_\theta(j)$$

The two add up to $\sum_{j\in\mathcal{V}} \ell_n(j)\,\nabla_\theta\pi_\theta(j)$. This is $\nabla_\theta\mathrm{KL}_n = \sum_{j\in\mathcal{V}}(\ell_n(j)+1)\,\nabla_\theta\pi_\theta(j)$, because $\sum_{j\in\mathcal{V}}\nabla_\theta\pi_\theta(j) = 0$.

Gradients, forward KL. Since $\nabla_\theta(\mathrm{FKL}_{\text{trun}})_n = -\sum_{j\in q_n}\pi_{\text{ref}}(j)\,\nabla_\theta\log\pi_\theta(j)$ and $\pi_\theta(j)\,w_n(j) = \pi_{\text{ref}}(j)$,

$$\nabla_\theta\left[(\mathrm{FKL}_{\text{trun}})_n + \Delta_n\right] = -\sum\nolimits_{j\in q_n}\pi_{\text{ref}}(j)\,\nabla_\theta\log\pi_\theta(j) + \sum\nolimits_{j\in q_n}\nabla_\theta\pi_\theta(j)$$
$$\mathbb{E}_{z_n}\left[\nabla_\theta(\widehat{\mathrm{FKL}}_{\text{tail}})_n\right] = -\sum\nolimits_{j\notin q_n}\pi_{\text{ref}}(j)\,\nabla_\theta\log\pi_\theta(j) + \sum\nolimits_{j\notin q_n}\nabla_\theta\pi_\theta(j)$$

The two add up to $-\sum_{j\in\mathcal{V}}\pi_{\text{ref}}(j)\,\nabla_\theta\log\pi_\theta(j) = \nabla_\theta\mathrm{FKL}_n$, again because $\sum_{j\in\mathcal{V}}\nabla_\theta\pi_\theta(j) = 0$. □

The vanilla forms. Without Δ_n, the same sums give $\nabla_\theta\mathrm{KL}_n + \sum_{j\in q_n}\nabla_\theta\pi_\theta(j)$ in the reverse case, which is (27), and $\nabla_\theta\mathrm{FKL}_n - \sum_{j\in q_n}\nabla_\theta\pi_\theta(j)$ in the forward case, which is (30).

K.2. Tail token versus rollout token

The tail term of Top-k KL can be estimated with a separate tail token $z_n \sim \mu_n$, as in (29) and (31), or with the rollout token itself. This section shows that the two estimates have the same expectation, and compares their variance.

Setup. Let $y_n \sim \pi_{\text{sampling}}$ be the rollout token, and let $\mathbf{K}_n(j)$ denote K4 (for reverse KL) or K5 (for forward KL) evaluated at token j. The rollout-token estimators are (29) and (31) with the tail term replaced by

$$\mathbb{1}(y_n \notin q_n)\, \mathrm{sg}\Big(\frac{\pi_\theta(y_n)}{\pi_{\text{sampling}}(y_n)}\Big)\, \mathbf{K}_n(y_n) \tag{171}$$

This is (26) with the importance weight of §5.2 for an off-policy rollout. The exact top-k term and Δ_n are the same in both kinds of estimators and are not random, so only the tail terms need to be compared.

Proposition K.1 (Lower variance than the rollout token)**.** *The rollout-token estimators have the same expected values and gradients as (29) and (31). If $\mu_n(j) \geq \pi_{\text{sampling}}(j)$ for all $j \notin q_n$, the covariance of their gradients is larger or equal in the positive semi-definite order, and the variance of their values is larger or equal. In particular, this holds for $\mu_n(j) \propto \pi_{\text{sampling}}(j)\, \mathbb{1}(j \notin q_n)$, where the tail token shrinks the second moment of the tail term by the factor $m_n \triangleq \sum_{j \notin q_n} \pi_{\text{sampling}}(j)$, the probability mass of the non-top-k indices.*

Proof. Let $c_n(j) \triangleq \nabla_\theta \mathbf{K}_n(j)$. Consider a token $j \notin q_n$ that is drawn with probability $p(j)$ and contributes the tail term $\mathrm{sg}(\pi_\theta(j)/p(j))\, \mathbf{K}_n(j)$, with no contribution otherwise. The gradient G of this tail term satisfies

$$\mathbb{E}[G] = \sum\nolimits_{j \notin q_n} p(j)\, \frac{\pi_\theta(j)}{p(j)}\, c_n(j) = \sum\nolimits_{j \notin q_n} \pi_\theta(j)\, c_n(j)$$
$$\mathbb{E}[G\, G^\top] = \sum\nolimits_{j \notin q_n} \frac{\pi_\theta(j)^2}{p(j)}\, c_n(j)\, c_n(j)^\top$$

The rollout token (171) is the case $p = \pi_{\text{sampling}}$, and the tail token is the case $p = \mu_n$. The mean does not depend on p, so the two have the same expected gradient, and

$$\mathrm{Cov}(G_{\text{rollout}}) - \mathrm{Cov}(G_{\text{tail}}) = \sum\nolimits_{j \notin q_n} \pi_\theta(j)^2 \Big(\frac{1}{\pi_{\text{sampling}}(j)} - \frac{1}{\mu_n(j)}\Big)\, c_n(j)\, c_n(j)^\top \tag{172}$$

which is positive semi-definite when $\mu_n(j) \geq \pi_{\text{sampling}}(j)$ for all $j \notin q_n$. The same computation with the value of $\mathbf{K}_n(j)$ in place of $c_n(j)$ gives the statement for the values. For $\mu_n(j) = \pi_{\text{sampling}}(j)/m_n$ on the non-top-k indices, $\mathbb{E}[G_{\text{tail}}\, G_{\text{tail}}^\top] = m_n\, \mathbb{E}[G_{\text{rollout}}\, G_{\text{rollout}}^\top]$, and (172) equals $(1 - m_n)\, \mathbb{E}[G_{\text{rollout}}\, G_{\text{rollout}}^\top]$. □

Remarks.

- *Same policy.* When the tail token is drawn from the sampling policy (Alg 1), the condition of Proposition K.1 is automatic. The rollout token falls outside q_n only with probability m_n, whereas the tail token always does and carries the factor m_n in its weight instead: the tail token replaces the indicator $\mathbb{1}(y_n \notin q_n)$ by its expectation.
- *Reference policy.* When the tail token is drawn from the reference policy (Alg 2), the condition requires that no non-top-k token is more likely under the sampling policy than under μ_n. If it fails for some tokens, (172) is no longer positive semi-definite in general, and which estimator has the lower variance depends on the policies.
- *Per token.* Like the conditions in (20), the statement is for one position given its prefix h_n.

K.3. Top-k KL versus sampled KL

Sampled KL (§5.2) draws one token $y_n \sim p$ from a sampling distribution p over $\mathcal{V}$ and uses $\mathrm{sg}(\pi_\theta(y_n)/p(y_n))\, \mathbf{K}_n(y_n)$, with $\mathbf{K}_n$ as in §K.2. Top-k KL under the same sampling distribution computes the indices in q_n exactly, and draws its tail token from p outside of them.

Proposition K.2 (Lower variance than sampled KL)**.** *Let p be any distribution with $p(j) > 0$ for all $j \in \mathcal{V}$, and let q_n be any index set. Top-k reverse KL (29) and Top-k forward KL (31) with $\mu_n(j) \propto p(j)\, \mathbb{1}(j \notin q_n)$ have the same expected values and gradients as sampled K4 and K5 with $y_n \sim p$. The covariance of their gradients is smaller or equal in the positive semi-definite order, and the variance of their values is smaller or equal.*

Proof. The expectations are equal by Proposition 5.1 and §5.2. Let $\phi(j)$ be the value of $\mathbf{K}_n(j)$, or its gradient $c_n(j)$ projected on a fixed direction. The sampled estimator is $X = (\pi_\theta(y_n)/p(y_n))\,\phi(y_n)$, with

$$\mathbb{E}[X] = \underbrace{\sum\nolimits_{j\in q_n} \pi_\theta(j)\,\phi(j)}_{a} + \underbrace{\sum\nolimits_{j\notin q_n} \pi_\theta(j)\,\phi(j)}_{b} \qquad \mathbb{E}[X^2] = \underbrace{\sum\nolimits_{j\in q_n} \frac{\pi_\theta(j)^2}{p(j)}\,\phi(j)^2}_{A} + \underbrace{\sum\nolimits_{j\notin q_n} \frac{\pi_\theta(j)^2}{p(j)}\,\phi(j)^2}_{B}$$

In Top-k KL, the exact terms equal a and are not random (§K.1), and the tail term $Y = s_n\,\phi(z_n)$ has $\mathbb{E}[Y] = b$ and $\mathbb{E}[Y^2] = P_t\,B$, where $P_t \triangleq \sum_{j\notin q_n} p(j)$ is the mass of p on the non-top-k indices; let $P_h \triangleq 1 - P_t$. By the Cauchy–Schwarz inequality, $a^2 \le P_h\,A$ and $b^2 \le P_t\,B$. Hence, for $0 < P_h < 1$,

$$\mathrm{Var}(X) - \mathrm{Var}(a+Y) = A + P_h\,B - a^2 - 2ab \;\ge\; \frac{P_t}{P_h}\,a^2 + \frac{P_h}{P_t}\,b^2 - 2ab = \left(\sqrt{\frac{P_t}{P_h}}\,a - \sqrt{\frac{P_h}{P_t}}\,b\right)^2 \ge 0$$

The cases $P_h = 0$ and $P_h = 1$ are sampled KL and exact KL themselves. Since the direction of the projection is arbitrary, the gradient covariances are ordered. □

Remarks.

- *Reverse KL.* In Alg 1, p is the sampling policy, so the comparison is with sampled K4 on the rollout token (§5.2).
- *Forward KL.* In Alg 2, p is the reference policy, so the comparison is with sampled K5 on a token drawn from the reference policy. Against sampled K5 on the rollout token, which is drawn from a different distribution, which estimator has the lower variance depends on the policies, as in §K.2.