RETHINKING KL REGULARIZATION IN RLHF: FROM VALUE ESTIMATION TO GRADIENT OPTIMIZATION

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ABSTRACT

Reinforcement Learning from Human Feedback (RLHF) leverages a Kullback-Leibler (KL) divergence loss to stabilize training and prevent overfitting. However, in methods such as GRPO, its implementation may be guided by principles from numerical value estimation—a practice that overlooks the term's functional role as an optimization loss. To analyze this issue, we establish a unified framework that connects two seemingly distinct implementation styles: using the mathematical term k_n as a detached coefficient for the policy's score function (' k_n in **reward**') or as a direct loss function through which gradients are propagated (' k_n as loss'). We show that the latter can always be analyzed via an equivalent gradient coefficient in the former, unifying the two perspectives. Through this framework, we prove that the conventional ' k_1 in reward' (like PPO) is the principled loss for Reverse KL (RKL) regularization. We further establish a key finding: under on-policy conditions, the ' k_2 as loss' formulation is, in fact, gradient-equivalent to k_1 in reward. This equivalence, first proven in our work, identifies both as the theoretically sound implementations of the RKL objective. In contrast, we show that the recently adopted 'k₃ as loss' (like GRPO) is merely a first-order, biased approximation of the principled loss. Furthermore, we argue that common off-policy implementations of k_n as loss' methods are biased due to neglected importance sampling, and we propose a principled correction. Our findings provide a comprehensive, gradient-based rationale for choosing and correctly implementing KL regularization, paving the way for more robust and effective RLHF systems.

1 Introduction

The training of state-of-the-art Large Language Models (LLMs) is a multistage process. Following large-scale pretraining, models are refined through Supervised Fine-Tuning (SFT) to learn instruction-following behaviors. To further elevate these SFT models, a final post-training stage, Reinforcement Learning from Human Feedback (RLHF), is often employed. The objective of RLHF is twofold; it serves to align the model more closely with complex human values (Ouyang et al., 2022) and, increasingly, to push the performance limits in specialized reasoning tasks such as mathematics and code generation, as seen in models such as DeepSeek-Math (Shao et al., 2024). A core component of this RLHF process is **KL regularization**, implemented through a loss term derived from the Kullback-Leibler (KL) divergence (Kullback & Leibler, 1951). The **KL loss** serves not only to stabilize the training process but also to improve generalization by preventing the policy from overfitting the reward signal and deviating excessively from the initial SFT model (Ouyang et al., 2022; Stiennon et al., 2020).

Despite the critical role of the KL loss, its theoretical foundations in the optimization context remain underexplored. The choice of its specific mathematical form is often guided by principles from numerical *value estimation*, not from the perspective of gradient-based *optimization*. This category error has led to a proliferation of ad-hoc implementations and suboptimal algorithm designs, exemplified by recent methods like GRPO that adopt sure estimators under the mistaken assumption that good value estimation properties translate to effective gradients. This paper argues that a gradient-centric perspective is essential for designing robust and effective RLHF algorithms.

We perform a systematic, gradient-based analysis of the KL loss to address these issues. We first establish a unified framework that connects two seemingly distinct implementation styles: using the

mathematical term k_n as a detached coefficient (' k_n in reward') or as a direct loss function (' k_n as loss'). This framework allows us to analyze any implementation by examining its equivalent gradient coefficient. Using this lens, we first use the ' k_1 as loss' case as a counterexample to demonstrate the mistakes of the value estimation perspective. We then prove that the conventional ' k_1 in reward' and the ' k_2 as loss' formulations are, in fact, gradient equivalent and represent the principled approach to reverse KL regularization. Finally, we analyze popular alternatives like ' k_3 as loss', revealing their nature as biased approximations, and address a common but critical bug in their off-policy implementation.

Our main contributions are threefold:

- 1. A Gradient-Centric Framework for KL Regularization. We revisit KL regularization in RLHF, shifting the focus from value estimation to gradient optimization. We demonstrate the necessity of this perspective using ' k_1 as loss' as a powerful counterexample, showing how an unbiased value estimator yields a completely ineffective optimization signal.
- 2. **Identification of Principled KL Implementations.** We prove that the conventional ' k_1 in reward' formulation correctly implements the KL gradient. We further establish a key, previously unrecognized equivalence: ' k_1 in reward' is gradient-equivalent to ' k_2 as loss'. This discovery solidifies both as theoretically sound choices for KL regularization.
- 3. Analysis of Alternative Implementations and a Practical Correction. We analyze popular alternative approaches, showing that ' k_3 as loss' (used in GRPO) is a biased first-order approximation of the principled gradient, leading to weaker regularization or potential instability. Furthermore, we identify a common pitfall in off-policy algorithms where ' k_n as loss' methods are often implemented without correct importance sampling, and we provide a principled correction for this bias.

2 RELATED WORK

KL Value Estimation. Since the expectation of the KL divergence is often intractable, it is typically estimated by Monte Carlo sampling. Prior analyses have primarily assessed these estimators as value estimators (John, 2020), characterizing k_1 as unbiased but high variance, k_2 as biased but lower variance, and k_3 as an "optimal", low variance and unbiased choice. We first challenge the claimed superiority of k_3 as a value estimator, showing that its advertised properties often fail to hold in practical settings. More importantly, this emphasis is misplaced when these estimators are used for regularization in RLHF. We show that a gradient-centric perspective is essential: conclusions drawn from value estimation do not necessarily translate into effective optimization.

RLHF Methods. OpenRLHF (Hu et al., 2024) is the first framework that uses vLLM Kwon et al. (2023) to accelerate the rollout phase in RLHF training, and incorporates a variety of techniques that make RLHF training more stable. Since then, several training frameworks have emerged, including Verl Sheng et al. (2024), slimeZhu et al. (2025), and ROLL Wang et al. (2025). These frameworks primarily support PPO (Ouyang et al., 2022) and its variants, focusing on improving training stability, particularly addressing challenges in training the critic model. VAPO Yue et al. (2025) proposed pretraining the critic model to mitigate these issues, while GRPO and Reinforce++ advocate removing it altogether, leading to larger actor model scaling. Most RLHF methods incorporate the KL loss, although some recent rule-based reward algorithms, such as DAPO, have suggested removing the KL loss to enhance performance. However, Prorl (Liu et al., 2025a) solves the performance problem by periodically resetting the reference models, and helps prove where the KL loss still plays a crucial role in preventing overfitting and ensuring long-term training stability. In particular, the KL loss used in Prorl is the 'k2 as loss' we propose and advocate in this paper.

KL Loss in RLHF. The practice of introducing a KL penalty *in the reward* is primarily based on the OpenAI InstructGPT paper (Ouyang et al., 2022), which effectively applies the log-ratio term as a coefficient for the policy's score function, although without a formal justification. Earlier work (Jaques et al., 2019) noted the potential equivalence of adding the KL term to the reward versus the loss, but this was not formally proven. More recently, the GRPO method (Shao et al., 2024), utilized in influential models such as DeepSeek-R1 (Guo et al., 2025), has gained prominence by adopting the term k_3 directly as a KL loss. This choice is justified by citing (John, 2020) and its claim of

 k_3 being an "unbiased estimator", exemplifying the flawed practice of transferring value estimation principles to loss design, a central issue we address.

3 PRELIMINARY

3.1 VALUE ESTIMATION OF KL DIVERGENCE

The Kullback-Leibler (KL) divergence from a distribution q(x) to a reference p(x) is defined as:

$$D_{\mathrm{KL}}(q \parallel p) = \mathbb{E}_{x \sim q} \left[\log \frac{q(x)}{p(x)} \right]. \tag{1}$$

As this expectation is often intractable, it is estimated from Monte Carlo samples. Given the importance ratio $\delta(x) = p(x)/q(x)$, common estimators for the term within the expectation include:

$$k_1(x) = -\log \delta(x),$$

$$k_2(x) = \frac{1}{2} (\log \delta(x))^2,$$

$$k_3(x) = \delta(x) - 1 - \log \delta(x).$$

Except for the property mentioned in Section 2, the estimator k_3 is particularly interesting, designed to reduce the high variance. Although it can be effective when distributions p and q are close, the claim that it is a 'strictly better estimator' (John, 2020) does not hold in the general case. Potential issues of severe bias and infinite variance can arise when the support or tail of the distribution differs significantly. Therefore, its application requires careful verification of some assumptions. A detailed analysis of these statistical instabilities, supported by counterexamples, is provided in Appendix I.

3.2 REINFORCEMENT LEARNING FROM HUMAN FEEDBACK (RLHF)

RLHF fine-tunes a policy(actor model) π_{θ} to produce responses y to prompts x that maximize a reward r(x,y) derived from human preferences. Pure reward maximization may cause reward hacking and distribution drift from a trusted SFT policy. To counteract this, RLHF adds a KL penalty loss that regularizes the policy toward a fixed reference π_{ref} :

$$\mathcal{J}_{\text{RLHF}}(\boldsymbol{\theta}) = \underbrace{\mathbb{E}_{x \sim D, y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[r(x, y) \right]}_{\text{Reward Maximization Term}} - \beta \underbrace{D_{\text{KL}} \left(\pi_{\boldsymbol{\theta}}(\cdot|x) \parallel \pi_{\text{ref}}(\cdot|x) \right)}_{\text{KL Regularization Term}}$$

$$= \mathcal{J}_{\text{Reward}}(\boldsymbol{\theta}) - \beta \mathcal{J}_{\text{KL}}(\boldsymbol{\theta}).$$
(2)

Here, \mathcal{D} is the prompt distribution, y is sampled on-policy from the detached snapshot π_{θ} (numerically equal to π_{θ} at sampling time), and β trades off reward maximization and deviation from π_{ref} .

4 A Unified Framework for KL Regularization in RLHF

Although most RLHF algorithms optimize for the same high-level objective as eq. (2), their specific implementations differ significantly. To analyze these differences systematically, we establish a unified framework that decomposes the objective into its core components and categorizes the different KL implementation styles.

Convention In our analysis, we use π_{θ} to denote the trainable policy that carries gradients, and follow the standard bandit setting. ¹ Samples y are drawn from a detached and numerically identical snapshot policy $\pi_{\theta}(\cdot|x)$, evaluated in the current iterate; gradients flow only through π_{θ} . All scalar coefficients that multiply the score function $\nabla_{\theta} \log \pi_{\theta}(y|x)$ are treated as detached.

¹To simplify analysis of core gradient properties, we model the entire response y as a single action. Our derivations therefore operate on the joint probability $\pi(y|x)$ of the sequence, rather than the token-level probabilities used in standard sequential PPO.

4.1 Core Components of the RLHF Objective

The practical RLHF objective consists of two parts estimated via Monte Carlo sampling.

Reward Maximization The primary goal is to maximize the expected reward. The gradient of this objective is typically estimated using the score function estimator (Williams, 1992), whose detailed derivation is provided in Appendix B:

$$\nabla_{\theta} \mathcal{J}_{\text{reward}}(\theta) = \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(\cdot|x)} \left[r(x, y) \cdot \nabla_{\theta} \log \pi_{\theta}(y|x) \right]. \tag{3}$$

Practical implementations replace the raw reward r(x, y) with a shaped advantage signal. The specific shaping techniques are detailed in Appendix A.

KL Regularization. RLHF regularizes the actor model to the reference model via the RKL:

$$\mathcal{J}_{\text{RKL}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim \mathcal{D}} \left[D_{\text{KL}} \left(\pi_{\boldsymbol{\theta}}(\cdot|x) \parallel \pi_{\text{ref}}(\cdot|x) \right) \right] = \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[\log \pi_{\boldsymbol{\theta}}(y|x) - \log \pi_{\text{ref}}(y|x) \right]. \tag{4}$$

Its expectation is taken under the current policy, making on-policy Monte Carlo estimation a natural choice.²

In implementation, we optimize this objective via surrogate terms k_n , whose forms are borrowed from value estimators. Expectations are evaluated using samples from the detached snapshot π_{θ} that is numerically equal to π_{θ} at sampling time. There are two primary formulations:

1. k_n as a Detached Coefficient (' k_n in reward'): Treats k_n as a detached coefficient weight for the score function. A typical choice is $k_1(y|x) = \log \pi_{\theta}(y|x) - \log \pi_{\text{ref}}(y|x)$.

$$\mathcal{J}_{k_n \text{ in reward}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(\cdot|x)} \left[\underbrace{k_n(\pi_{\theta}(y|x), \pi_{\text{ref}}(y|x))}_{\text{detached coefficient}} \cdot \log \pi_{\boldsymbol{\theta}}(y|x) \right]. \tag{5}$$

2. k_n as a Direct Loss (' k_n as loss'): Treats k_n as a standalone loss with gradients propagated directly through it. Common choices include $k_2(y|x) = \frac{1}{2} \left(\log \frac{\pi_{\theta}(y|x)}{\pi_{\text{ref}}(y|x)}\right)^2$ and

$$k_3(y|x) = \frac{\pi_{\text{ref}}(y|x)}{\pi_{\theta}(y|x)} - 1 - \log \frac{\pi_{\text{ref}}(y|x)}{\pi_{\theta}(y|x)}.$$

$$\mathcal{J}_{k_n \text{ as loss}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[k_n \left(\pi_{\boldsymbol{\theta}}(y|x), \, \pi_{\text{ref}}(y|x) \right) \right]. \tag{6}$$

The gradient of the 'as loss' is computed directly through k_n without an explicit score-function term, yet as we will prove, it matches the 'in reward' gradient under on-policy conditions in Section 5. And under on-policy sampling, the ' k_1 in reward' and ' k_2 as loss' are gradient-equivalent implementations of the RKL objective (see Appendix C for the full proof).

4.2 KL Integration Forms and Algorithm Mapping

The choice of KL formulation dictates how it is integrated with the reward objective.

Combined vs. Decoupled Forms. Since k_n in reward' uses the same score function as the reward objective, its coefficient can be merged into the reward coefficient to produce a **Combined Form**—hence the name 'in reward':

$$\mathcal{L}_{\text{combined}}(\theta) = -\mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(\cdot|x)} \left[\left(r(x, y) - \beta \, k_n \left(\pi_{\theta}(y|x), \pi_{\text{ref}}(y|x) \right) \right) \cdot \log \pi_{\theta}(y|x) \right]. \tag{7}$$

In contrast, ' k_n as loss' necessitates a **Decoupled form** with a separate loss form:

$$\mathcal{L}_{\text{decoupled}}(\boldsymbol{\theta}) = -\mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[r(x, y) \cdot \log \pi_{\boldsymbol{\theta}}(y|x) \right] + \beta \, \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[k_n \left(\pi_{\boldsymbol{\theta}}(y|x), \pi_{\text{ref}}(y|x) \right) \right]. \tag{8}$$

The decoupled form can also be used with ' k_n in reward' by separating the two score function terms. In off-policy updates, the merged coefficient in the combined form, $r-\beta$ k_n , must be corrected with importance sampling; when combined with PPO, this correction is automatically inherited via the clipped surrogate objective $\pi_\theta/\pi_{\theta_k}$. In contrast, 'as loss' implementations also explicitly require applying IS and PPO clip, but these have always been omitted in practice (see Appendix G).

²By contrast, Forward KL expectation is under $\pi_{ref}(\cdot|x)$ and thus hard to be estimated from on-policy samples, making it rarely used in RLHF.

Positioning PPO and GRPO. This framework can position the main algorithms, as summarized in Table 1. PPO is a canonical example of using ' k_1 in reward' in a combined form. GRPO exemplifies the use of ' k_3 as loss' in a decoupled form.

Table 1: Decomposition of RLHF algorithms. Note: ' k_n in reward' can also be implemented in a decoupled form.

Algorithm	Typical k_n	KL Formulation Style	Integration Form	Notes on Off-Policy Implementation				
PPO / REINFORCE GRPO	$k_1 \\ k_3$	k_n in reward' k_n as loss'	Combined (typical) Decoupled	Inherits IS/clipping when paired with PPO. Requires explicit IS/clipping, commonly omitted in practice.				

5 GRADIENT-BASED ANALYSIS OF KL IMPLEMENTATIONS

In RLHF, KL regularizers should be selected for gradient properties rather than for accurate estimation of values. In this section, we first use ' k_1 as loss' as a counterexample to show that adopting estimators without auditing the induced gradients can lead to vacuous updates. Then we derive the principal surrogate loss of RKL and demonstrate that ' k_3 as loss' is a first-order approximation. Meanwhile, we also prove that ' k_n as loss' and ' $k_{n'}$ in reward' are often gradient equivalent and can be converted to each other with the on-policy setting.

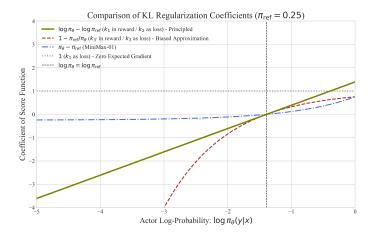


Figure 1: Comparison of KL regularization gradient coefficients. Each curve shows the scalar coefficient c(x,y) which would multiply the score function $\nabla_{\theta} \log \pi_{\theta}(y|x)$, plotted against $\log \pi_{\theta}(y|x)$ with $\pi_{\text{ref}}(y|x) = 0.25$ (vertical dashed line). Principled implementations $(k_1$ in reward or k_2 as loss) yield $c = \log(\pi_{\theta}/\pi_{\text{ref}})$, a linear restoring force in log-probability. The k_3 as loss uses $c = 1 - \pi_{\text{ref}}/\pi_{\theta}$, a first-order Taylor surrogate of $-\log \delta$ at $\delta = \pi_{\text{ref}}/\pi_{\theta} = 1$: it is loose when $\log \pi_{\theta}$ is large $(\pi_{\theta} \gg \pi_{\text{ref}})$ and can blow up when $\log \pi_{\theta}$ is small $(\pi_{\theta} \ll \pi_{\text{ref}})$. The naive k_1 as loss gives $c \equiv 1$, producing a zero-mean, non-regularizing gradient in expectation.

5.1 THE COUNTEREXAMPLE: WHY k_1 AS LOSS FAILS

A central lesson of this work is that the desirable properties of value estimation do not automatically translate into effective losses of optimization. The case of using ' k_1 as loss' provides a clean counterexample: although k_1 is an unbiased estimator of the KL value, it is ineffective as a loss for enforcing a KL constraint.

Consider the direct-loss formulation with on-policy sampling from a detached snapshot $y \sim \pi_{\theta}(\cdot|x)$:

$$\mathcal{J}_{k_1 \text{ as loss}}(\theta) = \mathbb{E}_{x \sim D, \ y \sim \pi_{\theta}(\cdot|x)} \left[\log \pi_{\theta}(y|x) - \log \pi_{\text{ref}}(y|x) \right]. \tag{9}$$

Since π_{ref} does not depend on θ , its term vanishes upon differentiation, leaving

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}_{k_1 \text{ as loss}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim D, y \sim \pi_{\boldsymbol{\theta}}(\cdot | x)} \left[\nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(y | x) \right]. \tag{10}$$

The result exposes a fundamental flaw: the gradient is entirely independent of the reference policy π_{ref} ; therefore, it carries *no* KL regularization signal.

 By the zero-mean score identity in Lemma C.2, the gradient has expectation exactly zero, precisely the exact mechanism that underlies the subtraction of the baseline in policy gradients such as REIN-FORCE (Williams, 1992). Consequently, in Monte Carlo practice, the term injects only zero-mean noise, which inflates the gradient variance and potentially destabilizes learning.

This counterexample is decisive: an "unbiased value estimator" can produce a useless optimization signal. It directly challenges the assumption that favorable value estimation properties are sufficient for designing effective KL losses, an assumption that has implicitly motivated certain recent implementations, such as GRPO.

THE PRINCIPLED KL LOSS IN RLHF: k_1 IN REWARD $\Leftrightarrow k_2$ AS LOSS

In the following, we derive the exact on-policy gradient of the Reverse KL objective in Equation (4) and use it as the reference gradient to design surrogates KL loss. Applying the product rule and the log-derivative trick to RKL (see Appendix C) gives:

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}_{RKL}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim \mathcal{D}} \left[\sum_{y} \nabla_{\boldsymbol{\theta}} \pi_{\boldsymbol{\theta}}(y|x) \left(\log \frac{\pi_{\boldsymbol{\theta}}(y|x)}{\pi_{ref}(y|x)} + 1 \right) \right]. \tag{11}$$

By the zero-mean score identity in Lemma C.2, the term '+1' vanishes in expectation, resulting in the practical form of the policy gradient:

$$\nabla_{\theta} \mathcal{J}_{RKL}(\theta) = \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(\cdot|x)} \left[\underbrace{\left(\log \frac{\pi_{\theta}(y|x)}{\pi_{ref}(y|x)} \right)}_{k_{1} \text{ (detached) coefficient}} \nabla_{\theta} \log \pi_{\theta}(y|x) \right]. \tag{12}$$

Any principled KL regularization loss should reproduce this target gradient in expectation. The following theorem shows that two structurally different surrogate losses do so exactly.

Theorem 5.1 (On-policy gradient equivalence of principled RKL surrogate losses). Let π_{θ} be a detached snapshot of the trainable policy π_{θ} whose parameters coincide at the time of gradient evaluation. For samples y drawn on-policy from $\pi_{\theta}(\cdot|x)$, the following objectives have the same expected gradient as the target in Equation (12):

$$\mathcal{J}_{k_1 \text{ in reward}}(\theta) = \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(\cdot|x)} \left[\underbrace{\left(\log \frac{\pi_{\theta}(y|x)}{\pi_{ref}(y|x)} \right)}_{k_1 \text{ (detached) coefficient}} \log \pi_{\theta}(y|x) \right], \tag{13}$$

$$\mathcal{J}_{k_2 \text{ as loss}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(\cdot|x)} \left[\frac{1}{2} \left(\log \frac{\pi_{\theta}(y|x)}{\pi_{ref}(y|x)} \right)^2 \right]. \tag{14}$$

Sketch (full proof in Appendix C). For Equation (13), it could recover Equation (12) because the term k_1 is a detached scalar multiplying $\nabla_{\theta} \log \pi_{\theta}$. For Equation (14), differentiating gives $\nabla_{\theta} \frac{1}{2} (\log \frac{\pi_{\theta}}{\pi_{\text{ref}}})^2 = (\log \frac{\pi_{\theta}}{\pi_{\text{ref}}}) \nabla_{\theta} \log \pi_{\theta}$, so here ' $k_{2'}$ ' is ' k_1 ', and the general $k_{n'}$ solution formula is in Equation (71), it also yields the same coefficient as Equation (12).

Consequently, conventional ' k_1 in reward' (as used in PPO / REINFORCE) and the newly proposed 'k₂ as loss' are principled, gradient-equivalent, and interchangeable implementations of RKL regularization under on-policy sampling. For off-policy updates, explicit importance sampling and PPO clip are required, as discussed in Appendix G.

FIRST-ORDER APPROXIMATION OF k_2 AS LOSS: k_3 AS LOSS $\Leftrightarrow k_{3'}$ IN REWARD

$$\mathcal{J}_{k_3 \text{ as loss}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[\frac{\pi_{\text{ref}}(y|x)}{\pi_{\boldsymbol{\theta}}(y|x)} - \log \frac{\pi_{\text{ref}}(y|x)}{\pi_{\boldsymbol{\theta}}(y|x)} - 1 \right], \tag{15}$$

where expectations are taken over on-policy samples from the detached snapshot π_{θ} . Taking the gradient of ' k_3 as loss' yields the equivalent coefficient $k_{3'}$ and could get ' $k_{n'}$ in reward' form loss:

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}_{k_{3} \text{ as loss}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim \mathcal{D}, \ y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[\underbrace{\left(1 - \frac{\pi_{\text{ref}}(y|x)}{\pi_{\boldsymbol{\theta}}(y|x)}\right)}_{k_{3'} \text{ (detached) coefficient}} \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(y|x) \right] = \nabla_{\boldsymbol{\theta}} \mathcal{J}_{k_{3'} \text{ in reward}}(\boldsymbol{\theta}).$$

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Let $\delta = \frac{\pi_{\text{ref}}(y|x)}{\pi_{\theta}(y|x)}$. The principled ' k_1 in reward' in Section 5.2 and ' $k_{3'}$ in reward' share the same score function but differ only in their scalar coefficients:

Principled (
$$k_1$$
 in reward / k_2 as loss):
$$-\log \delta \qquad \cdot \nabla_{\theta} \log \pi_{\theta}(y|x),$$
 (17)

Approximation
$$(k_3 \text{ as loss / } k_{3'} \text{ in reward}) : \underbrace{-(\delta - 1)}_{\text{(detached) coefficient}} \cdot \nabla_{\theta} \log \pi_{\theta}(y|x).$$
 (18)

The Taylor trap. Around $\delta = 1$, the identity $\log \delta = (\delta - 1) + \mathcal{O}((\delta - 1)^2)$ implies $-\log \delta \approx$ $1-\delta$. Thus, $1-\delta$ is only a *first-order* surrogate of the principal coefficient $-\log \delta$. The mismatch beyond first-order leads to three concrete issues (see Appendix E for formal statements). For visualization, the coefficient curves are plotted in Figure 1, with the code in Appendix H.

- 1. **Bias.** For all $\delta \neq 1$, $1 \delta \neq -\log \delta$, the update direction is biased relative to the true RKL gradient.
- 2. Pathological asymmetry. The two coefficients agree near $\delta = 1$, but behave very differently in the tails:
 - Over-coverage $(\delta \to 0)$: $-\log \delta \to +\infty$ (a strong, sustained restoring force), whereas $1-\delta \to 1$ (saturates), yielding a much weaker regularizer. This often occurs late in RLHF training when $\pi_{\theta} > \pi_{\text{ref}}$, making the $k_{3'}$ constraint weaker.
 - $Under-coverage\ (\delta \to \infty)$: $-\log \delta$ decays only logarithmically, but $1-\delta \to -\infty$ much faster, inducing explosive updates.
- 3. Statistical instability. Under $y \sim \pi_{\theta}(\cdot|x)$, $\mathbb{E}[\delta] = 1$ and $\text{Var}[1 \delta] = \mathbb{E}[(\delta 1)^2] = 1$ $\chi^2(\pi_{\rm ref}||\pi_{\theta})$, the chi-square divergence, which is notoriously unstable. The stochastic gradient inherits this high variance.

5.4 PRACTICAL RECOMMENDATIONS

Based on our gradient-centric analysis, we offer the following practical recommendations for implementing KL regularization loss in RLHF, and the last two points will be discussed in Appendix G and Appendix F:

Do not use 'k₁ as a loss'. Its expected gradient is zero and independent of the reference model, providing no regularization signal, only noise.

Prefer 'k_1 in reward' or 'k_2 as loss' for theoretical soundness. In the on-policy setting, these two formulations are gradient equivalent and correctly implement the RKL objective. They are the principal default choices for KL regularization (see Appendix C for a detailed proof).

Understand the properties of k_3 as loss'. This formulation should be recognized as a biased firstorder approximation of k_2 as loss' (see Appendix Appendix E for a formal analysis). Although its weaker regularization strength at high policy probabilities might offer practical benefits in some scenarios, practitioners should be aware of its theoretical deviation from the true KL gradient and its potential for pathological updates when the policy probability is low.

Correct for off-policy bias. When using any k_n as loss' formulation in an off-policy setting like PPO, it is crucial to apply importance sampling corrections to the KL term itself. Neglecting this introduces a systematic bias. The combined approach ' k_n in reward' naturally avoids this trap. A detailed discussion and our proposed correction are available in Appendix G.

Consider bounded alternatives for enhanced stability. If maximum stability is required, especially under significant policy updates, alternatives that produce bounded gradient coefficients can be beneficial. For example, the MSE-based penalty, like the MiniMax-01 loss, induces a coefficient bounded within [-1, 1]. Its derivation and properties are detailed in Appendix F.

EXPERIMENTAL VALIDATION

We conduct controlled GRPO experiments on a mathematical reasoning task to examine gradient analysis in Section 5. Our experiment design isolates the effects of different KL formulations, allowing us to: (i) validate that ' k_1 as loss' does not provide a proper regularization term and (ii) compare the principled ' k_2 as loss' with its first-order surrogate, ' k_3 as loss'. We put the large scale experiment in Appendix K and downstream benchmark performance in Appendix L

6.1 SETUP AND BASELINES

Dataset Construction. We use a curated subset of OpenR1-Math-220k³, primarily composed of NuminaMath 1.5 prompts. Reasoning traces are generated by a strong model, Deepseek-R1, and filtered by MathVerify⁴ for formatting and correctness. Sequences greater than 2048 tokens are removed, and we yield 7.3K prompts with high-quality off-policy reasoning traces.

RL Configuration. To isolate the gradient properties of each KL term, we employ a fully onpolicy training configuration: rollout batch size 32, 8 responses per prompt, and an update batch size of 256. The sampling temperature is 1.0. We compute the format reward using regular expressions, use Math-Verify for the accuracy reward, and the actor model is Qwen2.5-Math-1.5B Yang et al. (2024). We turn off the entropy loss (coefficient 0) and set $\beta = 0.5$ for all KL regularized losses.

6.2 KEY RESULTS

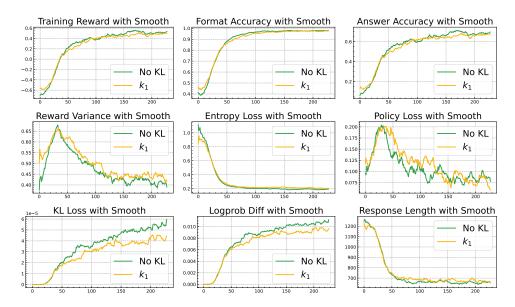


Figure 2: Comparison of " k_1 as loss" versus no KL regularization. The training dynamics are nearly indistinguishable, empirically confirming the theoretical prediction from Section 5: ' k_1 as loss' is ineffective as a KL regularizer due to its gradient's independence from the reference model and its zero-mean gradient expectation.

The empirical results shown in fig. 2 strongly support our theoretical analysis of ' k_1 as loss'. As derived in Section 5, the gradient of this loss term is fundamentally flawed for regularization: first, it is entirely independent of the reference policy π_{ref} , and second, its expectation over on-policy samples is exactly zero. In practice, this term is equivalent to adding a scaled score function, $\beta \cdot \nabla_{\theta} \log \pi_{\theta}$, to the gradient. Although this does not alter the expected update direction, it injects zero-mean noise, thereby increasing gradient variance. It is the inverse of the variance reduction technique used in REINFORCE with a baseline.

Consequently, the theoretical expectation for ' k_1 as loss' is that its performance will be, at best, comparable to that of having no KL penalty and could potentially be worse due to the increased variance that hinders optimization. Our experimental findings, where the training trajectories of ' k_1

³https://huggingface.co/datasets/open-r1/OpenR1-Math-220k

⁴https://github.com/huggingface/Math-Verify

as loss' are nearly indistinguishable from the baseline without KL, fall squarely within this predicted range of outcomes. This observation provides compelling evidence that ' k_1 as loss' should be avoided, as it does not benefit regularization while posing a potential risk to the stability of training.

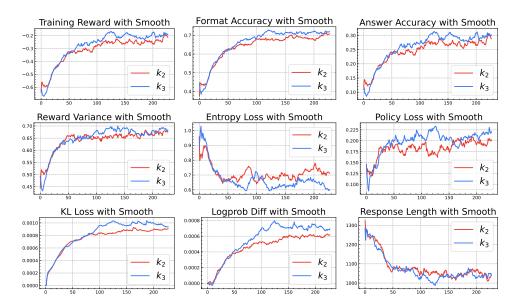


Figure 3: Comparison of the principled " k_2 as loss" against its first-order surrogate " k_3 as loss". Both variants effectively constrain the policy, but ' k_2 as loss' demonstrates superior regularization properties, maintaining a tighter coupling to the reference policy and yielding a more stable optimization path, evidenced by lower reward variance.

In Figure 3, we compare the principled ' k_2 as loss' with its approximation, ' k_3 as loss'. Both methods successfully regularize the policy; a cross-figure comparison with Figure 2 shows that their reward curves are suppressed relative to the baseline without KL, confirming that the KL penalty actively constrains the optimization to stay closer to the reference model.

Both variants regularize the policy, and the principled ' k_2 as loss' exhibits some advantages. It delivers greater training stability and stronger regularization, reflected in lower variance of rewards and response lengths, indicative of a smoother optimization landscape. It also maintains tighter coupling to the reference policy, with a smaller actor—reference probability gap (see "Logprob Diff with Smooth") and slightly higher entropy, suggesting ' k_2 as loss' preserves more exploration ability while remaining stable. These empirical observations align with its role as the correct surrogate loss for the RKL objective. In contrast, ' k_3 as loss' is a first-order surrogate that imposes weaker constraints, yielding larger probability gaps and reduced entropy. Although ' k_3 as loss' may be a viable choice when a milder late-stage constraint is desired, our results indicate that ' k_2 as loss' offers a more robust and principled route to stable, effective regularization.

7 Conclusion

This paper has presented a systematic, gradient-centric analysis of the KL loss in RLHF, challenging the common practice of borrowing principles from numerical value estimation to design optimization losses. We established a unified framework that connects the implementations of k_n in reward and k_n as loss, allowing a direct comparison of their gradient properties. Our analysis identifies conventional k_1 in reward and its newly revealed equivalent, k_2 as loss, as the principled loss of Reverse KL regularization. And showing the recent k_3 as loss to be a biased first-order approximation of the principal KL loss. Our experimental results validate these theoretical distinctions. Our work offers a clear and theoretically grounded foundation for implementing KL regularization. This addresses long-standing ambiguities in the field and provides practitioners with a robust rationale for designing more effective and reliable RLHF systems.

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A DETAILED IMPLEMENTATION OF RLHF METHODS

In a typical RLHF training step, we draw N prompts $\{x^{(i)}\}_{i=1}^N$ from the dataset \mathcal{D} . For each prompt $x^{(i)}$, we sample G responses $y^{(i,1)},\ldots,y^{(i,G)}\sim\pi_{\theta}(\cdot\mid x^{(i)})$ from the (detached) current policy. The G responses associated with the same prompt form a group, and the full minibatch contains $N\times G$ prompt—response pairs. We use π_{θ} for the trainable policy (which carries gradients) and π_{θ} for its numerically identical, detached snapshot (which does not).

Baseline Subtraction and Normalization Proposed by REINFORCE (Williams, 1992), subtracting an action-independent baseline does not change the expected policy gradient (unbiased; see Equation (34)) and typically reduces variance, accelerating convergence. We consider the following baseline operators applied to a scalar signal r:

$$f_{\text{group-bl}}(r) = r - \text{mean}_{\text{group}}(r),$$
 (19)

$$f_{\text{batch-bl}}(r) = r - \text{mean}_{\text{batch}}(r).$$
 (20)

In practice, normalization is also used. Normalization is *not* unbiased but can improve numerical stability by controlling the scale of the reward signal:

$$f_{\rm BN}(r) = \frac{r - {\rm mean_{batch}}(r)}{{\rm std_{batch}}(r)},$$
 (21)

$$f_{\rm GN}(r) = \frac{r - \text{mean}_{\rm group}(r)}{\text{std}_{\rm group}(r)}.$$
 (22)

How Common Algorithms Shape the Reward Signal Let $r_{\text{raw}}(x, y)$ denote the raw score from the reward model before any shaping. The following variants differ in how they post-process r_{raw} :

REINFORCE:
$$r(x,y) = f_{BN}(r_{raw}(x,y)),$$
 (23)

PPO/REINFORCE++:
$$r(x,y) = f_{\text{BN}}(r_{\text{raw}}(x,y)),$$
 (24)

GRPO:
$$r(x,y) = f_{GN}(r_{raw}(x,y)),$$
 (25)

Dr-GRPO (Liu et al., 2025b):
$$r(x, y) = f_{\text{group-bl}}(r_{\text{raw}}(x, y)),$$
 (26)

REINFORCE++baseline:
$$r(x,y) = f_{BN}(f_{group-bl}(r_{raw}(x,y))).$$
 (27)

Integration of the KL Regularization Loss The transforms above shape only the reward signal. The KL regularizer is typically integrated in one of two ways:

(i) **Combined Form** (k_n in reward'): Used by REINFORCE/PPO methods. A combined reward signal is formed first,

$$A_{\text{combined}}(x, y) = r_{\text{raw}}(x, y) - \beta k_1 \Big(\pi_{\theta}(y \mid x), \, \pi_{\text{ref}}(y \mid x) \Big),$$

and then baseline/normalization is applied to this combined signal A_{combined} before it multiplies the score function.

(ii) **Decoupled Form ('k_n as loss'):** Used by GRPO methods. The KL penalty $k_n(\pi_{\theta}(\cdot \mid x), \pi_{\text{ref}}(\cdot \mid x))$ is optimized as a separate, unnormalized loss term, added to the policy-gradient loss driven by the shaped reward r(x, y).

Complete On-Policy Objectives for REINFORCE/PPO and GRPO REINFORCE/PPO (Monte Carlo minibatch):

$$\mathcal{L}_{\text{REINFORCE/PPO,MC}}(\theta) = -\frac{1}{NG} \sum_{i=1}^{N} \sum_{j=1}^{G} \left\{ A(x^{(i)}, y^{(i,j)}) \log \pi_{\theta}(y^{(i,j)} \mid x^{(i)}) \right\}, \tag{28}$$

where
$$A(x,y) = f_{\text{BN}} \Big(r_{\text{raw}}(x,y) - \beta k_1 \Big(\pi_{\theta}(y \mid x), \, \pi_{\text{ref}}(y \mid x) \Big) \Big)$$
. (29)

Here, the k_1 term is evaluated using detached probabilities, consistent with the policy-gradient framework where it acts as a coefficient for the score function.

GRPO (Monte Carlo minibatch):

$$\mathcal{L}_{GRPO,MC}(\theta) = -\frac{1}{NG} \sum_{i=1}^{N} \sum_{j=1}^{G} \left\{ r(x^{(i)}, y^{(i,j)}) \log \pi_{\theta}(y^{(i,j)} \mid x^{(i)}) \right\}$$

$$+ \frac{\beta}{NG} \sum_{i=1}^{N} \sum_{j=1}^{G} k_{3} \left(\pi_{\theta}(y^{(i,j)} \mid x^{(i)}), \pi_{ref}(y^{(i,j)} \mid x^{(i)}) \right).$$
(30)

In this decoupled form, the shaped reward r(x, y) drives the policy-gradient term, while the KL penalty is a separate loss where gradients flow directly through π_{θ} inside $k_3(\cdot)$.

Remark. While baseline subtraction is an unbiased variance-reduction technique, normalization is a biased but often crucial heuristic for practical stability. Both are important engineering details, even if omitted from simplified theoretical analyses.

B POLICY GRADIENT DERIVATION FOR REWARD MAXIMIZATION

This section provides a detailed derivation of the policy gradient for the reward maximization objective. We clarify the distinction between the true objective, its gradient, and the surrogate loss function, adhering to a strict notation where θ indicates a variable subject to differentiation and θ indicates a detached parameter, such as in a sampling distribution.

The Objective Function The goal is to find parameters θ for a policy π_{θ} that maximize the expected reward:

$$\mathcal{J}_{\text{reward}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[r(x, y) \right] = \mathbb{E}_{x \sim \mathcal{D}} \sum_{y} \left[r(x, y) \cdot \pi_{\boldsymbol{\theta}}(y|x) \right]. \tag{31}$$

We assume standard regularity conditions that permit the interchange of differentiation and expectation operators.

Policy Gradient Derivation We compute the gradient of the objective function $\mathcal{J}_{reward}(\theta)$ using the log-derivative trick. The distinction between θ and θ is crucial in the derivation steps:

$$\nabla_{\theta} \mathcal{J}_{\text{reward}}(\theta) = \nabla_{\theta} \mathbb{E}_{x \sim \mathcal{D}} \sum_{y} \left[r(x, y) \cdot \pi_{\theta}(y|x) \right]$$

$$= \mathbb{E}_{x \sim \mathcal{D}} \sum_{y} \left[r(x, y) \cdot \nabla_{\theta} \pi_{\theta}(y|x) \right]$$

$$= \mathbb{E}_{x \sim \mathcal{D}} \sum_{y} \left[r(x, y) \cdot \pi_{\theta}(y|x) \cdot \frac{\nabla_{\theta} \pi_{\theta}(y|x)}{\pi_{\theta}(y|x)} \right]$$

$$= \mathbb{E}_{x \sim \mathcal{D}} \sum_{y} \pi_{\theta}(y|x) \left[r(x, y) \cdot \nabla_{\theta} \log \pi_{\theta}(y|x) \right]$$

$$= \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(\cdot|x)} \left[r(x, y) \cdot \nabla_{\theta} \log \pi_{\theta}(y|x) \right].$$
(32)

In the third and fourth lines, π_{θ} represents the current policy's probability value, which is treated as a constant factor in the application of the chain rule for logarithms, while π_{θ} is the function being differentiated. The final line expresses the gradient as an expectation over samples from π_{θ} , where the sampling process itself is treated as having no gradient path.

C FORMAL PROOF OF THE PRINCIPLE KL REGULARIZATION

This appendix provides a formal, step-by-step derivation showing that, under Assumptions (A1)–(A4), the true KL divergence objective and two common surrogates—' k_1 in reward' and ' k_2 as loss'—share the same expected gradient. We employ two numerically identical copies of the policy: a gradient-carrying one, $\pi_{\theta}(\cdot|x)$, and its detached counterpart, $\pi_{\theta}(\cdot|x)$. Parameters marked with θ carry gradients; black θ denotes detached parameters. Sampling measures, denominators, and scalar coefficients multiplying a gradient term are always treated as detached by using π_{θ} .

C.1 ASSUMPTIONS AND NOTATION

Let D be a data distribution over x, $\pi_{\text{ref}}(\cdot|x)$ a fixed reference policy, and $\pi_{\theta}(\cdot|x)$ a differentiable policy. All logarithms are natural.

- (A1) For each x, the function $y \mapsto \pi_{\theta}(y|x)$ is a valid probability mass/density: $\pi_{\theta}(y|x) > 0$ on its support, it is differentiable in θ , and normalizes to one, i.e., $\sum_{y} \pi_{\theta}(y|x) = 1$ (or $\int \pi_{\theta}(y|x) dy = 1$).
- (A2) The interchange of expectation/summation and differentiation is valid.
- (A3) The data distribution D and reference policy π_{ref} do not depend on θ .
- (A4) The KL divergence is well-defined: for all x and all y in the support of $\pi_{\theta}(\cdot|x)$, we have $\pi_{\text{ref}}(y|x) > 0$.

Notation: π_{θ} denotes the detached copy of π_{θ} , numerically equal at the current iterate. Expectations over y are taken with respect to $y \sim \pi_{\theta}(\cdot|x)$ unless stated otherwise.

C.2 FUNDAMENTAL IDENTITIES

Lemma C.1 (Log-derivative identity with detached denominator). For any fixed x and any y with $\pi_{\theta}(y|x) > 0$,

$$\nabla_{\theta} \log \pi_{\theta}(y|x) = \frac{\nabla_{\theta} \pi_{\theta}(y|x)}{\pi_{\theta}(y|x)}.$$
(33)

Proof. By the chain rule, $\nabla_{\theta} \log \pi_{\theta} = (\nabla_{\theta} \pi_{\theta})/\pi_{\theta}$. Replacing the denominator with its detached, numerically identical copy π_{θ} preserves the numerical value while making the no-gradient path explicit.

Lemma C.2 (Zero-mean score). For any fixed x,

$$\mathbb{E}_{y \sim \pi_{\theta}(\cdot|x)} \left[\nabla_{\theta} \log \pi_{\theta}(y|x) \right] = 0. \tag{34}$$

Proof. Using Lemma C.1,

$$\sum_{y} \pi_{\theta}(y|x) \frac{\nabla_{\theta} \pi_{\theta}(y|x)}{\pi_{\theta}(y|x)} = \sum_{y} \nabla_{\theta} \pi_{\theta}(y|x) = \nabla_{\theta} \sum_{y} \pi_{\theta}(y|x) = \nabla_{\theta}(1) = 0.$$
 (35)

Corollary C.0.1 (Score-function reweighting). For any function z(y,x) detached with respect to θ ,

$$\sum_{y} \nabla_{\theta} \pi_{\theta}(y|x) z(y,x) = \mathbb{E}_{y \sim \pi_{\theta}(\cdot|x)} \left[z(y,x) \nabla_{\theta} \log \pi_{\theta}(y|x) \right]. \tag{36}$$

Corollary C.0.2 (Baseline invariance). For any function b(x) detached with respect to θ ,

$$\mathbb{E}_{y \sim \pi_{\theta}(\cdot|x)} \left[b(x) \nabla_{\theta} \log \pi_{\theta}(y|x) \right] = b(x) \cdot \mathbb{E}_{y \sim \pi_{\theta}(\cdot|x)} \left[\nabla_{\theta} \log \pi_{\theta}(y|x) \right] = 0. \tag{37}$$

Thus, adding a detached, action-independent baseline b(x) to any coefficient does not change the expected gradient.

C.3 DERIVATION OF THE TRUE KL GRADIENT

The KL divergence objective is:

$$\mathcal{J}_{\mathrm{KL}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim D} \left[\sum_{y} \pi_{\boldsymbol{\theta}}(y|x) \log \frac{\pi_{\boldsymbol{\theta}}(y|x)}{\pi_{\mathrm{ref}}(y|x)} \right]. \tag{38}$$

Step 1 (Differentiate under the expectation). By (A2), the gradient operator is moved inside the expectation and sum.

Step 2 (Apply product rule). For each y, we apply the product rule and display detached copies for undifferentiated factors:

$$\nabla_{\theta} \left[\pi_{\theta}(y|x) \log \pi_{\theta}(y|x) \right] = (\nabla_{\theta} \pi_{\theta}) \log \pi_{\theta} + \pi_{\theta} \cdot \nabla_{\theta} \log \pi_{\theta}$$
$$= (\nabla_{\theta} \pi_{\theta}) (\log \pi_{\theta} + 1). \tag{39}$$

By (A3), the gradient of the reference term is $\nabla_{\theta}[-\pi_{\theta}(y|x)\log \pi_{\text{ref}}(y|x)] = -(\nabla_{\theta}\pi_{\theta}(y|x))\log \pi_{\text{ref}}(y|x)$.

Step 3 (Collect terms). Combining terms yields an expression with a detached coefficient:

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}_{\mathrm{KL}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim D} \left[\sum_{y} \nabla_{\boldsymbol{\theta}} \pi_{\boldsymbol{\theta}}(y|x) \left(\log \frac{\pi_{\boldsymbol{\theta}}(y|x)}{\pi_{\mathrm{ref}}(y|x)} + 1 \right) \right]. \tag{40}$$

Step 4 (Apply score-function reweighting). Using Corollary C.0.1 with the detached coefficient $z(y,x) := \log \frac{\pi_{\theta}(y|x)}{\pi_{\text{ref}}(y|x)} + 1$:

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}_{\mathrm{KL}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim D, \ y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[\left(\log \frac{\pi_{\boldsymbol{\theta}}(y|x)}{\pi_{\mathrm{ref}}(y|x)} + 1 \right) \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(y|x) \right]. \tag{41}$$

Step 5 (**Simplify using the zero-mean score property**). The expectation of the '+1' term is zero by Lemma C.2, yielding the final gradient:

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}_{\mathrm{KL}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim D, \ y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[\log \frac{\pi_{\boldsymbol{\theta}}(y|x)}{\pi_{\mathrm{ref}}(y|x)} \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(y|x) \right]. \tag{42}$$

C.4 THE GOLD STANDARD: k_1 IN REWARD $\Leftrightarrow k_2$ AS LOSS

Surrogate 1: k_1 in reward'.

$$\mathcal{J}_{k_1 \text{ in reward}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim D, \ y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[\underbrace{\left(\log \frac{\pi_{\boldsymbol{\theta}}(y|x)}{\pi_{\text{ref}}(y|x)} \right)}_{\text{deteched coefficient}} \log \pi_{\boldsymbol{\theta}}(y|x) \right]. \tag{43}$$

Since the coefficient is detached, its gradient is identical to Equation (42).

Surrogate 2: k_2 as loss.

$$\mathcal{J}_{k_2 \text{ as loss}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim D, \ y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[\frac{1}{2} \left(\log \pi_{\boldsymbol{\theta}}(y|x) - \log \pi_{\text{ref}}(y|x) \right)^2 \right]. \tag{44}$$

By the chain rule, and displaying the resulting scalar multiplier as its detached copy for clarity:

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}_{k_2 \text{ as loss}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim D, \ y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[\left(\log \pi_{\boldsymbol{\theta}}(y|x) - \log \pi_{\text{ref}}(y|x) \right) \ \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(y|x) \right], \tag{45}$$

which is also identical to Equation (42).

C.5 CONCLUSION AND IMPLEMENTATION GUIDANCE

Under Assumptions (A1)–(A4), the true KL objective and both surrogates share the same expected gradient, given by Equation (42). This equivalence is based on the following key conventions.

Sampling Measure: The samples are drawn from a detached policy $y \sim \pi_{\theta}(\cdot|x)$ (usually vLLM).

Detached Coefficients: The scale coefficients that multiply the score function are treated as detached. Applying Corollary C.0.2, any detached baseline b(x) can be added to reduce variance.

Gradient Path: Gradients propagate only through terms explicitly parameterized by θ .

 Implementation Notes. For a single on-policy sample $y \sim \pi_{\theta}(\cdot|x)$:

- ' k_1 in reward': To minimize $\mathcal{J}_{\mathrm{KL}}$, define the loss as weight := $\log \pi_{\theta}(y|x) \log \pi_{\mathrm{ref}}(y|x)$ (detached) and Loss := weight $\cdot \log \pi_{\theta}(y|x)$. A gradient descent step on this loss performs descent on $\mathcal{J}_{\mathrm{KL}}$. The common RL loss, -weight $\cdot \log \pi_{\theta}$, implements objective *ascent*.
- ' k_2 as loss': To minimize $\mathcal{J}_{\mathrm{KL}}$, define log_ratio := $\log \pi_{\theta}(y|x) \log \pi_{\mathrm{ref}}(y|x)$ and Loss := $\frac{1}{2} (\log_{-1} \pi_{\mathrm{to}})^2$.

Remarks. (i) For continuous spaces, replace sums by integrals; the proof is unchanged provided densities are positive on their support. (ii) The equivalence requires on-policy sampling. If samples are drawn from a stale policy π_{old} , exact correction uses importance weights $\rho(x,y) = \pi_{\theta}(y|x)/\pi_{\text{old}}(y|x)$ inside the expectations.

D SURROGATE OBJECTIVE: FULL-VOCABULARY VS. MONTE CARLO

This section formalizes the connection between the theoretical policy-gradient objective and its practical mini-batch implementations. We detail two key estimators: a **full-vocabulary loss**, which is exact but computationally infeasible, and a **Monte Carlo** (**MC**) **loss**, which provides an unbiased, practical approximation.

Conventions and gradient paths.

- 1. The trainable policy π_{θ} carries gradients; its detached, numerically identical snapshot at the current iterate is denoted π_{θ} .
- 2. All scalars that multiply the score function are detached: the reward r(x,y), any KL-derived term $k_n(\cdot)$, and their combination $r(x,y) \beta k_n(\cdot)$.
- 3. Gradients flow only through $\log \pi_{\theta}(y|x)$; everything inside the coefficient c(x,y) is detached.
- 4. We adopt the naming used in the main text: reward (detached) coefficient, k_n (detached) coefficient, and combined form coefficient.

We express the objective using a generic, detached scalar coefficient c(x, y), which can take several forms:

$$c(x,y) \in \left\{ \begin{array}{ll} r(x,y) & \text{reward (detached) coefficient} \\ k_n(\pi_{\theta}(y|x), \ \pi_{\text{ref}}(y|x)) & k_n \text{ (detached) coefficient} \\ r(x,y) - \beta \ k_n(\pi_{\theta}(y|x), \ \pi_{\text{ref}}(y|x)) & \text{combined form coefficient} \end{array} \right\}. \tag{46}$$

A typical KL choice is

$$k_1(y|x) = \log \pi_{\theta}(y|x) - \log \pi_{\text{ref}}(y|x). \tag{47}$$

Policy gradient in expectation form (with baseline). For the population objective $\mathcal{J}_{true}(\theta) = \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(\cdot|x)}[c(x,y)]$, using a detached, action-independent baseline b(x) and the log-derivative identity with a detached denominator,

$$\nabla_{\theta} \log \pi_{\theta}(y|x) = \frac{\nabla_{\theta} \pi_{\theta}(y|x)}{\pi_{\theta}(y|x)},\tag{48}$$

the unbiased policy gradient is

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}_{\text{true}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim \mathcal{D}, \ y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \Big[(c(x, y) - b(x)) \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(y|x) \Big]. \tag{49}$$

This relies on the zero-mean score property under $y \sim \pi_{\theta}(\cdot|x)$ as proved in Equation (34), ensuring b(x) does not change the expected gradient.

Population surrogate loss. A surrogate loss whose negative gradient recovers Equation (49) is

$$\mathcal{L}_{\text{sur}}(\boldsymbol{\theta}) = -\mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(\cdot|x)} \Big[\big(c(x, y) - b(x) \big) \log \pi_{\boldsymbol{\theta}}(y|x) \Big].$$
 (50)

Two interchangeable mini-batch implementations. We provide two equivalent mini-batch estimators of Equation (50). The first computes the exact inner expectation over the discrete action space \mathcal{V} by summing all actions with a detached sampling weight; the second replaces this inner sum with i.i.d. on-policy samples, yielding an unbiased estimate conditional on the mini-batch prompts.

$$\mathcal{L}_{\text{sur,Full}}(\boldsymbol{\theta}) = -\frac{1}{N} \sum_{i=1}^{N} \sum_{y^{(i)} \in \mathcal{V}} \underbrace{\pi_{\boldsymbol{\theta}}(y^{(i)} \mid x^{(i)})}_{\text{detached weight}} \left(c(x^{(i)}, y^{(i)}) - b(x^{(i)}) \right) \log \pi_{\boldsymbol{\theta}}(y^{(i)} \mid x^{(i)}). \tag{51}$$

Here, "detached weight" indicates that gradients do not flow through π_{θ} ; the score path is solely via $\log \pi_{\theta}$.

$$\mathcal{L}_{\text{sur,MC}}(\theta) = -\frac{1}{N} \sum_{i=1}^{N} \frac{1}{G} \sum_{j=1}^{G} \left(c(x^{(i)}, y^{(i,j)}) - b(x^{(i)}) \right) \log \pi_{\theta} (y^{(i,j)} \mid x^{(i)}), \quad y^{(i,j)} \sim \pi_{\theta} (\cdot \mid x^{(i)}).$$
(52)

In Equation (52), $\{y^{(i,j)}\}_{j=1}^G$ are i.i.d. samples from the detached snapshot $\pi_{\theta}(\cdot|x^{(i)})$; increasing G reduces variance while preserving unbiasedness.

Unbiasedness and practical considerations. For any fixed $x^{(i)}$ and function f,

$$\mathbb{E}_{\{y^{(i,j)}\}_{j=1}^{G} \text{ i.i.d.} \sim \pi_{\theta}(\cdot | x^{(i)})} \left[\frac{1}{G} \sum_{j=1}^{G} f(y^{(i,j)}) \right] = \sum_{y^{(i)} \in \mathcal{V}} \pi_{\theta}(y^{(i)} | x^{(i)}) f(y^{(i)}), \tag{53}$$

hence $\mathbb{E}\left[\mathcal{L}_{\text{sur,MC}} \mid \{x^{(i)}\}\right] = \mathcal{L}_{\text{sur,Full}}$. In practice, computing r(x,y) or $k_n(\cdot)$ over the full vocabulary is infeasible for LLMs due to GPU memory constraints; MC estimation is therefore standard.

Alternative decoupled formulation: ' k_n as loss'. In addition to incorporating KL via the coefficient c(x,y), one may add a separate penalty-only loss that differentiates directly through the log-ratio. Let $\psi_n : \mathbb{R} \to \mathbb{R}$ be differentiable (e.g., $\psi_1(t) = t$, $\psi_2(t) = \frac{1}{2}t^2$). Define

$$\mathcal{L}_{k_n \text{ as loss,MC}}(\boldsymbol{\theta}) = -\frac{1}{NG} \sum_{i=1}^{N} \sum_{j=1}^{G} \psi_n \left(\underbrace{\log \pi_{\boldsymbol{\theta}}(y^{(i,j)}|x^{(i)})}_{\text{with grad}} - \underbrace{\log \pi_{\text{ref}}(y^{(i,j)}|x^{(i)})}_{\text{detached}} \right). \tag{54}$$

Its gradient takes the score-like form

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}_{k_n \text{ as loss,MC}}(\boldsymbol{\theta}) = -\frac{1}{NG} \sum_{i=1}^{N} \sum_{j=1}^{G} \psi'_n(\cdot) \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(y^{(i,j)} | x^{(i)}), \tag{55}$$

where (\cdot) denotes the log-ratio in Equation (54). Here the prime denotes differentiation with respect to the scalar argument:

$$\psi_n'(t) \triangleq \frac{\mathrm{d}}{\mathrm{d}t} \psi_n(t).$$
 (56)

Under on-policy sampling, evaluating the scalar coefficient $\psi_n'(\cdot)$ at the current iterate (i.e., treating it as detached) yields the gradient-equivalence established in the main text (see Theorem in Section 5.2 and Appendix C). A common choice $\psi_2(t) = \frac{1}{2}t^2$ recovers the squared log-ratio penalty. The total objective is then $\mathcal{L}_{\text{reward,MC}} - \beta \cdot \mathcal{L}_{k_n \text{ as loss,MC}}$, with π_{ref} fixed and detached.

E FORMAL ANALYSIS OF THE ' k_3 AS LOSS' GRADIENT SURROGATE

This appendix provides the formal analysis underpinning Section 5.3, proving that the ' k_3 as loss' formulation acts as a first-order, biased surrogate for the principled Reverse KL (RKL) gradient. We first derive its gradient-equivalent 'in-reward' coefficient under on-policy sampling, then dissect its three core deficiencies: local bias, global asymmetry, and statistical instability.

Throughout, we fix a prompt x and consider samples $y \sim \pi_{\theta}(\cdot|x)$ drawn on-policy from a detached snapshot of the trainable policy π_{θ} . We define the probability ratio as:

$$\delta(y) := \frac{\pi_{\text{ref}}(y|x)}{\pi_{\theta}(y|x)}.$$
(57)

Our analysis compares the coefficient induced by ' k_3 as loss' against the principled RKL gradient coefficient, $c^{\star}(y) = -\log \delta(y)$. All scalar coefficients multiplying the score function $\nabla_{\theta} \log \pi_{\theta}(y|x)$ are treated as detached.

Gradient-Equivalent Coefficient of ' k_3 **as loss'.** The ' k_3 as loss' objective is given by:

$$\mathcal{J}_{k_3 \text{ as loss}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(\cdot|x)} \left[\frac{\pi_{\text{ref}}(y|x)}{\pi_{\boldsymbol{\theta}}(y|x)} - 1 - \log \frac{\pi_{\text{ref}}(y|x)}{\pi_{\boldsymbol{\theta}}(y|x)} \right]. \tag{58}$$

Differentiating and evaluating the resulting scalar multiplier at the detached snapshot yields:

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}_{k_3 \text{ as loss}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\boldsymbol{\theta}}(\cdot|x)} \left[\left(1 - \frac{\pi_{\text{ref}}(y|x)}{\pi_{\boldsymbol{\theta}}(y|x)} \right) \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(y|x) \right]. \tag{59}$$

This confirms that ' k_3 as loss' is gradient-equivalent (under on-policy sampling) to an 'in-reward' update with the detached coefficient:

$$c_{3'}(y) := 1 - \delta(y). \tag{60}$$

$$\mathcal{J}_{k_{3'} \text{ in reward}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(\cdot|x)} \left[\left(1 - \frac{\pi_{\text{ref}}(y|x)}{\pi_{\theta}(y|x)} \right) \log \pi_{\boldsymbol{\theta}}(y|x) \right]. \tag{61}$$

The remainder of this section formally analyzes the deficiencies of this proxy, $c_{3'}$, when compared to the principled target, $c^* = -\log \delta$.

Lemma E.1 (First-order agreement and second-order bias). The proxy $1 - \delta$ is the first-order Taylor approximation of the principled coefficient $-\log \delta$ around $\delta = 1$. The approximation error (bias) is of second order:

$$Bias(\delta) = (-\log \delta) - (1 - \delta) = \frac{1}{2}(\delta - 1)^2 - \frac{1}{3}(\delta - 1)^3 + O((\delta - 1)^4).$$
 (62)

Proof sketch. The result is obtained by expanding $-\log \delta$ in a Taylor series at r=1 and subtracting the term $(1-\delta)$.

Lemma E.2 (One-sided domination and asymmetric tails). For all $\delta > 0$, the proxy is a strict lower bound, $1 - \delta \le -\log \delta$, with equality holding only at $\delta = 1$. Their tail behaviors are pathologically asymmetric:

- Over-coverage ($\delta \to 0^+$): The proxy provides a weak, saturating restoring force $(\lim_{\delta \to 0^+} (1 \delta) = 1)$, whereas the principled coefficient provides an unbounded penalty $(\lim_{\delta \to 0^+} (-\log \delta) = +\infty)$.
- Under-coverage ($\delta \to \infty$): The proxy induces an aggressive, linearly explosive penalty ($\lim_{\delta \to \infty} (1 \delta) = -\infty$), while the principled coefficient's penalty grows only logarithmically.

Proof sketch. The inequality follows from the fundamental property $\log \delta \leq \delta - 1$. The limits are elementary.

Theorem E.1 (Variance equals chi-squared divergence). Assuming $\sup(\pi_{ref}(\cdot|x)) \subseteq \sup(\pi_{\theta}(\cdot|x))$, the proxy coefficient $c_{3'}$ has zero mean under the on-policy sampling distribution, and its variance is exactly the chi-squared divergence:

$$\mathbb{E}_{y \sim \pi_{\theta}}[1 - \delta(y)] = 0, \qquad \operatorname{Var}_{y \sim \pi_{\theta}}[1 - \delta(y)] = \chi^{2}(\pi_{ref}(\cdot|x) \parallel \pi_{\theta}(\cdot|x)). \tag{63}$$

If the support condition is violated, the variance is infinite.

Proof sketch. $\mathbb{E}[\delta] = \sum_{y} \pi_{\theta}(y|x) \frac{\pi_{\text{ref}}(y|x)}{\pi_{\theta}(y|x)} = 1$, thus $\mathbb{E}[1-r] = 0$. The variance identity then follows directly from the definition of $\chi^2(p \parallel q)$.

Corollary E.1.1 (Implication for stochastic gradient variance). The variance of the stochastic gradient term induced by ' k_3 as loss' is directly governed by the chi-squared divergence, a notoriously unstable metric:

$$\mathbb{E}\left[\left\|(1-\delta(y))\nabla_{\boldsymbol{\theta}}\log \pi_{\boldsymbol{\theta}}(y|x)\right\|^{2}\right] = \mathbb{E}\left[(1-\delta(y))^{2}\left\|\nabla_{\boldsymbol{\theta}}\log \pi_{\boldsymbol{\theta}}(y|x)\right\|^{2}\right]. \tag{64}$$

Conclusion. These results provide a rigorous, gradient-centric justification for the claims in the main text. The ' k_3 as loss' formulation does not implement the true RKL gradient. Instead, it deploys a first-order proxy ($c_{3'}=1-\delta$) that is accurate only when the policy is very close to the reference ($\delta\approx 1$). Its pathological tail behavior and high variance, linked to the chi-squared divergence, introduce optimization challenges not present in the principled ' k_1 in reward' or ' k_2 as loss' formulations. This analysis underscores the critical importance of selecting regularization losses based on their gradient properties, not merely their characteristics as value estimators.

F DERIVATION OF AN ALTERNATIVE REGULARIZER: THE MINIMAX-01 LOSS FROM MSE DISTANCE

As an alternative to KL regularization, this section derives the MiniMax-01 loss (Li et al., 2025). We will prove it originates from a mean squared error (MSE) objective and fits within our gradient-centric framework. We adhere to the established on-policy conventions: π_{θ} is the trainable policy, π_{θ} is its detached snapshot (numerically equal at the current iterate), and all scalar coefficients that multiply the score function are treated as detached during backpropagation.

Objective. We minimize the full-vocabulary MSE between the policy and the reference:

$$\mathcal{J}_{\text{MSE}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim \mathcal{D}} \left[\frac{1}{2} \sum_{y} \left(\pi_{\boldsymbol{\theta}}(y \mid x) - \pi_{\text{ref}}(y \mid x) \right)^{2} \right]. \tag{65}$$

On-policy gradient. Differentiating Equation (65) with respect to θ , evaluating the scalar multiplier at the detached snapshot π_{θ} (our standard on-policy convention), and converting to the score-function form yields:

$$\nabla_{\theta} \mathcal{J}_{MSE}(\theta) = \mathbb{E}_{x \sim D} \sum_{y} \left[\frac{1}{2} \nabla_{\theta} (\pi_{\theta}(y|x) - \pi_{ref}(y|x))^{2} \right]$$

$$= \mathbb{E}_{x \sim D} \sum_{y} \underbrace{\left(\pi_{\theta}(y \mid x) - \pi_{ref}(y \mid x) \right)}_{\text{detached coefficient}} \nabla_{\theta} \pi_{\theta}(y \mid x)$$

$$= \mathbb{E}_{x \sim D} \sum_{y} \pi_{\theta}(y \mid x) \left(\pi_{\theta}(y \mid x) - \pi_{ref}(y \mid x) \right) \nabla_{\theta} \log \pi_{\theta}(y \mid x)$$

$$= \mathbb{E}_{x \sim D, y \sim \pi_{\theta}(\cdot|x)} \left[\left(\pi_{\theta}(y \mid x) - \pi_{ref}(y \mid x) \right) \nabla_{\theta} \log \pi_{\theta}(y \mid x) \right].$$
(66)

The last line reveals that MSE regularization induces a score-function update whose scalar coefficient is the probability difference $\pi_{\theta} - \pi_{\text{ref}}$.

MiniMax-01 surrogate loss (Monte Carlo). Using a on-policy sampler that draws G responses $y^{(i,j)} \sim \pi_{\theta}(\cdot \mid x^{(i)})$ per prompt, the unbiased minibatch surrogate whose negative gradient recovers Equation (66) is

$$\mathcal{L}_{\text{MSE,MC(MiniMax-01)}}(\boldsymbol{\theta}) = -\frac{1}{NG} \sum_{i=1}^{N} \sum_{j=1}^{G} \left(\pi_{\boldsymbol{\theta}}(y^{(i,j)} \mid x^{(i)}) - \pi_{\text{ref}}(y^{(i,j)} \mid x^{(i)}) \right) \log \pi_{\boldsymbol{\theta}}(y^{(i,j)} \mid x^{(i)}).$$
(67)

This head shares the same in-reward score-function structure as our principled KL implementations: the coefficient is detached, and gradients flow only through $\log \pi_{\theta}$.

Key properties and implications.

- 1. Bounded gradient coefficient. Since $0 \le \pi_{\theta}(y \mid x), \pi_{\text{ref}}(y \mid x) \le 1$, the coefficient satisfies $-1 \le \pi_{\theta}(y \mid x) \pi_{\text{ref}}(y \mid x) \le 1$. This boundedness enhances stability against large or pathological updates, in contrast to the unbounded log-ratio used by KL (see Figure 1). This supports our recommendation in Section 5 to consider bounded alternatives when stability is paramount.
- 2. Symmetry in probability space. The MSE penalty is symmetric with respect to probability differences, providing more conservative corrections when policies diverge, compared to the logarithmic penalty of Reverse KL.
- 3. Off-policy compatibility. Owing to its in-reward form with a detached coefficient, this head is fully compatible with importance sampling and clipping, following the same correction rules as in Appendix G.

Remark. Consistent with our KL analysis, Equation (66) is obtained by evaluating scalar multipliers at the detached snapshot π_{θ} (on-policy). This keeps all regularizers within a unified k_n multiply score-function lens and enables direct, apples-to-apples comparison of their induced update dynamics.

G OFF-POLICY CORRECTION FOR KL REGULARIZATION

Many RLHF implementations harbor a subtle yet critical off-policy bias, particularly when the KL term is implemented "as loss." Such formulations are only gradient-correct under on-policy sampling. For off-policy updates, they require explicit importance sampling (IS) and PPO-style clipping. Omitting these steps systematically biases the update and undermines training stability. This section provides the principled correction, fully aligned with our gradient-centric framework.

G.1 From On-Policy to Off-Policy Gradients

We operate in the policy-gradient view, where updates are driven by a detached (stop-gradient) coefficient c(x, y) multiplying the score function. The on-policy gradient estimator is:

$$\nabla_{\theta} \mathcal{J}_{c}(\theta) = \mathbb{E}_{x \sim D, \ y \sim \pi_{\theta}(\cdot \mid x)} [c(x, y) \nabla_{\theta} \log \pi_{\theta}(y \mid x)], \tag{68}$$

where π_{θ} is a detached snapshot numerically equal to π_{θ} at the time of gradient evaluation. For samples drawn from a behavior policy $y \sim \pi_{\theta_k}(\cdot \mid x)$, an unbiased off-policy estimator requires IS, assuming the behavior policy has support over the sampled data $(\pi_{\theta_k}(y \mid x) > 0)$:

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}_{c}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim D, y \sim \pi_{\theta_{k}}(\cdot \mid x)} \left[\underbrace{\frac{\pi_{\boldsymbol{\theta}}(y \mid x)}{\pi_{\theta_{k}}(y \mid x)}}_{\text{detached IS weight}} c(x, y) \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(y \mid x) \right]. \tag{69}$$

In practice, PPO replaces this detached IS weight with the gradient-carrying ratio $\rho_k(\theta) = \frac{\pi_{\theta}(y|x)}{\pi_{\theta_k}(y|x)}$ (where gradients flow only through the numerator) and employs a clipped surrogate objective to reduce variance. For any detached coefficient c(x, y), the clipped objective to be maximized is:

$$\mathcal{J}_{c,\text{clipped}}(\boldsymbol{\theta}) = \mathbb{E}_{x \sim D, y \sim \pi_{\theta_k}(\cdot|x)} \left[\min \left(\rho_k(\boldsymbol{\theta}) c(x, y), \text{ clip}(\rho_k(\boldsymbol{\theta}), 1 - \epsilon, 1 + \epsilon) c(x, y) \right) \right]. \tag{70}$$

G.2 Correcting " k_n as loss" by Converting to an "in Reward" Head

A " k_n as loss" head is gradient-correct only on-policy. To adapt it for off-policy use, it must first be converted to its gradient-equivalent "in reward" form. This is achieved by defining a detached (stop-gradient) coefficient $k_{n'}(x,y)$ that reproduces the on-policy gradient of the original loss. For a differentiable penalty $k_n(\pi_{\theta}(y|x),\pi_{\text{ref}}(y|x))$, this coefficient is its derivative with respect to the policy's log-probability, evaluated at the *current* detached snapshot:

$$k_{n'}\big(\pi_{\theta}(y|x), \pi_{\text{ref}}(y|x)\big) := \frac{\partial}{\partial \log \pi_{\theta}} k_n\big(\pi_{\theta}(y|x), \pi_{\text{ref}}(y|x)\big) \bigg|_{\log \pi = \log \pi_{\theta}(y|x)}. \tag{71}$$

This conversion precisely aligns with the theoretical equivalences established in the main text:

- Principled k_2 as loss: $k_2 = \frac{1}{2}(\log \pi_{\theta} \log \pi_{\text{ref}})^2 \Rightarrow k_{2'} = \log \pi_{\theta} \log \pi_{\text{ref}}$ (the k_1 in reward coefficient).
- Proxy k_3 as loss: $k_3 = \frac{\pi_{\text{ref}}}{\pi_{\theta}} 1 \log \frac{\pi_{\text{ref}}}{\pi_{\theta}} \implies k_{3'} = 1 \frac{\pi_{\text{ref}}}{\pi_{\theta}}$ (the $k_{3'}$ in reward coefficient).

Once expressed as a detached coefficient $k_{n'}(x,y)$, the KL head is handled off-policy exactly like any other score-function head via Equation (70). In PPO with multiple epochs per batch, $k_{n'}$ should be recomputed at each epoch using the updated detached snapshot π_{θ} to maintain strict gradient equivalence (the denominator π_{θ_k} remains fixed from the rollout).

G.3 Two Principled Off-Policy Integration Strategies

With the correctly derived coefficient $k_{n'}$ in hand, there are two principled ways to integrate it into the PPO objective, mirroring the on-policy discussion in Section 4.

1. Combined Form (Single Clipped Head). Merge the reward advantage and the KL coefficient *before* applying the PPO machinery:

$$A_{\text{combined}}(x,y) := r(x,y) - \beta k_{n'} (\pi_{\theta}(y|x), \pi_{\text{ref}}(y|x)). \tag{72}$$

The clipped surrogate is then applied to this combined head:

$$\mathcal{J}_{\text{RLHF}}(\boldsymbol{\theta}) = \mathbb{E}_{y \sim \pi_{\theta_k}} \left[\min \left(\rho_k(\boldsymbol{\theta}) \, A_{\text{combined}}, \, \operatorname{clip}(\rho_k(\boldsymbol{\theta}), 1 - \epsilon, 1 + \epsilon) \, A_{\text{combined}} \right) \right]. \tag{73}$$

This is the most robust and straightforward approach, as IS and clipping are consistently applied to both components. For correct PPO semantics, form A_{combined} prior to any baseline subtraction or normalization. This preserves the trade-off set by β , which would be distorted by shifting or rescaling the KL component.

2. Decoupled Form (Two Clipped Heads). Maintain separate reward and KL objectives, each with its own IS correction and clipping scheme:

$$\mathcal{J}_{\text{reward}}(\boldsymbol{\theta}) = \mathbb{E}_{y \sim \pi_{\theta_k}} \left[\min \left(\rho_k(\boldsymbol{\theta}) \, r(x, y), \, \text{clip}(\rho_k(\boldsymbol{\theta}), \, 1 - \epsilon_1, \, 1 + \epsilon_2) \, r(x, y) \right) \right], \tag{74}$$

$$\mathcal{J}_{KL}(\boldsymbol{\theta}) = \mathbb{E}_{y \sim \pi_{\theta_k}} \left[\min \left(\rho_k(\boldsymbol{\theta}) k_{n'} \left(\pi_{\boldsymbol{\theta}}(y|x), \pi_{ref}(y|x) \right), \\ \operatorname{clip} \left(\rho_k(\boldsymbol{\theta}), 1 - \epsilon, 1 + \epsilon \right) k_{n'} \left(\pi_{\boldsymbol{\theta}}(y|x), \pi_{ref}(y|x) \right) \right) \right]. \tag{75}$$

The final objective to maximize is:

$$\mathcal{J}_{\text{RLHF}}(\theta) := \mathcal{J}_{\text{reward}}(\theta) - \beta \mathcal{J}_{\text{KL}}(\theta). \tag{76}$$

This decoupled design affords greater flexibility, such as using asymmetric clipping for the reward head (e.g., $\epsilon_2 > \epsilon_1$) to accelerate learning, while retaining conservative, symmetric clipping for the KL head to ensure stable regularization. Baselines or normalization should be applied only to A_{reward} , not to $k_{n'}(x,y)$, to avoid implicitly altering the regularization strength β .

Implementation Notes.

- Token vs. Sequence Level: Our derivations use sequence-level probabilities. In token-level PPO, it is often more stable to compute the ratio as $\rho_k = \exp\left(\sum_t \log \pi_{\theta}(y_t \mid \cdot) \sum_t \log \pi_{\theta_k}(y_t \mid \cdot)\right)$ and apply clipping at the sequence level; per-token clipping can be overly conservative.
- Masking Consistency: Sum log-probabilities only over action tokens that contribute to the reward/KL (exclude prompt, padding, or masked tokens) to keep ρ_k aligned with the heads being optimized.
- Numerical Stability and Support: Ensure $\pi_{\theta_k}(y \mid x) > 0$ for all sampled (x, y) and consider numerically capping ρ_k to prevent overflows under extreme ratios.
- Adaptive β : If targeting a desired KL via an adaptive schedule, update β outside the gradient path (detached) and avoid mixing it with advantage normalization; adaptation is orthogonal to IS/clipping and works for both combined and decoupled forms.

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Sign Convention. We present objectives for *maximization*. Implementations that *minimize* a loss should negate these expressions, e.g., by minimizing $-\mathcal{J}_{\text{combined}}$ or $-(\mathcal{J}_{\text{reward}} - \beta \mathcal{J}_{\text{KL}})$.

H VISUALIZATION OF KL REGULARIZATION GRADIENT COEFFICIENTS

To visualize the theoretical arguments discussed in Section 5, this section presents the Python code used to generate Figure 1. The plot compares the behavior of the different scalar coefficients that multiply the policy's score function $\nabla_{\theta} \log \pi_{\theta}(y|x)$, as a function of the actor's log-probability for a given token. These coefficients are derived from the respective KL regularization Loss: k_1 in reward, k_2 as loss, k_3 as loss, and the MiniMax-01 loss.

The visualization clearly contrasts the stable, linear behavior of the principled coefficients derived from ' k_1 in reward' / ' k_2 as loss' with the asymmetric behavior of the first-order approximate ' k_3 as loss'. The k_3 proxy's tendency to saturate for over-sampled tokens and explode for under-sampled ones, as argued in the main text. The following code, using 'matplotlib' and 'torch', generates the figure.

```
1150
    1 import torch
    2 import matplotlib.pyplot as plt
1152 3
1153 4 # --- Plotting Style ---
    5 plt.style.use('seaborn-v0_8-whitegrid')
    6 plt.rcParams.update({
1155
         "text.usetex": False, # Disable LaTeX rendering
1156 <sub>8</sub>
          "font.family": "serif", # Use a generic serif font
         "font.serif": ["Times New Roman"], # Specify Times New Roman as the
1157 9
             serif font
1158
       "font.size": 14,
"axes.labelsize": 16,
1159 10
    11
1160 <sub>12</sub>
         "legend.fontsize": 12,
1161 <sub>13</sub>
          "xtick.labelsize": 12,
1162 14
          "ytick.labelsize": 12,
1163 15 })
1164 16
    17 # --- Data Generation ---
1165 18 log_pi_actor = torch.linspace(-5, 0, steps=400)
1166 pi_actor = torch.exp(log_pi_actor)
1168 21 pi_ref_val = 0.25
1169 22 log_pi_ref = torch.log(torch.tensor(pi_ref_val))
1170
    24 # --- Coefficients Calculation ---
1171 25 coeff_k1_loss = torch.ones_like(log_pi_actor)
1172 26 coeff_k1_reward = log_pi_actor - log_pi_ref
1173 27 coeff_k3_loss = 1 - pi_ref_val / pi_actor
1174 28 coeff_minimax = pi_actor - pi_ref_val
1175 <sub>30</sub> # --- Plotting ---
1176 31 plt.figure(figsize=(10, 6.5))
1178 33 plt.plot(log_pi_actor, coeff_k1_reward,
1180 <sub>35</sub>
             color='#808000', linewidth=3, zorder=10)
1181 36
1182 37 plt.plot(log_pi_actor, coeff_k3_loss,
         label=r'\$1 - \pi_{\text{ref}}/\pi_{\text{theta}} (\$k_{3^{\rm prime}}) in
1183 38
               reward / $k_3$ as loss) - Biased Approximation',
1184
              color='Firebrick', linestyle='--', linewidth=2)
1185 <sub>40</sub>
1186 41 plt.plot(log_pi_actor, coeff_minimax,
color='RoyalBlue', linestyle='-.', linewidth=2)
```

```
1188
1189
    45 plt.plot(log_pi_actor, coeff_k1_loss,
               label=r'$1$ ($k_1$ as loss) - Zero Expected Gradient',
                color='Gray', linestyle=':', linewidth=2)
1191 47
1192 48
    49 plt.axvline(x=log_pi_ref.item(), color='black', linestyle='--', linewidth
1193
1194
                   label=r'$\log\pi_{\theta} = \log\pi_{\text{ref}}$')
1195 51
1196 52 plt.xlabel(r'Actor Log-Probability: $\log \pi_{\theta}(y|x)$')
1197 53 plt.ylabel(r'Coefficient of Score Function')
    54 plt.title(r'Comparison of KL Regularization Coefficients ($\pi_{\text{ref}}
           }=0.25)', fontsize=18)
1199 55 plt.legend(loc='upper left')
1200 56
1201 57 plt.ylim(-4, 4)
1202 58 plt.xlim(-5, 0)
1203
    60 plt.tight_layout()
1204
    61 plt.savefig('comparison_kl_regularization_coefficients.png', dpi=300,
          bbox_inches='tight')
1206 62 plt.show()
```

Listing 1: Python code to generate the comparison plot of KL gradient coefficients.

I ON THE STATISTICAL INSTABILITY OF THE k_3 VALUE ESTIMATOR

I.1 THE STRICT PRECONDITION FOR UNBIASEDNESS

An estimator is unbiased if its expectation equals the true value. For k_3 , the expectation is:

$$\mathbb{E}_q[k_3] = \mathbb{E}_q[\delta(x) - 1 - \log \delta(x)] = (\mathbb{E}_q[\delta(x)] - 1) + D_{KL}(q \parallel p) \tag{77}$$

For k_3 to be unbiased, it is necessary that $\mathbb{E}_q[\delta(x)] = 1$. This condition is met if p is absolutely continuous with respect to q ($p \ll q$), which means that the support of p must be contained within the support of q.

The condition of a finite KL divergence $(D_{KL}(q \parallel p) < \infty)$ is **not sufficient** to guarantee unbiasedness. For example, let q be the uniform distribution in [0,1] and p be the uniform distribution on [0,2].

- The KL divergence $D_{KL}(q \parallel p) = \int_0^1 1 \cdot \log(\frac{1}{0.5}) dx = \log 2$, which is finite.
- However, $\mathbb{E}_q[r(x)] = \int_0^1 1 \cdot \frac{p(x)}{q(x)} dx = \int_0^1 \frac{0.5}{1} dx = 0.5.$
- The estimator expectation is therefore $\mathbb{E}_q[k_3] = (0.5 1) + \log 2 = \log 2 0.5$, which is biased.

I.2 Infinite Variance and the Chi-Squared Divergence

The variance of k_3 is dominated by the second moment of the importance ratio, $\mathbb{E}_q[\delta(x)^2]$. This term is directly related to the Chi-squared divergence.

When $p \ll q$, the identity holds: $\chi^2(p \parallel q) = \mathbb{E}_q[(\delta(x)-1)^2] = \mathbb{E}_q[\delta(x)^2] - 1$. If p is not absolutely continuous with respect to q ($p \ll q$), $\chi^2(p \parallel q)$ is defined to be infinite.

Therefore, the variance of k_3 will be infinite if $\mathbb{E}_q[\delta(x)^2]$ is infinite. This occurs if $p \not\ll q$ or if $p \ll q$ but the tails of q are sufficiently lighter than the tails of p. While the divergence of $\mathbb{E}_q[\delta(x)^2]$ is the primary cause of instability, the finiteness of $\operatorname{Var}(k_3)$ also technically requires the finiteness of $\mathbb{E}_q[(\log \delta(x))^2]$.

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I.3 THE GAUSSIAN CASE AND AN EMPIRICAL DEMONSTRATION

For two Gaussian distributions, $p \sim \mathcal{N}(\mu_p, \sigma_p^2)$ and $q \sim \mathcal{N}(\mu_q, \sigma_q^2)$, the variance of k_3 is finite if and only if $\sigma_q^2 > \sigma_p^2/2$. This condition illustrates that the sampling distribution q must be sufficiently "wide" relative to the reference distribution p. This condition generalizes for multivariate Gaussians with covariance matrices Σ_p and Σ_q . The expectation $\mathbb{E}_q[r(x)^2]$ is calculated via an integral involving the ratio of two Gaussian probability densities. For this integral to converge (and thus for the variance to be finite), it is required that the matrix $2\Sigma_q - \Sigma_p$ be positive definite.

This failure mode is empirically illustrated below, where a narrow Gaussian q(x) ($\sigma_q = 0.2$) is used to estimate the KL divergence to a standard Gaussian p(x) ($\sigma_p = 1$). This configuration violates the condition, since $0.2^2 \ge 1^2/2$.

```
1254 1 import torch
1255 2 import torch.distributions as dist
1257 4 # p: reference distribution, q: sampling distribution
    5 p = dist.Normal(loc=0, scale=1)
1258
    6 q = dist.Normal(loc=0.1, scale=0.2) # A narrow distribution where Var[k3]
          is infinite
1260 7
1261 8 # Sample from the narrow distribution q
    y = q.sample(sample\_shape=(10\_000,))
1262
    # Ground truth KL divergence D_KL(q || p)
1264 12 true_kl = dist.kl_divergence(q, p)
1266 14 # Compute the log-ratio log(p(x)/q(x))
1267 15 log_r = p.log_prob(x) - q.log_prob(x)
    r = torch.exp(log_r)
1269 <sub>18</sub> # Define estimators
1270 	 19 	 k1 = -log_r
1271 \ 20 \ k2 = log_r.pow(2) / 2
1272 21 k3 = r - 1 - log_r
1273 \frac{22}{23} # --- Code to generate output ---
1274 24 print(f"True KL Divergence: {true_kl:.4f}\n")
1275 25 print ("Estimator | Sample Mean | Sample Std. Dev.")
1276 26 print ("-----")
1277 27 estimators = {"k1": k1, "k2": k2, "k3": k3}
1278 \frac{28}{29} for name, k in estimators.items():
1279 _{30} mean = k.mean()
1280 31
          std = k.std()
         print(f"{name:<17} | {mean:>13.4f} | {std:>16.4f}")
1281 32
    34 # --- Actual Output 1 ---
1283 35 True KL Divergence: 1.1344
1285 37 Estimator | Sample Mean | Sample Std. Dev.
1286 38 ------
1287 39 k1 | 1.1272 |

1287 40 k2 | 0.8742 |

1288 41 k3 | 0.8136 |
                                            0.6912
                                 0.8136 |
                                                    8.8244
1289 <sub>42</sub> # --- Actual Output 2 ---
1290 43 True KL Divergence: 1.1344
1291 44
1292 45 Estimator | Sample Mean | Sample Std. Dev.
    46 -----
1293 <sub>47</sub> k1
          1.1336 | 0.6611
| 0.8611 | 0.5210
| 0.6817 | 4.1082
1294 <sub>48</sub> k2
1295 49 k3
    50 # --- Actual Output 3 ---
```

Listing 2: Code illustrating the high variance of the k_3 value estimator when the sampling distribution q(x) is too narrow.

The results vividly illustrate the issue. The sample standard deviation of k_3 is **several times larger** than that of k_1 . And several repeated experiments show that the numerical instability of k_3 is obviously more severe than k_1 and k_2 . The large gap between the sample mean of k_3 and the true KL value is not estimator bias, but rather a large **sampling error**, which is characteristic of an estimator with immense or infinite variance. This demonstrates that an impractically large number of samples would be required for the estimate to converge reliably, making k_3 an unreliable choice in such scenarios.

J GROUP NORMALIZATION STABILITY ISSUES

GRPO performs per-prompt group normalization: for a prompt with G responses and rewards $\mathbf{r} = \{r_1, \dots, r_G\}$, the advantage is

$$A_i = \frac{r_i - \text{mean}_{\text{group}}(\mathbf{r})}{\text{std}_{\text{group}}(\mathbf{r})}.$$
 (78)

Stability issue. When the within-group variance is very small (e.g., $\mathbf{r}=[0.99999,\ 1.00001,\ 0.99999,\ 1.00001]$), normalization can dramatically amplify tiny numerical differences. For the above example, the resulting advantages become approximately $[-0.8660,\ 0.8660,\ -0.8660,\ 0.8660]$ (using the unbiased sample standard deviation), which destabilizes optimization by turning near-constant rewards into large-magnitude updates.

Proposed solution. Clip the standard deviation to prevent pathological amplification:

$$A_{i} = \frac{r_{i} - \operatorname{mean}_{\operatorname{group}}(\mathbf{r})}{\operatorname{clip_std}_{\operatorname{group}}(\mathbf{r})}, \quad \operatorname{clip_std}_{\operatorname{group}}(\mathbf{r}) = \max(\min(\operatorname{std}_{\operatorname{group}}(\mathbf{r}), \operatorname{std}_{\operatorname{max}}), \operatorname{std}_{\min}). \quad (79)$$

Here, $\mathrm{std}_{\min} > 0$ is a small floor that prevents exploding normalization when variance collapses, and std_{\max} avoids under-normalization when variance is unusually large. In practice, setting std_{\min} as a small constant relative to the reward scale (e.g., 10^{-1}) may be effective.

Why this matters beyond binary rewards. Although binary 0/1 rewards in RLVR can sometimes mitigate extreme cases, more general regression reward models—such as those trained with Bradley–Terry (BT) losses—often produce continuous scores that may become highly concentrated (e.g., near 0 or 1) on easy or very hard prompts. In such regimes, within-group standard deviations can be arbitrarily small even when rewards are bounded in [0,1], and group normalization will over-scale negligible differences unless a variance floor (or clipping) is used. Therefore, std clipping is important not only for numerical stability but also to avoid over-amplifying noise when reward predictions saturate.

Remark. For reward scores bounded in [0,1], $std(\mathbf{r}) < 1$ always holds, but it can be orders of magnitude smaller than 1 in practice; the smaller the variance, the stronger the amplification effect from group normalization. Clipping $std_{group}(\mathbf{r})$ preserves the intended scale-invariance when variance is moderate, while guarding against instability when variance collapses.

K LARGE SCALE EXPERIMENT

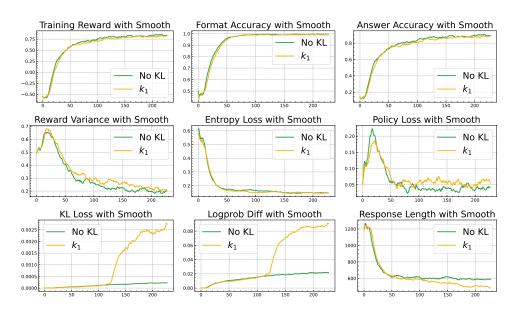


Figure 4: Comparison of " k_1 as loss" versus no KL regularization. The training dynamics are nearly indistinguishable, empirically confirming the theoretical prediction from Section 5: ' k_1 as loss' is ineffective as a KL regularizer due to its gradient's independence from the reference model and its zero-mean gradient expectation.

The empirical results on the larger 7B-scale model in Figure 4 further corroborate our theoretical analysis of ' k_1 as loss'. As derived in Section 5, the gradient of this loss term is fundamentally unsuitable for regularization: it is independent of the reference policy π_{ref} and has an expectation of exactly zero under on-policy sampling. In practice, this is equivalent to injecting a scaled score function, $\beta \cdot \nabla_{\theta} \log \pi_{\theta}$, which introduces zero mean but potentially high variance noise. Although the expected update direction remains unchanged, increased gradient variance can occasionally produce large deviations in a single update step. This phenomenon is clearly reflected in the experimental curves. As shown in the **KL Loss** and **Logprob Diff**, the actor model under ' k_1 as loss' not only fails to stay closer to the reference model but, in fact, drifts further away at later stages. The trajectories of both settings are initially aligned, but the ' k_1 as loss' variant suddenly diverges, indicating a sharp fluctuation induced by variance. Although the final task-level performance (e.g., reward/accuracy) remains broadly similar, achieving such results requires substantially higher KL magnitudes, which is ultimately inefficient and provides no meaningful regularization. In short, applying ' k_1 as a loss' on a larger model scale is not only ineffective, but also counterproductive, as it destabilizes training and weakens alignment with the reference model.

The empirical results on the 7B scale model in Figure 5 highlight the contrasting behaviors of ' k_2 as loss' and ' k_3 as loss'. Under the same coefficient, ' k_2 as loss' imposes a visibly stronger constraint: both the KL Loss and Logprob Diff curves remain consistently lower than those of ' k_3 as loss', indicating that the actor stays closer to the reference model. In contrast, ' k_3 as loss' tends to diverge more during training, as seen from higher KL magnitudes and larger log-probability differences. This divergence is further reflected in the response length, where k_3 produces shorter and more variable outputs, suggesting weaker control over generation. Although ' k_3 as loss' sometimes achieves higher Reward and Accuracy in the early and middle phases, this advantage comes at the cost of instability. The Reward Variance and Policy Loss under ' k_3 as loss' are substantially higher,

showing that its weaker constraint allows for larger fluctuations during optimization. In comparison, k_2 as loss' provides a more stable training trajectory, maintaining a lower variance and keeping the policy tightly aligned with the reference. These results imply that, on larger model scales, k_2 as loss' is the more effective choice for consistent and controlled regularization, while k_3 as loss' risks greater drift and instability despite temporary performance gains.

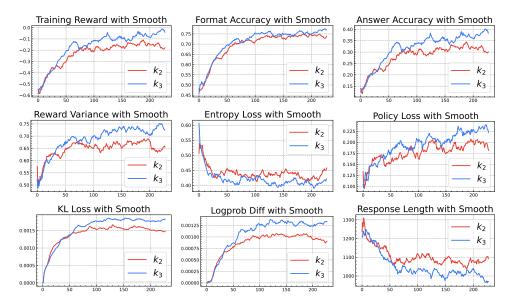


Figure 5: Comparison of the principled " k_2 as loss" against its first-order surrogate " k_3 as loss". Both variants effectively constrain the policy, but ' k_2 as loss' demonstrates superior regularization properties, maintaining a tighter coupling to the reference policy and yielding a more stable optimization path, evidenced by lower reward variance.

L DOWNSTREAM BENCHMARK PERFORMANCE

The main results on the math and general reasoning benchmarks are summarized in table 2. Several consistent patterns emerge across the 7B and 1.5B models.

First, the setting with k_1 as loss' does not provide a significant benefit of regularization. This aligns with our theoretical analysis, which suggests that the expected gradient vanishes, thereby failing to constrain the actor with respect to the reference model. Empirically, its performance remains very close to the baseline 'RL without KL' in both mathematical and general domain tasks, demonstrating that k_1 as loss' is ineffective as a regularizer.

Second, under the same coefficient, the behaviors of k_2 as loss' and k_3 as loss' diverge significantly. The k_2 as loss enforces a much tighter constraint on the actor: the model remains closer to the reference policy, but this tighter coupling comes at the cost of substantially degraded performance, as reflected in both math reasoning (e.g., AIME (Li et al., 2024), AMC (Li et al., 2024), MATH-500 (Hendrycks et al., 2021)) and general reasoning benchmarks (e.g., ARC-c (Clark et al., 2018), GPQA* (Rein et al., 2024), MMLU-Pro (Wang et al., 2024)). In contrast, k_3 as loss' imposes a weaker constraint and allows the model to drift more, as also observed in training dynamics (higher KL and log-prob differences). Although k_3 as loss' appears slightly better than k_2 as loss' in the final benchmark scores, its more divergent behavior highlights the lack of effective regularization and greater instability.

Taken together, these results confirm our theoretical expectations: k_1 as loss' does not act as a constraint; k_2 as loss' imposes stronger and rigid regularization that suppresses overall performance; and k_3 as loss', though less restrictive, allows excessive divergence, may leads to unstable training.

Table 2: Main experiment results on math and general reasoning benchmarks based on **Qwen2.5-Math-7B** and **Qwen2.5-Math-1.5B**.

Model	Math Reasoning Performance						General Domain Reasoning Performance			
	AIME 24/25	AMC	MATH-500	Minerva	Olympiad	Avg.	ARC-c	GPQA*	MMLU-Pro	Avg.
Qwen2.5-Math-7B	11.5/4.9	31.3	43.6	7.4	15.6	19.0	18.2	11.1	16.9	15.4
RL w/o KL	20.5/14.4	55.6	78.6	36.8	42.4	41.4	81.7	33.8	46.9	54.1
RL w/. $k1$ as loss	19.1/11.6	56.0	80.6	40.8	43.0	41.8	79.7	29.8	45.1	51.5
RL w/. $k2$ as loss	15.4/7.5	48.5	64.2	16.9	24.9	29.6	31.3	15.2	27.1	24.5
RL w/. $k3$ as loss	19.0/7.3	48.9	65.4	18.8	29.0	31.4	29.6	19.2	27.7	25.5
Qwen2.5-Math-1.5B	7.2/3.6	26.4	28.0	9.6	21.2	16.0	3.5	4.0	2.5	3.3
RL w/o KL	12.5/4.8	43.7	66.8	28.3	31.9	31.3	43.7	19.2	23.1	28.7
RL w/. $k1$ as loss	13.8/4.7	41.5	68.0	25.7	31.9	30.9	36.6	18.2	21.0	25.3
RL w/. $k2$ as loss	7.0/5.5	35.2	52.8	14.7	29.0	24.0	7.8	7.6	4.9	6.8
RL w/. $k3$ as loss	7.7/3.8	34.9	54.2	15.8	28.0	24.1	11.3	8.1	5.5	8.3

M STATEMENT ON THE USE OF LARGE LANGUAGE MODELS

We used LLMs solely for language polishing and editing. All retrieval of related work, algorithmic design, and theoretical derivations are carried out by the authors.

N IMPACT

Our " k_2 as loss" formulation has been merged into OpenRLHF and has been adopted and cited by Reinforce++. Prorl also integrates it with periodic resetting of the reference model. By providing a gradient-correct, off-policy-ready treatment of KL regularization, our work clarifies long-standing ambiguities and offers practical guidance for building stable, effective, and reproducible RLHF systems. We anticipate that these contributions will enable the community to design more reliable training pipelines and make significant advances in the field.