
$Q\sharp$: Provably Optimal Distributional RL for LLM Post-Training

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Abstract

Reinforcement learning (RL) post-training is crucial for LLM alignment and reasoning, but existing policy-based methods, such as PPO and DPO, can fall short of fixing shortcuts inherited from pre-training. In this work, we introduce $Q\sharp$, a value-based algorithm for KL-regularized RL that guides the reference policy using the optimal regularized Q function. We propose to learn the optimal Q function using distributional RL on an aggregated online dataset. Unlike prior value-based baselines that guide the model using unregularized Q -values, our method is theoretically principled and provably learns the optimal policy for the KL-regularized RL problem. Empirically, $Q\sharp$ outperforms prior baselines in math reasoning benchmarks while maintaining a smaller KL divergence to the reference policy. Theoretically, we establish a reduction from KL-regularized RL to no-regret online learning, providing the first bounds for deterministic MDPs under only realizability. Thanks to distributional RL, our bounds are also variance-dependent and converge faster when the reference policy has small variance. In sum, our results highlight $Q\sharp$ as an effective approach for post-training LLMs, offering both improved performance and theoretical guarantees. The code can be found at https://github.com/jinpz/q_sharp.

1 Introduction

Reinforcement learning (RL) post-training is a crucial step in training large language models (LLMs), aligning their generations with human preferences [1] and enhancing their reasoning capabilities [2, 3]. This stage typically follows supervised learning (next-token prediction), where the model is further trained to maximize expected cumulative reward while minimizing KL divergence from the reference policy π^{ref} obtained via supervised learning. The KL penalty plays a critical role by keeping the model close to π^{ref} , mitigating issues such as reward hacking and catastrophic forgetting.

Most state-of-the-art LLMs [4, 5, 6] are post-trained using *policy-based* RL methods, which update model weights via stochastic gradient descent using algorithms like RLOO [7], PPO [8], and DPO [9]. However, these methods are computationally expensive, requiring full backpropagation through the LLM during training. In this paper, we propose a more efficient alternative: a *value-based* RL approach that guides the generations of the reference policy π^{ref} using a learned value function, without modifying π^{ref} model weights. This approach is particularly attractive because, for many tasks, evaluating generations is easier than producing them [4, 10], suggesting we can use much smaller models to learn value functions for guidance. For instance, in our experiments (Section 3.2), we show that a 1B parameter value model can effectively steer and improve a 70B parameter LLM.

Existing value-based methods for LLM post-training, such as CD [11] and VAS [12], fall short of faithfully optimizing the KL-constrained RL objective. These approaches guide π^{ref} using $Q^{\pi^{\text{ref}}}$ —the

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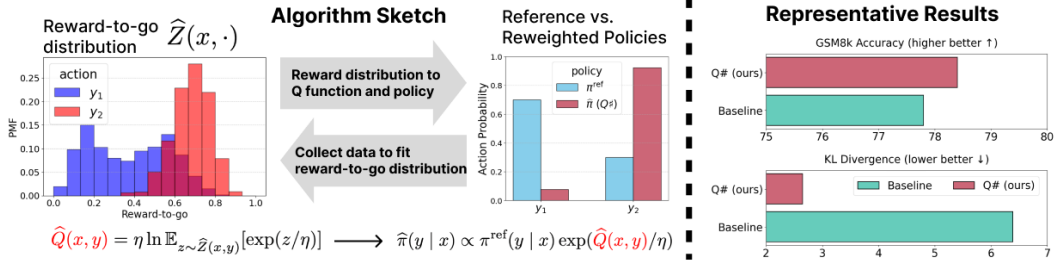


Figure 1: (Left) A sketch of our post-training algorithm ($Q^\#$) based on distributional RL. $Q^\#$ alternates between learning Z^* – the reward-to-go distribution of π^{ref} – and using the induced policy to collect new data and further improve the distributional estimate. (Right) Evaluation result on the GSM8K dataset [19]. We see that $Q^\#$ achieves both higher accuracy and lower KL compared to prior value-based post-training algorithms [11, 12].

expected reward-to-go under π^{ref} without KL regularization—which does not guarantee convergence to the optimal policy $\pi^{*,\eta}$. In contrast, under the classical KL-regularized RL framework, we show that it is provably optimal to guide π^{ref} using $Q^{*,\eta}$, the expected reward-to-go under the optimal policy $\pi^{*,\eta}$, which accounts for KL regularization. This theoretical insight ensures convergence to $\pi^{*,\eta}$ and addresses the shortcomings of previous methods. As we demonstrate empirically and theoretically, prior approaches can lead to suboptimal rewards or large KL divergence—issues that our algorithm, $Q^\#$, provably avoids.

Our method exploits special properties of $Q^{*,\eta}$ in deterministic MDPs and iteratively trains a model to estimate it through supervised distributional learning such as MLE. The iterative training procedure is motivated by the classic imitation learning algorithm DAgger [13], which addresses covariate shift and ensures that the learned $Q^{*,\eta}$ estimator remains accurate when used to guide π^{ref} at inference time. This distributional learning approach not only enhances empirical performance but also enables second-order style regret bounds - instance-dependent bounds that adapt to the variance of the model’s generation.

$Q^\#$ differs from traditional RL methods in two key aspects. First, we avoid complex temporal difference (TD) learning [14] or Q-learning techniques [15, 16], instead relying on direct supervised learning of a fixed critic. Second, while we adopt a distributional perspective, $Q^\#$ is conceptually simpler than classical distributional RL algorithms like C51 [17]: we directly learn outcome distributions via supervised maximum likelihood, without invoking distributional Bellman updates. We elaborate on this and related works in Appendix A. In summary, our contributions are as follows:

1. We propose $Q^\#$, a principled algorithm for KL-regularized RL in deterministic MDPs, which includes LLMs, based on guiding π^{ref} with the soft Q^* learned with *distributional RL* (Section 2.2).
2. We prove variance-dependent PAC bounds for convergence to the optimal policy, which only requires realizability in the function class (Section 4).
3. We show that value-based post-training, which includes $Q^\#$, can fix biases and shortcuts in a star-graph environment [18], while popular policy-based methods cannot (Section 3.1).
4. We provide extensive experiments on math reasoning tasks that validate the effectiveness of our method at maximizing reward while maintaining small KL deviations from the reference policy (Section 3.2).

2 Method

2.1 Preliminaries

We study KL-regularized reinforcement learning (RL) in deterministic Markov Decision Processes (MDPs), where large language model (LLM) post-training is a motivating special case. An MDP is defined by a state space $\mathcal{X}$, action space $\mathcal{Y}$, horizon H , transition kernels $(P_1, \dots, P_H)$ with $P_h : \mathcal{X} \times \mathcal{Y} \mapsto \Delta(\mathcal{X})$, and known reward functions $(r_1, \dots, r_H)$ where $r_h : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$. A policy $\pi = (\pi_1, \dots, \pi_H)$ consists of decision rules $\pi_h : \mathcal{X} \rightarrow \Delta(\mathcal{Y})$. For a given $\eta > 0$, the KL-regularized

value of a policy π is defined as

$$V^{\pi, \eta} := \mathbb{E}_{\pi} \left[\sum_{h=1}^H r_h(x_h, y_h) - \eta \text{KL}(\pi_h(x_h) \parallel \pi_h^{\text{ref}}(x_h)) \right]. \quad (1)$$

A classical result shows that KL-regularized RL can be solved via soft Bellman equations [20]. Starting from $h = H$ and proceeding backward, we define:

$$\begin{aligned} V_{H+1}^{\star, \eta}(x) &= 0, & Q_h^{\star, \eta}(x, y) &= r_h(x, y) + \mathbb{E}_{x' \sim P_h(x, y)} [V_{h+1}^{\star, \eta}(x')], \\ \pi_h^{\star, \eta}(y \mid x) &\propto \pi_h^{\text{ref}}(y \mid x) \exp(\eta^{-1} Q_h^{\star, \eta}(x, y)), & V_h^{\star, \eta}(x) &= \eta \ln \mathbb{E}_{y \sim \pi_h^{\text{ref}}(x)} \exp(\eta^{-1} Q_h^{\star, \eta}(x, y)). \end{aligned} \quad (2)$$

This expresses the optimal policy as a softmax over $Q_h^{\star, \eta}$, weighted by π_h^{ref} . Moreover, $Q_h^{\star, \eta}(x, y)$ is the maximal expected KL-regularized return starting from (x, y) at time h . We now focus on deterministic MDPs, which covers LLM post-training and other structured generation tasks such as diffusion models [21].

Assumption 2.1. The transitions P_h are deterministic.

Under this assumption, the value function simplifies significantly:

$$\begin{aligned} \exp(\eta^{-1} V_h^{\star, \eta}(x)) &= \mathbb{E}_{y \sim \pi_h^{\text{ref}}(x)} [\exp(\eta^{-1} r_h(x, y) + \eta^{-1} V_{h+1}^{\star, \eta}(x'))] \\ &= \mathbb{E}_{\pi^{\text{ref}}} [\exp(\eta^{-1} \sum_{t \geq h} r_t(x_t, y_t)) \mid x_h = x], \end{aligned} \quad (3)$$

$$= \mathbb{E}_{\pi^{\text{ref}}} [\exp(\eta^{-1} \sum_{t \geq h} r_t(x_t, y_t)) \mid x_h = x], \quad (4)$$

where Equation (3) is due to the determinism of P_h , while Equation (4) follows by recursively unrolling until the final step. Note that although $V_h^{\star, \eta}(x_h)$ corresponds to the soft value of the optimal policy, its recursion is expressed via expectations over π^{ref} . We summarize this in the following known result [22, 23, 21]:

Theorem 2.2. Under Assumption 2.1, we have $V_h^{\star, \eta}(x_h) = \eta \ln \mathbb{E}_{\pi^{\text{ref}}} [\exp(\eta^{-1} \sum_{t \geq h} r_t(x_t, y_t)) \mid x_h]$ and $Q_h^{\star, \eta}(x_h, y_h) = \eta \ln \mathbb{E}_{\pi^{\text{ref}}} [\exp(\eta^{-1} \sum_{t \geq h} r_t(x_t, y_t)) \mid x_h, y_h]$.

This shows $V^{\star, \eta}$ and $Q^{\star, \eta}$ are simple functionals of Z^* – the cumulative reward distribution of π^{ref} – where the functional is $f(P) = \eta \ln \mathbb{E}_P \exp(X/\eta)$. In other words, if we learn the cumulative reward distribution of π^{ref} , then we can directly compute $V^{\star, \eta}$ and $Q^{\star, \eta}$, without any dynamic programming.

This offers several benefits. First, we do not require temporal difference (TD) learning (*i.e.*, bootstrapping) which is notoriously unstable with deep networks [24] and requires completeness-type assumptions to guarantee convergence in theory [25]. Second, fitting the reward-to-go distribution Z^* or regressing $\mathbb{E}_{\pi^{\text{ref}}} [\exp(\eta^{-1} \sum_{t \geq h} r_t)]$ is a standard supervised learning task with a fixed target, which is much more stable in practice and well-understood in theory. Notably, there is no bootstrapping or changing targets which is what renders deep RL fragile. Third, we can apply distributional RL methods, where we directly fit the distribution Z^* via supervised learning (*e.g.*, maximum likelihood). Importantly, our approach *does not* involve distributional Bellman equation nor distributional TD update, which are known to be non-contractive under certain metrics [17]. Prior work has shown that fitting Z^* in this manner yields benefits in representation learning [17, 26], lower variance updates [27], and second-order bounds [28, 29].

Applicability to LLMs. Our deterministic MDP framework directly models LLM post-training as a special case [4]. The initial state x_1 corresponds to the input prompt, each intermediate state x_h is the current generation prefix, and the action y_h is the next token. The policy thus reflects the LLM’s autoregressive decoding process. The transition function is deterministic: $P_h(x_h, y_h) = x_h y_h$, which simply appends the new token to the prefix. In many post-training settings, the reward is sparse, meaning only r_H is nonzero. Under this assumption, Theorem 2.2 simplifies to $Q_h^{\star, \eta}(x_h, y_h) = \eta \ln \mathbb{E}_{\pi^{\text{ref}}} [\exp(\eta^{-1} r(x_H, y_H)) \mid x_h, y_h]$. For example, the reward may indicate solution correctness in math tasks or reflect user preference in dialogue, as determined by a learned reward model.

Inference with cumulative reward distribution. Let Z^* denote the conditional distribution over cumulative rewards under rollouts from π^{ref} , that is, $Z_h^*(x, y) \stackrel{D}{=} \sum_{t \geq h} r_t(x_t, y_t) \mid x_h = x, y_h = y$, where the trajectory $(x_h, y_h, \dots, x_H, y_H)$ is sampled under π^{ref} , and $\stackrel{D}{=}$ denotes equality in distribution. Combining Theorem 2.2 and Equation (2), the optimal policy can be rewritten in terms

of Z^* as $\pi_h^{*,\eta}(y | x) \propto \pi_h^{\text{ref}}(y | x) \mathbb{E}_{z \sim Z_h^*(x,y)}[\exp(z/\eta)]$. This motivates defining a general family of policies induced by any distribution $Z : \mathcal{X} \times \mathcal{Y} \rightarrow \Delta(\mathbb{R})$ via

$$\pi_h^{Z,\eta}(y | x) \propto \pi_h^{\text{ref}}(y | x) \mathbb{E}_{z \sim Z_h(x,y)}[\exp(z/\eta)]. \quad (5)$$

Since $\pi^{*,\eta} = \pi^{Z^*,\eta}$, we can approximate the optimal policy by estimating Z^* with $\hat{Z} \approx Z^*$ using distributional learning techniques such as maximum likelihood estimation (MLE), and then instantiating $\pi^{Z,\eta}$. This forms the core of our proposed $Q^\sharp$ algorithm.

2.2 Algorithm $Q^\sharp$

We propose Q-Sharp ($Q^\sharp$), a distributional value-based algorithm for KL-regularized RL in deterministic MDPs. $Q^\sharp$ iteratively collects data from progressively improved policies to approximate the target distribution Z^* (Algorithm 1). In this section, we describe $Q^\sharp$ in practical terms for deep neural networks and LLMs; in Section 4, we formalize it using online learning oracles and prove convergence under a mild realizability assumption.

Algorithm 1 $Q^\sharp$

- 1: **Input:** reference policy π^{ref} .
- 2: Initialize parameters θ^1 of conditional distribution $Z^\theta : \mathcal{X} \times \mathcal{Y} \rightarrow \Delta(\mathbb{R})$ and dataset $\mathcal{D}_h = \emptyset$ for all h .
- 3: **for** $k = 1, 2, \dots$ **until** convergence **do**
- 4: Let $\pi^k \leftarrow \pi^{Z_{\theta^k}, \eta}$ be policy induced by Z_{θ^k} (using Equation (5)).
- 5: **for** $i = 1, 2, \dots, N$ **do**
- 6: Sample a switching time $h \sim [H]$.
- 7: Roll-in with π^k for $h - 1$ steps.
- 8: Resume trajectory with π^{ref} from x_h .
- 9: Let R_t denote cumulative rewards after time t .
- 10: Add (x_t, y_t, R_t) to $\mathcal{D}_t, \forall t \geq h$.
- 11: **end for**
- 12: Update θ^k by minimizing the distributional loss on the aggregated data:

$$\theta^{k+1} \leftarrow \arg \min_{\theta} \sum_h \mathbb{E}_{\mathcal{D}_h} [\mathcal{L}(R_h, Z^\theta(x_h, y_h))].$$
- 13: **end for**
- 14: **Output:** Final θ^k .

Let $Z_h^\theta : \mathcal{X} \times \mathcal{Y} \rightarrow \Delta(\mathbb{R})$ denote a parametric conditional distribution with parameters θ . Given a sample $R \in \mathbb{R}$ (e.g., drawn from Z^*) and a model prediction $\hat{Z}$, let $L(R, \hat{Z})$ be a distributional loss for training the model. We denote by θ^* the parameter that minimizes the distance between Z^* and Z^θ . For example, if $Z_h^*(x, y)$ is $\text{Ber}(p_h^*(x, y))$, we can parameterize $Z_h^\theta(x, y)$ by a neural network that outputs a scalar estimate $\hat{p}$ of $p_h^*(x, y)$. The natural loss in this case is binary cross-entropy (BCE): $L_{\text{bce}}(r, \hat{p}) = -r \ln \hat{p} - (1 - r) \ln(1 - \hat{p})$. This binary setup is appropriate for tasks such as math or multiple-choice questions where the reward is binary. If the reward distribution has no known parametric form, one can use a non-parametric model (e.g., a histogram that discretizes the reward space) trained via maximum likelihood (MLE) [17]: $L_{\text{mle}}(r, \hat{z}) = -\ln \hat{z}[\text{idx}(r)]$, where $\text{idx}(r)$ returns the index of the bin containing r , and $\hat{z}[i]$ denotes the probability estimate for bin i . In general, $Q^\sharp$ can incorporate any distributional RL loss function [30]. Once Z^θ closely approximates

Z^* , we instantiate a near-optimal policy $\pi^{\theta,\eta}$ via Equation (5). In Section 4, we prove that this procedure converges to the optimal policy under a mild realizability assumption.

Then, the key idea of $Q^\sharp$ is an iterative data-collection and update process. At iteration k , with current parameters θ^k , we deploy the induced policy $\pi^k := \pi^{Z_{\theta^k}, \eta}$ to gather new data. Specifically, we roll in with π^k for $h - 1$ steps to reach a state x_h , then switch to π^{ref} to complete the trajectory. The cumulative reward from step h to the end, denoted $R_{h,k}$, is a sample from $Z_h^*(x_h)$. We add these samples to the dataset and update θ via gradient descent on the distributional loss. This process repeats until convergence.

Our iterative approach is similar in spirit to DAgger [13], AggreVaTe [31, 32], and RLGF [33], which likewise mitigate distribution shift to ensure the learned estimator remains accurate at test time. In contrast, prior value-based methods such as CD [11] and entropy-regularized PRM [34] train their estimators only on data from π^{ref} . While such an estimator may perform well on π^{ref} 's distribution, it offers no guarantee of accuracy when used to steer π^{ref} 's generation at inference time.

Comparison with CD and VAS. The most closely related value-based baselines are CD [11] and VAS [12], yet they exhibit three critical limitations. (i) Incorrect value target. Both methods re-weight π^{ref} using $Q^{\pi^{\text{ref}}, 0}$ —the *unregularized* Q -function of π^{ref} —thereby ignoring the KL term. As shown in Section 4, this choice can yield policies that are either sub-optimal in reward or far from π^{ref} . $Q^\sharp$

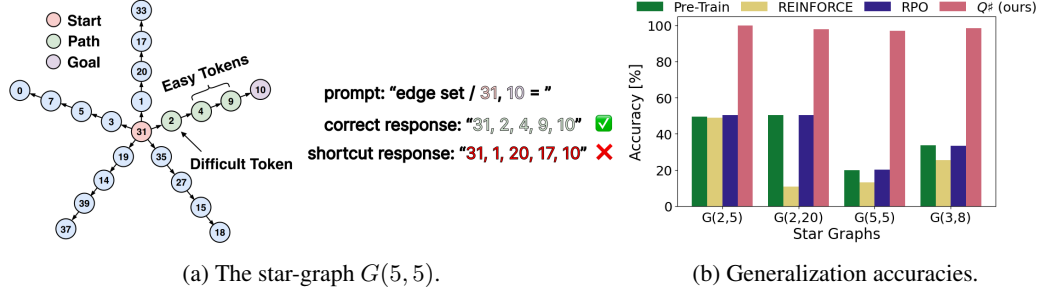


Figure 2: (a) The star-graph with degree $d = 5$ and path length $\ell = 5$. Next-token prediction, the standard pre-training loss, learns a sub-optimal shortcut that selects a random first node and follows it until the end. (b) Accuracies on held-out test graphs for various models. Policy-based post-training methods such as REINFORCE and RPO (a variant of DPO) still exhibit the shortcut and has test accuracy $1/d$, while our value-based $Q^\#$ fixes the shortcut and achieves near-perfect accuracy.

instead employs the principled target $Q^{*,\eta}$ and is guaranteed to converge to $\pi^{*,\eta}$ under realizability. (ii) Offline training. CD and VAS fit their value functions on a fixed dataset, whereas $Q^\#$ alternates data collection and updates, improving robustness to distribution shift [13, 31]. (iii) Squared-loss regression. Both baselines learn $Q^{\pi^{\text{ref}},0}$ with an ℓ_2 loss, implicitly assuming homoskedastic Gaussian rewards. $Q^\#$ leverages distributional RL losses, which are theoretically more sample-efficient [35, 29] and empirically superior [17, 26].

Relation to actor-critic methods. Although $Q^\#$ learns a value function, its target $V^{*,\eta}$ (or $Q^{*,\eta}$) is *fixed* throughout training. Standard actor-critic algorithms (e.g., PPO) continuously update V^π or Q^π as π evolves, and rely on bootstrap-based TD updates. In contrast, $Q^\#$ trains the value network via distributional supervised learning (e.g., MLE), thereby avoiding the instability of changing targets.

Relation to DPO [9]. While the form of Equation 5 resembles DPO’s policy expression, their derivations and scopes are fundamentally different. DPO begins from the same KL-regularized RL objective but, without exploiting the deterministic transition structure, operates at the **sequence level**, corresponding to the **one-step case** ($H = 1$). Its policy is given by $\pi_r(y | x) = \frac{1}{Z(x)} \pi^{\text{ref}}(y | x) \exp\left(\frac{1}{\beta} r(x, y)\right)$, where y denotes a full completion and $Z(x)$ is the partition function over all possible sequences. When $H = 1$, our Q^* reduces to the reward r , and the DPO expression naturally follows as a special case. However, the DPO partition function $Z(x)$ is intractable to normalize, and practical implementations must rely on pairwise preference data (e.g., Bradley-Terry modeling) to bypass it.

Inference with multiple η . Because the learned distribution $\hat{Z}^\theta$ is independent of η , a single trained network can support any choice of η at inference time simply by plugging it into Equation (5).

3 Experiments

3.1 Star-Graph

We begin with the star-graph task from [18], illustrated in Figure 2(a). A star-graph $G(d, \ell)$ has d paths of length ℓ from a central node. Given a start/goal node and the graph edges, the LM must generate a valid path. Though seemingly simple, [18] showed that next-token pre-training often learns a faulty shortcut: the model picks the first node at random (correct with probability $1/d$) and follows the path, yielding a test accuracy of only $1/d$. This highlights the limitations of next-token prediction on planning tasks. [36] also showed that the task embeds the "sparse parity" problem — determining whether the sum of a binary string is even or odd — which is known to be difficult for gradient-based optimizers and is widely studied in learning theory and optimization [37, 38, 39, 40].

Can this shortcut be fixed during post-training? We evaluate REINFORCE [41], DPO [9], RPO [42], and $Q^\#$, reporting test accuracies in Figure 2 (b). $Q^\#$ consistently corrects the shortcut, achieving near-perfect accuracy, even for long paths ($G(2, 20)$) or large degrees ($G(5, 5)$). CD [11] achieves similar performance as $Q^\#$. In contrast, policy-based methods like REINFORCE and RPO fail to

Table 1: Comparison of $Q_{\#}$ with π^{ref} and CD baseline on GSM8K (Left) and MATH (Right). For both Llama 3 and Llama 3.1 8B, $Q_{\#}$ consistently improves both pass@1 and majority voting accuracy upon baselines while incurring minimal KL deviation.

π^{ref}							π^{ref}						
Llama 3 8B							Llama 3 8B						
Methods	π^{ref}	CD	$Q_{\#}$	π^{ref}	CD	$Q_{\#}$	Methods	π^{ref}	CD	$Q_{\#}$	π^{ref}	CD	$Q_{\#}$
pass@1 $\uparrow$	69.1	77.8	78.4	82.9	84.5	85.1	pass@1 $\uparrow$	25.4	24.9	27.1	43.9	45.3	46.7
maj1@8 $\uparrow$	85.8	87.2	88.1	90.5	90.9	91.4	maj1@8 $\uparrow$	34.3	34.3	37.9	57.0	59.0	60.1
KL-Divergence $\downarrow$	-	6.39	2.65	-	7.43	3.67	KL-Divergence $\downarrow$	-	15.27	7.14	-	26.8	8.69

fix the shortcut, plateauing at $1/d$ accuracy. DPO performs worst, often collapsing the policy to zero accuracy by suppressing both chosen and rejected paths—a failure mode also noted by RPO. These results suggest that once shortcuts are learned, policy-based methods struggle to unlearn them, reinforcing the effectiveness of value-based approaches like $Q_{\#}$ and CD for LLM post-training. Please see Appendix C for a more detailed discussion on why REINFORCE and RPO cannot fix shortcuts and implementation details.

3.2 Math Reasoning

Datasets. We evaluate on two mathematical reasoning benchmarks: GSM8K [19], a dataset of grade school arithmetic word problems, and MATH [43], which features more challenging high school competition problems. We split each training set 90%-10% for training and validation. Test performance is reported on the full GSM8K test set and a 500-sample subset of MATH (MATH-500), following prior work [44, 45]. In Appendix G, we also evaluate $Q_{\#}$ on AIME-24 dataset.

Models. We experiment with Llama 3 [5] and Qwen 2.5 [46] model families, both of which are competitive on math reasoning tasks and span a wide range of parameter scales. Due to space constraints, we report results for Llama 3 in the main text and defer Qwen 2.5 results to Appendix G. Unless otherwise noted, the $Q^{*,\eta}$ function in $Q_{\#}$ is parameterized and initialized with a Llama 3.2 1B model, and we use $\eta = 0.1$, which yields consistent and strong performance. We run $Q_{\#}$ for two iterations, after which performance converges. Additional details on model configurations and $Q_{\#}$ training are provided in Appendices D and E.

Evaluation metrics. We report *single sample* accuracy (pass@1) and *majority voting* accuracy (maj1@k). pass@1 evaluates one sampled generation per problem against the ground truth, while maj1@k checks if the most frequent answer among k samples is correct. We use $k = 8$, temperature $T = 0.8$, and nucleus sampling $p = 0.9$. The evaluation prompt template is provided in Appendix F.

Main results. Table 1 presents $Q_{\#}$ performance on GSM8K (Left) and MATH (Right) with π^{ref} as Llama 3 or 3.1 8B. Although both have 8B parameters, Llama 3.1 performs significantly better. Across all settings, $Q_{\#}$ consistently improves over π^{ref} , boosting pass@1 by up to 9% on GSM8K with just 1B additional parameters. We also compare against the CD baseline [11], which incorrectly uses $Q^{\pi^{\text{ref}},0}$ to guide π^{ref} . $Q_{\#}$ outperforms CD on both accuracy metrics while maintaining lower KL divergence. Overall, $Q_{\#}$ Pareto-dominates CD in the KL-regularized RL setting by achieving higher reward and lower KL. We note that CD [11] and VAS [12] are concurrent work and differ only in minor aspects such as sampling strategy. Therefore, we use CD as a canonical baseline for empirical comparison. Since $Q_{\#}$ is complementary to policy-based methods, we further evaluate its effectiveness when guiding a PPO-trained model, as shown in Appendix I.

Larger π^{ref} and $Q_{\#}$ sizes. We evaluate how performance scales with larger π^{ref} and $Q_{\#}$ models on MATH (Table 2). Using 70B Llama 3 and 3.1 as π^{ref} significantly boosts baseline pass@1 (45.6% and 60.6%, respectively). Remarkably, a 1B $Q_{\#}$ still improves these large models—e.g., by 2.5% pass@1 and 3.5% maj1@8 for Llama 3.1. Increasing $Q_{\#}$ to 3B yields further gains, demonstrating scalability. Compared to Table 1 (right), we note that with 9B total parameters (8B π^{ref} + 1B $Q_{\#}$), the maj1@8 accuracy already matches the pass@1 of the 70B π^{ref} in Table 2, suggesting a promising low-resource alternative. For Llama 3, pass@1 improves while maj1@8 slightly drops, likely due to increased generation diversity benefiting harder problems but reducing consistency on easier ones.

$Q_{\#}$ as a reward model. Beyond guiding π^{ref} generation, $Q_{\#}$ ’s token-level Q function can also assess how good a complete generation is among many. We compute $Q(\text{generation}, \text{EOS})$ by applying $Q_{\#}$ as a reward model ($Q_{\#}$ -RM) on GSM8K and MATH, using both π^{ref} and $Q_{\#}$ generations. Table 3 reports two settings: $Q_{\#}$ -RM Best of 8 (selects top-scoring sample) and $Q_{\#}$ -RM maj1@8 (aggregates

Table 2: Performance of π^{ref} and $Q_{\#}$ on MATH with larger π^{ref} and $Q_{\#}$ model sizes. $Q_{\#}$ of size 1B is capable of guiding a 70B π^{ref} model. Increasing $Q_{\#}$ model sizes to 3B also leads to noticeably better performance for Llama 3.1 70B.

π^{ref}	Llama 3 70B			Llama 3.1 70B		
$Q_{\#}$ Model	None	Llama 3.2 1B	Llama 3.2 3B	None	Llama 3.2 1B	Llama 3.2 3B
pass@1 $\uparrow$	45.6	46.4	46.7	60.6	63.1	64.1
maj1@8 $\uparrow$	55.6	55.5	55.3	69.0	72.5	72.7
KL-Divergence $\downarrow$	-	3.12	5.15	-	4.98	4.99

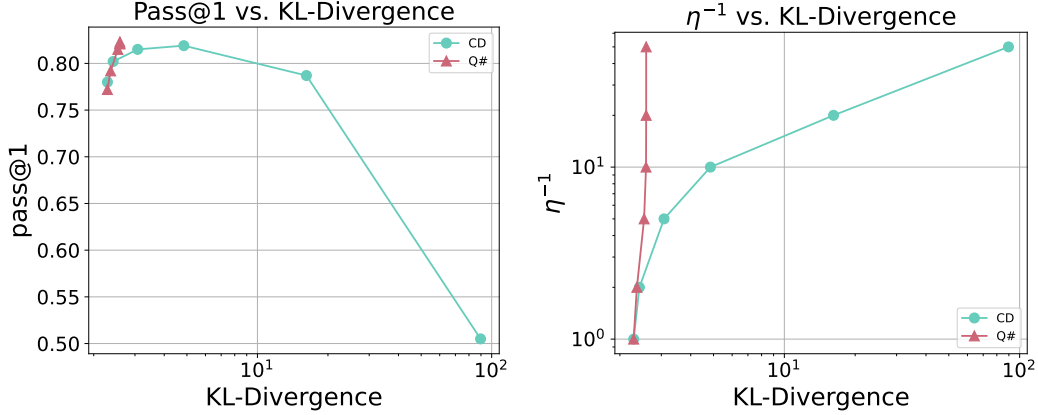


Figure 3: Performance tradeoff between CD and $Q_{\#}$ on the GSM8K validation set. **(Left)** pass@1 vs. KL divergence: $Q_{\#}$ outperforms CD with higher accuracy and lower KL. **(Right)** KL divergence across η : CD’s KL increases rapidly and deviates from π^{ref} , while $Q_{\#}$ remains stable.

majority voting with scores). $Q_{\#}$ -RM maj1@8 consistently improves over vanilla maj1@8, and Best of 8 yields more than 10% gains over pass@1 for π^{ref} . The reward model can be used on both π^{ref} and $Q_{\#}$ own generations to further improve performance, which suggests the (same) reward model has generalizability for evaluating diverse generations.

Effect of η . Figure 3 shows the performance–KL tradeoff between CD and $Q_{\#}$ on the GSM8K validation set. **(Left)** Increasing KL can improve pass@1 for both methods, but $Q_{\#}$ consistently achieves a better Pareto frontier. **(Right)** CD is highly sensitive to η : as η^{-1} increases, its KL grows rapidly and performance degrades below that of π^{ref} . In contrast, $Q_{\#}$ remains stable and requires less tuning of η .

Ablations. We ablate several design choices in Table 4 on the GSM8K and MATH validation sets using pass@1 accuracy. The “Prefix” column tests training on all $t \geq h$ prefixes after switching to π^{ref} (Algorithm 1, Line 10), as opposed to only $t = h$. Though this breaks IID assumptions, the increased training data improves $Q_{\#}$ performance by up to 4%. We compare two parameterizations of $Q^{*,\eta}$: Q-type, which computes $Q^{*,\eta}(x, y)$ for all y , and V-type, which predicts $Q^{*,\eta}(x, \hat{y})$ for a specific $\hat{y}$. V-type outperforms Q-type, likely due to its lower parameter count and per-token computation. Details are in Appendix D. We also compare distributional $Q_{\#}$ with MSE-based regression, which underperforms as expected under Bernoulli rewards. Finally, more iterations of Algorithm 1 yield marginal gains, with performance saturating after two iterations, which we adopt by default.

Qualitative comparison. Figure 6 shows side-by-side generations from π^{ref} and $Q_{\#}$ on math reasoning tasks. While both models often begin with similar prefixes—consistent with $Q_{\#}$ ’s low KL deviation— $Q_{\#}$ typically corrects π^{ref} ’s mistakes and produces more coherent reasoning. This behavior reflects $Q_{\#}$ ’s ability to assign higher value to correct tokens, thereby steering generation more effectively at critical decision points. Additional examples are provided in Appendix K.

Beyond math reasoning. To further validate the generality of $Q_{\#}$ beyond mathematical reasoning tasks, we evaluate its performance on QuALITY [47], a challenging multiple-choice reading comprehension benchmark with long-form passages drawn from Project Gutenberg. As shown in

Table 3: Performance of π^{ref} and $Q^\#$ with $Q^\#$ as a reward model. The reward model can determine the best generation among all generations for a problem and consistently improves maj1@8 for π^{ref} and $Q^\#$ own generations.

Setting	Llama 3 8B GSM8K		Llama 3.1 8B MATH	
Methods	π^{ref}	$Q^\#$	π^{ref}	$Q^\#$
pass@1	69.1	78.4	43.9	46.7
maj1@8	85.8	88.1	57.0	60.1
$Q^\#$ -RM Best of 8	85.9	86.0	54.0	54.0
$Q^\#$ -RM maj1@8	88.5	89.2	59.2	60.6

Table 4: Ablations of $Q^\#$ (last row) on pass@1 with various configurations on the validation set of GSM8K and MATH. The improvement suggests that our design choices all contribute positively to the final performance.

Prefix	Type	Opt.	# Iter.	Llama 3 8B GSM8K	Llama 3.1 8B MATH
Single	V	Dist.	1	80.5	64.5
All	Q	Dist.	1	81.4	66.4
All	V	MSE	1	81.4	65.4
All	V	Dist.	1	82.3	67.4
All	V	Dist.	2	83.5	68.5

Appendix H, Table 6, we compare $Q^\#$ with π^{ref} and CD baseline using Qwen 2.5 and Llama 3.1. Specifically, Qwen 2.5 1B guides Qwen 2.5 7B and Llama 3.2 1B guides Llama 3.1 8B. Across both architectures, $Q^\#$ consistently improves upon π^{ref} in all evaluation metrics, demonstrating its robustness beyond the mathematical domain.

4 Theory

4.1 CD & VAS are sub-optimal for KL-regularized RL

First, CD and VAS both propose to reweight $\pi^{\text{ref}}(\cdot | x)$ with the unregularized Q -function of π^{ref} :

$$\pi^{\text{CD},\eta}(y | x) \propto \pi^{\text{ref}}(y | x) \exp(Q^{\pi^{\text{ref}}}(x, y)/\eta), \quad (6)$$

where recall that $Q_h^{\pi^{\text{ref}}}(x_h, y_h) = \mathbb{E}_{\pi^{\text{ref}}}[\sum_{t \geq h} r_t | x_h, y_h]$. Comparing with Equation (2), we can already see that $\pi^{\text{CD},\eta}$ does not match the optimal policy $\pi^{*,\eta}$, as $Q^{\pi^{\text{ref}}}$ can be arbitrarily far from $Q^{*,\eta}$. In particular, π^{CD} may fail to optimize the KL-regularized RL objective and exhibit two failure cases, which we demonstrate with a simple MDP in Figure 4. First, we show that CD fails to maximize expected reward in this MDP, even as the KL-regularizer η decays to zero.

Theorem 4.1. *Under Figure 4, CD learns to always select the left sub-tree as $\eta \rightarrow 0$, which gives a sub-optimal reward of 0.1, while $\pi^{*,\eta}$ learns to always select the right sub-tree and chooses the path that gives reward 1.*

Proof. First, for CD, we have $Q^{\pi^{\text{ref}}}(x_1, a_L) = 0.1$ and $Q^{\pi^{\text{ref}}}(x_1, a_R) = 0.05$. Hence, CD’s probability of selecting the left sub-tree is $\frac{p_L \exp(0.1/\eta)}{p_L \exp(0.1/\eta) + p_R \exp(0.05/\eta)}$, which converges to 1 as $\eta \rightarrow 0$. Next, for $Q^\#$, we have $Q^{*,\eta}(x_1, a_L) = 0.1$ and $Q^{*,\eta}(x_1, a_R) = \eta \ln(0.05 \exp(1/\eta) + 0.95)$. Hence, $Q^\#$ ’s probability of selecting the left sub-tree is $\frac{p_L \exp(0.1/\eta)}{p_L \exp(0.1/\eta) + p_R (0.05 \exp(1/\eta) + 0.95)}$, which converges to 0 as $\eta \rightarrow 0$. Thus, CD learns the sub-optimal path. $\square$

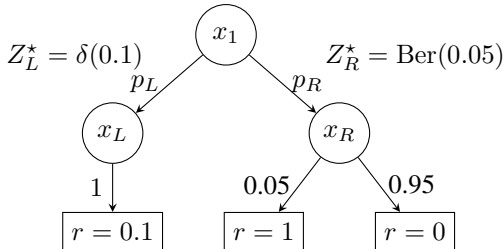


Figure 4: A tree MDP where edges are labeled with π^{ref} ’s action probability. π^{ref} goes to the left sub-tree w.p. p_L and the right sub-tree w.p. p_R , where $p_L, p_R > 0$. The left sub-tree gives $r = 0.1$ w.p. 1. In the right sub-tree, π^{ref} chooses reward 1 w.p. 0.05 and chooses reward 0 w.p. 0.95.

Next, we show that CD also incurs a higher KL than $Q^\#$.

Theorem 4.2. *Under Figure 4, CD’s KL converges to $\ln(1/p_L)$ while $Q^\#$ ’s KL converges to $\ln(1/p_R)$ as $\eta \rightarrow 0$. Thus if $p_L \ll p_R$, CD converges to a higher KL than $Q^\#$.*

Proof. As shown in Theorem 4.1, CD learns to select the left sub-tree while $Q^\#$ learns to select the right sub-tree as $\eta \rightarrow 0$. Then, the KLs simply follow by definition. $\square$

In sum, we proved that Figure 4, CD both incurs a higher KL and achieves a lower sub-optimal reward compared to $Q^\#$. Thus, $Q^\#$ generally Pareto-dominates CD in the reward-KL trade-off, which matches our empirical findings.

4.2 Performance Guarantee for $Q^\sharp$

We prove that the learned policy by $Q^\sharp$ is guaranteed to converge to the optimal policy with enough samples. This result holds in rich-observation MDPs where the size of the state space can be exponentially large or infinite, so long as the mild realizability assumption holds.

To setup, let $\mathcal{F}$ be a distributional function class for modeling Z^* , the reward-to-go distribution under π^{ref} . Each element of $\mathcal{F}$ has type $f = (f_1, \dots, f_H)$ and $f_h : \mathcal{X} \times \mathcal{Y} \mapsto \Delta([0, V^{\max}])$.¹ For the purpose of analysis, we assume access to a no-regret online learning oracle for the maximum likelihood (MLE) loss, which proceeds as follows: for each iteration $k = 1, 2, \dots, K$, given any $\{x_{h,k}, y_{h,k}, R_{h,k}\}_{h=1}^H$, the oracle outputs $\hat{Z}_k \in \mathcal{F}$ s.t.

$$\sum_{k=1}^K \sum_{h=1}^H (\log Z_h^*(R_{h,k} \mid x_{h,k}, y_{h,k}) - \log \hat{Z}_{h,k}(R_{h,k} \mid x_{h,k}, y_{h,k})) \leq \text{Reg}_{\text{mle}}(K).$$

Here, $\text{Reg}_{\text{mle}}(K)$ denotes the cumulative regret of the MLE oracle after K iterations. No-regret online learning is well-studied in the literature [48, 49] and is a standard tool when reducing decision making to supervised learning [13, 50, 35]. For example, if $\mathcal{F}$ is finite and satisfies realizability, then Vovk’s aggregating algorithm ensures that $\text{Reg}_{\text{mle}}(K) \lesssim \ln(|\mathcal{F}|)$ [51].²

Assumption 4.3 (Realizability). $Z^* \in \mathcal{F}$.

The following algorithm is a slightly modified version of Algorithm 1 amenable for theoretical analysis. The only differences with Algorithm 1 are: (1) we use the MLE oracle to learn $\hat{Z}_k$, and (2) for purpose of local exploration, we play a random action at the switching time h before following π^{ref} to the end of the trajectory [31].

We now state our main PAC bound for $Q^\sharp$.

Theorem 4.4. Fix any $\eta \in (0, V^{\max}]$ and $\delta \in (0, 1)$. Under Assumptions 2.1 and 4.3, Algorithm 2 ensures w.p. at least $1 - \delta$, setting $\beta = \ln(1/\delta) + \text{Reg}_{\text{mle}}(K)$, we have

$$\sum_{k=1}^K (V^{*,\eta} - V^{\pi^k,\eta}) \lesssim AV^{\max} (\sqrt{\sum_{h=1}^H \sum_{k=1}^K \text{CV}_{h,k}^2(x, y) \cdot \beta} + \max_{h \in [H]} E_h \cdot \beta),$$

where $\text{CV}_{h,k}(x, y) := \mathbb{E}_{x_h \sim \pi^k, y_h \sim \text{Unif}(\mathcal{A})} \left[\frac{\sqrt{\text{Var}(\exp(Z_h^*(x_h, y_h)/\eta))}}{\mathbb{E}[\exp(Z_h^*(x_h, y_h)/\eta)]} \right]$ is the coefficient of variation of $\exp(Z_h^*(x_h, y_h)/\eta)$, and $E_h := \|\exp((V^{\max} - Q_h^{*,\eta}(x_h, y_h))/\eta)\|_{L_\infty(\pi^{\text{ref}})}$ is the envelope of $\exp((V^{\max} - Q_h^{*,\eta}(x_h, y_h))/\eta)$, both under π^{ref} .

Algorithm 2 $Q^\sharp$ (Theory Version)

- 1: **Input:** reference π^{ref} , iteration count K , regularizer η .
 - 2: Initialize $\hat{Z}_1$ randomly.
 - 3: **for** $k = 1, 2, \dots, K$ **do**
 - 4: Let $\pi^k \leftarrow \pi^{\hat{Z}_k, \eta}$.
 - 5: **for** step $h = 1, 2, \dots, H$ **do**
 - 6: Roll-in with π^k for $h - 1$ steps and see $x_{h,k}$.
 - 7: Play random action $y_{h,k}$ and transit to $x_{h+1,k}$.
 - 8: Resume trajectory with π^{ref} from $x_{h+1,k}$.
 - 9: Let $R_{h,k}$ be cumulative rewards after time h .
 - 10: **end for**
 - 11: Input $\{x_{h,k}, y_{h,k}, R_{h,k}\}_{h \in [H]}$ to MLE oracle.
 - 12: Receive $\hat{Z}_k$ from MLE oracle.
 - 13: **end for**
 - 14: **Output:** $\hat{Z}_1, \dots, \hat{Z}_K$.
-

We highlight this applies to rich-observation MDPs where our only requirement for $\mathcal{F}$ is realizability. Our bound only scales with the function class’s complexity, *i.e.*, $\ln(|\mathcal{F}|)$, and does not contain structural complexity measures. In contrast, prior bounds in RL theory require stronger assumptions such as Bellman completeness [52, 53, 54, 55, 56, 57, 29], even in deterministic MDPs [58], and/or scale with structural complexity measures such as coverability [59, 60], eluder dimension [61, 55], and certain rank related complexity measures [62, 63, 64].

Computational efficiency. Algorithm 2 is model-free and computationally effi-

cient. In contrast, prior model-free algorithms for rich-observation MDPs perform exploration with version spaces and are computationally hard [62, 65, 55, 59, 29]. Thus, Theorem 4.4 shows that Algorithm 2 achieves *both statistical and computational* efficiency under mild assumptions by simply operating within the KL-regularized RL framework, which is of great relevance for post-training. We remark that [66] observed similar benefits in offline RL while we study the harder online setting.

¹Suppose rewards-to-go under π^{ref} lie in $[0, V^{\max}]$ w.p. 1.

² $a \lesssim b$ is short for $a \leq Cb$ for some universal constant C .

Second-order guarantee. Thanks to the distributional perspective, Theorem 4.4 is a *second-order bound* [28, 29]. Its leading term $\mathcal{O}(\sqrt{\sum_{h=1}^H \sum_{k=1}^K \text{CV}_{h,k}^2(x, y)})$ aggregates coefficients of variation.

In the worst case this is $\mathcal{O}(\sqrt{\sum_{h=1}^H E_h^2 K})$ but when Z_h^* has small or zero variance the term vanishes, leaving the lower-order $\mathcal{O}(\max_{h \in [H]} E_h \ln(K))$, logarithmical in K . Thus the bound adaptively improves from $\mathcal{O}(\sqrt{K})$ to $\mathcal{O}(\ln(K))$ in benign instances. Interestingly, the envelope term E_h is also instance-dependent; when $Q^{*,\eta} = V^{\max}$ it equals 1, eliminating the exponential dependence on η . In general, we can tolerate an η that is as small as the worst $V^{\max} - Q^{*,\eta}$ under rollouts from π^{ref} , which is reminiscent of the condition required for first-order or small-loss bounds [50, 35, 57].

Bernoulli rewards simplification. For closed-ended tasks (e.g. math or multiple-choice), the reward-to-go $Z_h^*(x, y)$ is Bernoulli, $Z_h^*(x, y) \sim \text{Ber}(p_h(x, y))$. Then the CV term can be bounded by $\text{CV}_{h,k} \leq \mathbb{E}_{\pi^k \circ \text{Unif}} \sqrt{(1 - p_h)/p_h}$ and the envelope term becomes $\|1/p_h\|_{L_\infty(\pi^{\text{ref}})}$, which notably does not have exponential dependence on $1/\eta$. Thus, as long as the reference model π^{ref} has sufficient probability of solving the problem, our bound can be made independent of η . Finally, we note that the distributional-realizability condition can also be weakened to mean-realizability, since the only parameter of a Bernoulli distribution is its mean; also the MLE loss reduces to the binary cross-entropy loss [50, 57]. We present the corollary below and the proof in Appendix B.1.

Corollary 4.5. *Suppose reward-to-gos are Bernoulli: $Z_h^*(x, y) \sim \text{Ber}(p_h(x, y))$. Then, under the setup of Theorem 4.4, the bound can be simplified to:*

$$\begin{aligned} \sum_{k=1}^K (V^{*,\eta} - V^{\pi^k, \eta}) &\lesssim A \left(\sqrt{\sum_{h=1}^H \sum_{k=1}^K \mathbb{E}_{x_h \sim \pi^k, y_h \sim \text{Unif}(\mathcal{A})} \left[\frac{1 - p_h(x_h, y_h)}{p_h(x_h, y_h)} \right]} \cdot \beta \right. \\ &\quad \left. + \max_{h \in [H]} \left\| \frac{1}{p_h(x_h, y_h)} \right\|_{L_\infty(\pi^{\text{ref}})} \cdot \beta \right), \end{aligned}$$

Remark: Modification for Regret Bound. It is possible to turn Theorem 4.4 into a regret bound by replacing random action in Line 7 of Algorithm 2 with a no-regret contextual bandit oracle, where “context” is x_h , action is y_h and “reward” is R_h . This is alike the steps needed to convert AggreVaTe’s PAC bound into a regret bound [31]. Our theory can be interpreted as a regret/PAC reduction from KL-regularized RL in deterministic MDPs to no-regret online learning, which mirrors the type of imitation learning guarantees obtained for AggreVaTe [31].

5 Limitations & Conclusion

Our results focus on deterministic MDPs including LLM post-training, where the optimal action-value $Q^{*,\eta}$ is a simple functional of the reference return distribution $Z^{\pi^{\text{ref}}}$ and Theorem 2.2 applies directly. For domains with stochastic transitions such as multi-agent game playing where the next state depends on the (potentially unpredictable) behavior of the other player, $Q^{*,\eta}$ need to be learned via temporal-difference methods, which typically rely on the stronger Bellman-completeness assumption and may introduce additional training instability. In summary, $Q^\#$ offers a principled and practical avenue for post-training LLMs. It combines a distributional-RL objective with supervised regression, enjoys provable convergence under mild assumptions, and consistently surpasses prior value-based baselines on synthetic planning and math-reasoning benchmarks—achieving higher accuracy while maintaining a lower KL divergence from the reference policy.

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A Related Works

From the empirical side, the most relevant works are controlled decoding (CD; [11]) and value augmented sampling (VAS; [12]). These two works both propose to guide the reference policy π^{ref} with $Q^{\pi^{\text{ref}},0}$, the expected reward-to-go under π^{ref} *without* KL regularization. As discussed in Section 4.1, guiding with $Q^{\pi^{\text{ref}},0}$ is not principled for the KL-regularized RL problem and can lead to both sub-optimal reward and large KL from π^{ref} . In contrast, we propose to guide π^{ref} with $Q^{*,\eta}$, the expected reward-to-go under the optimal policy *with* KL regularization, which is the correct closed-form of the optimal policy. A recent work [34] proposed a process reward model (PRM) of a similar form as our $Q^{*,\eta}$, but their PRM is applied to steps instead of tokens, and they do not use distributional RL or iterative training (i.e., data aggregation).

In terms of reweighting π^{ref} with classifier scores, FUDGE [67] is another closely related work but their derivation is based on Bayes rule and FUDGE does not solve KL-regularized RL. Sequential Monte Carlo (SMC) methods [22, 68] also reweight π^{ref} 's distribution with a twist function, where the optimal twist function is analogous to our $Q^{*,\eta}$. One key difference is that SMC performs resampling while we directly combine logits of π^{ref} and $\exp(Q^{*,\eta})$ to avoid importance sampling, which has higher variance. Finally, none of these prior works apply distributional RL losses [17, 69, 70, 57] or online data aggregation [13] to learn $Q^{*,\eta}$, which we showed to be beneficial in our ablations. Indeed, CD and VAS both use square loss regression over a fixed offline dataset. We also remark that risk-sensitive RL has been an important application of distributional RL [69, 71] and extending $Q^\#$ along those lines is a promising future direction.

We also discuss some of the recent advances in stable distributional RL. [72] shows that the categorical distributional RL loss, which we employ for our theory and experiments, enjoys smoothness and optimization stability under a bounded logit condition. [73] introduces a Sinkhorn distributional RL loss which is a computationally efficient alternative for Wasserstein distance, and was shown to be more stable for multi-dimensional rewards. [69] proposed a KL-regularized categorical loss which they showed is empirically more stable in Atari games. However, these references all apply TD-learning with function approximation and replay buffers, which [74] identified as a deadly triad that is notoriously difficult to scale, requiring many tricks such as double Q-learning and target networks. In contrast, our work obviates the need for TD-learning or tricks such as the target network by leveraging the special form of Q^* in deterministic KL-regularized MDPs, which perfectly captures the LLM post-training application we focus on.

We also cite some tangentially related works. Proxy tuning [75] and speculative decoding [76] both use a small model to guide the logit distribution of a large π^{ref} model. Speculative decoding is focused on maximizing the large model's likelihood, which does not relate to any extrinsic rewards. In our framework, the classifier model can be any size relative to π^{ref} , although deeper investigation into the computational benefits of using a small classifier is a promising direction for future work. We note that the star-graph problem can also be solved during pre-training by also predicting backwards via the belief state transformer [36].

Finally we discuss previous post-training methods for LLMs. First, online iterative DPO [77, 78], REBEL [79], PPO [8], etc. are based on policy gradient and require a good reset distribution which only guarantees local optimality. XPO [80], VPO [81], SELM [82], etc. treat this as an exploration setting but requires solving non-convex optimization oracles and relies on strong structure conditions such as coverability / eluder / linearity, similar to the theoretical works like [55, 59]. Instead, we approach post-training in a fundamentally different angle and solve it via simple computationally tractable regression and mle oracles, without any strong structural conditions or reset distribution assumptions.

From the theoretical side, KL-regularized RL is closely related to soft RL or maximum entropy RL which are well-studied [20, 83, 84, 22]. The optimal policy decomposition in deterministic MDPs is also known in prior works [23, 21]. Our contribution is an algorithm that provably learns $Q^{*,\eta}$ using distributional RL [17] and data aggregation [13]. This enables us to prove a reduction of KL-regularized RL (in deterministic MDPs) to no-regret online learning, which ensures convergence to the optimal policy with realizability being the only assumption for function approximation. Notably we are able to avoid more stringent conditions such as completeness or structural MDP conditions which are ubiquitous in the current literature [53, 55, 56, 35, 29, 57, 59]. [66] observed similar benefits in offline RL, while we provide guarantees for the harder online RL setting.

Complementary to our online, KL-regularized setting, DualDICE [85] and AlgaeDICE [86] tackle the high-variance "curse of horizon" that arises when one performs importance weighting for long trajectories in *offline* RL. Both methods replace per-step importance weights with stationary-distribution density ratios, learned through a dual (Lagrangian) formulation, and have shown empirical success on low-dimensional continuous-control benchmarks, although learning is also shown to be difficult in high-dimensional control tasks [56]. Because we continually collect on-policy data and constrain updates via an explicit KL penalty—which already limits distribution shift—we do not need such ratio estimation; nonetheless, density-ratio approaches remain a promising orthogonal direction for variance reduction in purely offline LLM post-training.

We remark that our theoretical guarantees are quite similar in structure to that of AggreVaTe [31, 32], which is a reduction of imitation learning to no-regret online learning. Besides the obvious difference in problem setting, another improvement from our work is using distributional RL theory to prove second-order bounds. Notably, we are able to prove second-order bounds without any completeness assumptions that were required in [35, 28, 29].

B Proofs

In this section, we provide the full proof for Theorem 4.4.

Theorem 4.4. *Fix any $\eta \in (0, V^{\max}]$ and $\delta \in (0, 1)$. Under Assumptions 2.1 and 4.3, Algorithm 2 ensures w.p. at least $1 - \delta$, setting $\beta = \ln(1/\delta) + \text{Reg}_{\text{mle}}(K)$, we have*

$$\sum_{k=1}^K (V^{\star, \eta} - V^{\pi^k, \eta}) \lesssim AV^{\max} (\sqrt{\sum_{h=1}^H \sum_{k=1}^K \mathbf{CV}_{h,k}^2(x, y) \cdot \beta} + \max_{h \in [H]} E_h \cdot \beta),$$

where $\mathbf{CV}_{h,k}(x, y) := \mathbb{E}_{x_h \sim \pi^k, y_h \sim \text{Unif}(\mathcal{A})} \left[\frac{\sqrt{\text{Var}(\exp(Z_h^*(x_h, y_h)/\eta))}}{\mathbb{E}[\exp(Z_h^*(x_h, y_h)/\eta)]} \right]$ is the coefficient of variation of $\exp(Z_h^*(x_h, y_h)/\eta)$, and $E_h := \|\exp((V^{\max} - Q_h^{\star, \eta}(x_h, y_h))/\eta)\|_{L_\infty(\pi^{\text{ref}})}$ is the envelope of $\exp((V^{\max} - Q_h^{\star, \eta}(x_h, y_h))/\eta)$, both under π^{ref} .

Proof. Fix any $\eta \in (0, V^{\max})$. Let $Q_{h,k}(x, y) = \eta \ln \mathbb{E}_{z \sim \hat{Z}_{h,k}(x, y)} \exp(z/\eta)$ denote the induced soft Q function from the distributional estimate $\hat{Z}_k$. Let $\pi_h^k(y | x) \propto \pi_h^{\text{ref}}(y | x) \exp(Q_{h,k}(x, y)/\eta)$ denote the induced policy from $Q_{h,k}$. Then,

$$\begin{aligned} V^{\star, \eta} - V^{\pi^k, \eta} & \stackrel{(i)}{=} \sum_{h=1}^H \mathbb{E}_{\pi^k} [Q_h^{\star, \eta}(x_h, \pi_h^{\star, \eta}) - Q_h^{\pi^k, \eta}(x_h, \pi_h^k) + \eta \text{KL}(\pi_h^k(x_h) \parallel \pi_h^{\text{ref}}(x_h)) - \eta \text{KL}(\pi_h^{\star, \eta}(x_h) \parallel \pi_h^{\text{ref}}(x_h))] \\ & = \sum_{h=1}^H \mathbb{E}_{\pi^k} [Q_h^{\star, \eta}(x_h, \pi_h^{\star, \eta}) - \eta \text{KL}(\pi_h^{\star, \eta}(x_h) \parallel \pi_h^{\text{ref}}(x_h)) - (Q_{h,k}(x_h, \pi_h^k) - \eta \text{KL}(\pi_h^k(x_h) \parallel \pi_h^{\text{ref}}(x_h))) \\ & \quad + Q_{h,k}(x_h, \pi_h^k) - Q_h^{\star, \eta}(x_h, \pi_h^k)] \\ & \stackrel{(ii)}{\leq} \sum_{h=1}^H \mathbb{E}_{\pi^k} [Q_h^{\star, \eta}(x_h, \pi_h^{\star, \eta}) - \eta \text{KL}(\pi_h^{\star, \eta}(x_h) \parallel \pi_h^{\text{ref}}(x_h)) - (Q_{h,k}(x_h, \pi_h^{\star, \eta}) - \eta \text{KL}(\pi_h^{\star, \eta}(x_h) \parallel \pi_h^{\text{ref}}(x_h))) \\ & \quad + Q_{h,k}(x_h, \pi_h^k) - Q_h^{\star, \eta}(x_h, \pi_h^k)] \\ & = \sum_{h=1}^H \mathbb{E}_{\pi^k} [Q_h^{\star, \eta}(x_h, \pi_h^{\star, \eta}) - Q_{h,k}(x_h, \pi_h^{\star, \eta}) + Q_{h,k}(x_h, \pi_h^k) - Q_h^{\star, \eta}(x_h, \pi_h^k)] \\ & \leq 2 \sum_{h=1}^H \mathbb{E}_{x_h \sim \pi^k} [\max_{\pi \in \{\pi^{\star}, \pi^k\}} |Q_h^{\star, \eta}(x_h, \pi) - Q_{h,k}(x_h, \pi)|] \\ & \leq 2A \sum_{h=1}^H \mathbb{E}_{x_h \sim \pi^k, y_h \sim \text{Unif}(\mathcal{A})} |Q_h^{\star, \eta}(x_h, y_h) - Q_{h,k}(x_h, y_h)|, \end{aligned}$$

where (i) is by the performance difference lemma in the soft MDP (Lemma B.2); (ii) is by Donsker-Varadhan (Lemma B.1) which proves that $\pi_h^{\star}(x_h) = \arg \max_{\pi} \mathbb{E}_{\pi} [Q_{h,k}(x_h, \pi) - \text{KL}(\pi(x_h) \parallel \pi_h^{\text{ref}}(x_h))]$. Now, we bound the difference between the optimal and learned Q functions:

$$\begin{aligned} & |Q_h^{\star, \eta}(x, y) - Q_{h,k}(x, y)| \\ & = \eta \left| \ln \mathbb{E}_{z \sim Z_h^*(x, y)} \exp(z/\eta) - \ln \mathbb{E}_{z \sim \hat{Z}_{h,k}(x, y)} \exp(z/\eta) \right| \\ & \stackrel{(i)}{\lesssim} \eta(1 + V_{\max}/\eta) \left(\mathbf{CV}_{z \sim Z_h^*(x, y)}(\exp(z/\eta)) H_{h,k}(x, y) + \frac{\exp(V_{\max}/\eta) - 1}{\mathbb{E}_{z \sim Z_h^*(x, y)} \exp(z/\eta)} H_{h,k}^2(x, y) \right) \\ & = (\eta + V_{\max}) \left(\mathbf{CV}_{z \sim Z_h^*(x, y)}(\exp(z/\eta)) H_{h,k}(x, y) + \frac{\exp(V_{\max}/\eta)}{\exp(Q_h^{\star, \eta}(x, y)/\eta)} H_{h,k}^2(x, y) \right), \end{aligned}$$

where (i) is by Lemma B.4 and the fact that $Z^*, \hat{Z}_k \in [0, V^{\max}]$ and $H_{h,k}(x, y) := H(Z_h^*(x, y), \hat{Z}_{h,k}(x, y))$ is the Hellinger distance between the learned $\hat{Z}_{h,k}$ and optimal Z_h^* .

Thus, if we let $x_h, y_h \sim \pi^k \circ_h \text{Unif}(\mathcal{A})$ denote the distribution of rolling in with π^k until x_h and taking a random $y_h \sim \text{Unif}(\mathcal{A})$, then we have:

$$\begin{aligned} & \sum_{k=1}^K V^{\star, \eta} - V^{\pi^k, \eta} \\ & \leq 2A \sum_{h=1}^H \sum_{k=1}^K \mathbb{E}_{\pi^k \circ_h \text{Unif}(\mathcal{A})} |Q_h^{\star, \eta}(x_h, y_h) - Q_{h,k}(x_h, y_h)| \\ & \lesssim AV_{\max} \sum_{h=1}^H \sum_{k=1}^K \mathbb{E}_{\pi^k \circ_h \text{Unif}(\mathcal{A})} \left[\mathbf{CV}_{z \sim Z_h^*(x, y)}(\exp(z/\eta)) H_{h,k}(x_h, y_h) + \frac{\exp(V_{\max}/\eta)}{\exp(Q_h^{\star, \eta}(x_h, y_h)/\eta)} H_{h,k}^2(x, y) \right] \\ & \leq AV_{\max} \sqrt{\sum_{h=1}^H \sum_{k=1}^K \mathbb{E}_{\pi^k \circ_h \text{Unif}(\mathcal{A})} [\mathbf{CV}_{h,k}^2(x_h, y_h)]} \sqrt{\sum_{h=1}^H \sum_{k=1}^K \mathbb{E}_{\pi^k \circ_h \text{Unif}(\mathcal{A})} [H_{h,k}^2(x_h, y_h)]} \\ & + AV_{\max} \left\| \frac{\exp(V_{\max}/\eta)}{\exp(Q_h^{\star, \eta}(x_h, y_h)/\eta)} \right\|_{L_{\infty}(\pi^k \circ_h \text{Unif}(\mathcal{A}))} \cdot \sum_{h=1}^H \sum_{k=1}^K \mathbb{E}_{\pi^k \circ_h \text{Unif}(\mathcal{A})} [H_{h,k}^2(x_h, y_h)]. \end{aligned}$$

The final step is to bound the summed Hellinger square terms. This can be done via Multiplicative Azuma's inequality and [87, Lemma A.14], which shows that for any $\delta \in (0, 1)$, we have $\sum_{h,k} \mathbb{E}_{\pi^k \circ_h \text{Unif}(\mathcal{A})} [H_{h,k}^2(x_h, y_h)] \lesssim \sum_{h,k} H_{h,k}^2(x_{h,k}, y_{h,k}) + \ln(1/\delta) \lesssim \text{Reg}_{\text{mle}}(K) + \ln(1/\delta)$, which recall is exactly the definition of β . This finishes the proof of Theorem 4.4. $\square$

Lemma B.1 (Donsker-Varadhan's Variational Formula; [88]). *For any prior $p \in \Delta(\Theta)$, consider the KL-regularized optimization:*

$$\pi^* = \arg \max_{\pi \in \Delta(\Theta)} V(\pi) := \mathbb{E}_{\pi}[Q(\theta) - \eta \text{KL}(\pi(\theta) \parallel p(\theta))].$$

The optimal policy π^ is given by $\pi^*(\theta) \propto p(\theta) \exp(Q(\theta)/\eta)$ and it has value $V(\pi^*) = \eta \ln \mathbb{E}_{\theta \sim p} \exp(Q(\theta)/\eta)$.*

Lemma B.2 (Soft Performance Difference Lemma (PDL)). *For any f and π ,*

$$V^{\pi} - f_1(x_1, \pi) = \sum_{h=1}^H \mathbb{E}_{\pi}[(\mathcal{T}_h^{\pi} f_{h+1} - f_h)(x_h, y_h)] - \eta \text{KL}(\pi_1(x_1) \parallel \pi_1^{\text{ref}}(x_1)).$$

For any π, π' ,

$$V^{\pi} - V^{\pi'} = \sum_{h=1}^H \mathbb{E}_{\pi} [Q_h^{\pi'}(x_h, y_h) - Q_h^{\pi}(x_h, \pi') + \eta \text{KL}(\pi_h'(x_h) \parallel \pi_h^{\text{ref}}(x_h)) - \eta \text{KL}(\pi_h(x_h) \parallel \pi_h^{\text{ref}}(x_h))].$$

Proof. Let $\text{KL}(\pi_h(x_h)) := \text{KL}(\pi_h(x_h) \parallel \pi_h^{\text{ref}}(x_h))$ denote KL-divergence w.r.t. π^{ref} . Then,

$$\begin{aligned} & V^{\pi} - V^{\pi'} \\ & = \sum_{h=1}^H \mathbb{E}_{\pi} [r_h - \eta \text{KL}(\pi_h(x_h))] - (Q_1^{\pi'}(x_1, \pi') - \eta \text{KL}(\pi_1'(x_1))) \\ & = \sum_{h=1}^H \mathbb{E}_{\pi} [r_h - \eta \text{KL}(\pi_{h+1}'(x_{h+1})) + \eta \text{KL}(\pi_{h+1}'(x_{h+1})) + Q_{h+1}^{\pi'}(x_{h+1}, \pi') - Q_h^{\pi'}(x_h, \pi') - \eta \text{KL}(\pi_h(x_h))] + \eta \text{KL}(\pi_1'(x_1)) \\ & = \sum_{h=1}^H \mathbb{E}_{\pi} [r_h - \eta \text{KL}(\pi_{h+1}'(x_{h+1})) + Q_{h+1}^{\pi'}(x_{h+1}, \pi') - Q_h^{\pi'}(x_h, \pi') + \eta \text{KL}(\pi_h'(x_h)) - \eta \text{KL}(\pi_h(x_h))] \\ & = \sum_{h=1}^H \mathbb{E}_{\pi} [\mathcal{T}_h^{\pi'} Q_{h+1}^{\pi'}(x_h, y_h) - Q_h^{\pi'}(x_h, \pi') + \eta \text{KL}(\pi_h'(x_h)) - \eta \text{KL}(\pi_h(x_h))] \\ & = \sum_{h=1}^H \mathbb{E}_{\pi} [Q_h^{\pi'}(x_h, y_h) - Q_h^{\pi'}(x_h, \pi') + \eta \text{KL}(\pi_h'(x_h)) - \eta \text{KL}(\pi_h(x_h))]. \end{aligned}$$

$\square$

Lemma B.3. *For any two numbers $x, y \in [\exp(a), \exp(b)]$, we have*

$$|\ln(x) - \ln(y)| \leq (1 + b - a) \left| \frac{x - y}{y} \right|.$$

If $b - a \geq \frac{1}{2}$, then $\max(1, \frac{b-a}{1-\exp(a-b)}) \leq 3(b-a)$.

Proof. If $x \geq y$, then $\ln(x) - \ln(y) = \ln(1 + (x-y)/y) \leq (x-y)/y$. If $x < y$, then $\ln(y) - \ln(x) = -\ln(1 + (x-y)/y)$. By premise, we have $0 \geq \frac{x-y}{y} \geq \exp(a-b) - 1$. Note that $-\ln(1+z)$ is convex and is thus upper bounded by the line connecting $(0, 0)$ and $(\exp(a-b) - 1, b-a)$, i.e., $-\ln(1+z) \leq \frac{b-a}{1-\exp(a-b)}|z|$ for $0 \geq z \geq \exp(a-b) - 1$. Thus, $-\ln(1 + (x-y)/y) \leq \frac{b-a}{1-\exp(a-b)} \left| \frac{x-y}{y} \right|$. Thus, we've shown that $|\ln(x) - \ln(y)| \leq \max\left(1, \frac{b-a}{1-\exp(a-b)}\right) \left| \frac{x-y}{y} \right|$. Finally, since $\frac{x}{1-\exp(-x)} \leq 1+x$ when $x \geq 0$, we have $\max(1, \frac{b-a}{1-\exp(a-b)}) \leq \max(1, 1+b-a) = 1+b-a$. $\square$

Lemma B.4. For any distributions p, q on $[a, b]$, we have

$$|\ln \sum_z p(z)e^z - \ln \sum_z q(z)e^z| \lesssim (1+b-a) \left(\frac{\sqrt{\text{Var}_q(e^z)}}{\mathbb{E}_q e^z} H(p, q) + \frac{\exp(b) - \exp(a)}{\mathbb{E}_q e^z} H^2(p, q) \right),$$

where $H^2(p, q) = \frac{1}{2} \sum_z (\sqrt{p(z)} - \sqrt{q(z)})^2$ is the squared Hellinger distance.

Proof. By Lemma B.3, we have $|\ln \sum_z p(z)e^z - \ln \sum_z q(z)e^z| \leq (1+b-a) \left| \frac{\sum_z (p(z) - q(z))e^z}{\sum_z q(z)e^z} \right|$. By Lemma B.5, we have that the numerator is bounded by $\sqrt{\text{Var}_q(e^z)} H(p, q) + (\exp(b) - \exp(a)) H^2(p, q)$. $\square$

Lemma B.5 (Second-Order Lemma). Suppose p, q are distributions on the interval $[a, b]$. Then, we have

$$|\bar{p} - \bar{q}| \lesssim \sqrt{\text{Var}(p)} H(p, q) + (b-a) H^2(p, q).$$

Proof. Define p', q' as the normalized distributions on $[0, 1]$, i.e., p' is the law of $X' = (X-a)/(b-a)$ where $X \sim p$. Then, we have

$$\begin{aligned} |\bar{p} - \bar{q}| &= (b-a) |\bar{p}' - \bar{q}'| \\ &\lesssim (b-a) (\sqrt{\text{Var}(p')} H(p', q') + H^2(p', q')) \\ &= \sqrt{\text{Var}(p)} H(p, q) + (b-a) H^2(p, q), \end{aligned}$$

where the $\lesssim$ step is due to the second-order lemma of [28]. $\square$

B.1 Case of Bernoulli reward-to-go

In this section, we focus on problems where $Z_h^*(x, y) = \text{Ber}(p_h(x, y))$ is a Bernoulli distribution, which is common for closed-ended problems such as math or multiple choice. Here, the envelope term can be bounded as follows:

Lemma B.6. If $Z_h^*(x, y) = \text{Ber}(p_h(x, y))$, then we have $V^{\max} = 1$ and for all $\eta > 0$, we have

$$\exp((1 - Q_h^{\star, \eta}(x, y))/\eta) \leq 1/p_h(x, y).$$

Proof. Fix x, y and let $p = p_h(x, y)$. Then, it suffices to show that

$$1/\eta - \ln(p \exp(1/\eta) + 1 - p) \leq \ln(1/p).$$

This is indeed true because

$$\begin{aligned} 1/\eta - \ln(p \exp(1/\eta) + 1 - p) &= \ln\left(\frac{\exp(1/\eta)}{p \exp(1/\eta) + 1 - p}\right) \\ &= \ln\left(\frac{1}{p + (1-p) \exp(-1/\eta)}\right) \leq \ln(1/p). \end{aligned}$$

$\square$

We can also bound the coefficient of variance in terms of the Bernoulli parameter.

Lemma B.7. If $Z_h^*(x, y) = \text{Ber}(p_h(x, y))$, then for all $\eta > 0$, we have

$$\frac{\sqrt{\text{Var}(\exp(Z_h^*(x, y)/\eta))}}{\mathbb{E}[\exp(Z_h^*(x, y)/\eta)]} \leq \sqrt{(1-p)/p}.$$

Proof. Fix x, y and let $p = p_h(x, y)$. Then, the variance term is:

$$\begin{aligned}
\text{Var}(\exp(Z_h^*(x, y)/\eta)) &= \mathbb{E}[\exp(2Z_h^*(x, y)/\eta)] - (\mathbb{E}[\exp(Z_h^*(x, y)/\eta)])^2 \\
&= p \exp(2/\eta) + (1 - p) - (p \exp(1/\eta) + (1 - p))^2 \\
&= p \exp(2/\eta) + (1 - p) - p^2 \exp(2/\eta) - 2p \exp(1/\eta)(1 - p) - (1 - p)^2 \\
&= p(1 - p) \exp(2/\eta) + (1 - p)p - 2p \exp(1/\eta)(1 - p) \\
&= p(1 - p)(\exp(2/\eta) + 1 - 2 \exp(1/\eta)) \\
&= p(1 - p)(\exp(1/\eta) - 1)^2.
\end{aligned}$$

Thus, the CV is:

$$\frac{\sqrt{p(1 - p)(\exp(1/\eta) - 1)^2}}{p \exp(1/\eta) + 1 - p} = \frac{\sqrt{p(1 - p)(\exp(1/\eta) - 1)^2}}{p(\exp(1/\eta) - 1) + 1} \leq \frac{\sqrt{p(1 - p)}}{p} = \sqrt{(1 - p)/p}.$$

□

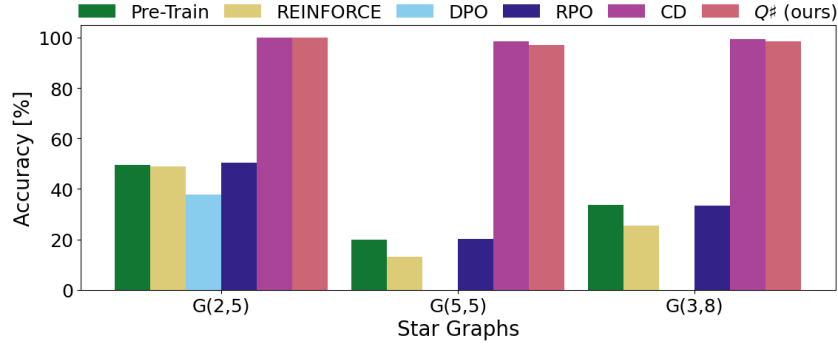


Figure 5: Full results for star-graph experiments. The empty bar for $G(5, 5)$ and $G(3, 8)$ are for DPO, which pushed down both the chosen and reject paths resulting in 0 accuracy.

C Additional Discussion and Implementation Details for Star-Graph

The shortcut behavior, also known as the Clever Hans Trick [18], in the star-graph task arises directly from the auto-regressive next-token prediction objective. Specifically, the model minimizes loss by memorizing the first token seen during training and following the corresponding edge, achieving low training error but generalizing poorly at test time when the initial token is not provided. This leads to a brittle, shortcut-based policy.

Policy-based methods such as REINFORCE and RPO attempt to correct this by upweighting high-reward trajectories. However, because their loss is still based on the product of next-token prediction probabilities, the same as in pretraining, they are vulnerable to the same shortcut and require exponentially many samples via gradient descent on the policy to correct it once it is learned (Theorem 1 of [89]).

In contrast, $Q^\#$ does not depend on myopic next-token supervision. Instead, it learns to predict the cumulative reward-to-go from each (prefix, token) pair under the reference policy, and uses this to guide generation toward optimal completions. This token-level value modeling allows $Q^\#$ to predict future outcome and assign higher value to early tokens that lead to long-term reward. In other words, $Q^\#$ ’s loss function is directly trained to perform planning, making it robust to the Clever Hans Trick [18] that undermines next-token-based methods. As shown in Figure 5, both $Q^\#$ and CD are able to solve the star-graph task near-perfectly, while policy-based methods perform at random-guess level.

We follow the setup of [18] and reused their official code for producing the star-graph results. We used the GPT-2 small model for graphs $G(2, 5)$, $G(5, 5)$ and the GPT-2 medium model for $G(3, 8)$ [90].³ We first pretrain these models with next-token prediction on a pretraining set of 200k random graphs and correct paths. We call this the resultant model the “pre-trained” model, and as observed by [18], these models have the Clever Hans shortcut so they do not generalize well on unseen test graphs. We highlight that this is a failure in generalization, since the pre-trained model achieves near-perfect accuracy on the training set but only $1/d$ accuracy on the test set.

In order to fix the Clever Hans shortcut, we perform post-training with two common baselines – REINFORCE [41] and DPO [9], RPO [42] – as well as our algorithm $Q^\#$. The post-training is done on another set of 200k random graphs. For REINFORCE, the reward function we use is 1 if the response is correct, and -0.1 if incorrect. We noticed that if the incorrect reward is too negative, this causes model collapsing to accuracy of 0. For DPO and RPO, we sampled pairwise responses $(y_{\text{chosen}}, y_{\text{reject}})$ where y_{chosen} is the correct path and y_{reject} is an incorrect shortcut path sampled from the pretrained model. For $Q^\#$, we also trained the classifier on the same dataset of pairwise responses, where correct paths are marked with reward 1 and incorrect responses are marked with reward 0. Throughout, we used the AdamW optimizer with weight decay 0.1 and batch size of 256, and trained for 10 epochs. The learning rates were $2.5e-4$ for pre-training; $1e-5$ for REINFORCE; $1e-4$ for DPO and RPO; $1e-4$ for classifier-based CD and $Q^\#$. All models are trained on a single A100 or H100 GPU. All models were evaluated on a separate test set of 20k graphs, using top-k 10 and

³Models from <https://huggingface.co/openai-community/gpt2> and <https://huggingface.co/openai-community/gpt2-medium>.

temperature 1.0. For $Q_{\#}$ and CD, we use $\eta = 0.1$. We found that DPO often pushed down the probabilities of both the chosen and reject paths, leading to poor performance even on the training set; RPO fixed this issue and so we report the RPO numbers.

D Additional Model Details

π^{ref} models. All models we use in the experiments are the "Instruct" versions. That is, Llama 3 8B refers to meta-llama/Meta-Llama-3-8B-Instruct and we use the default chat template and system message from Meta to interact with them.

$Q_{\#}$ models. Two variants for $Q_{\#}$ are implemented and experimented: Q-type and V-type. Specifically, the Q-type takes input of a partial generation x and computes $Q^{*,\eta}(x, y)$ for all y in the vocabulary of the π^{ref} model whereas the V-type takes input of concatenated x and a specific token $\hat{y}$ and outputs a single value that represents $Q^{*,\eta}(x, \hat{y})$. Because of the key difference, Q-type therefore can efficiently calculate $Q^{*,\eta}$ with just one forward pass and its model architecture can also be identical to the original LLM. V-type, however, has a prohibitive inference cost with a naive implementation since it requires making $|V|$ forward passes at every decoding step to calculate the full Q function. In the paragraph below, we discuss our efficient implementation to address this issue. For Q-type, we initialize the model directly from Llama 3.2 1B and for V-type, we replace the last layer of Llama 3.2 1B with a randomly initialized fully connected layer with output size of 1. Therefore, V-type $Q_{\#}$ also has slightly fewer number of parameters than Q-type. We by default use V-type $Q_{\#}$ in our experiments.

Efficient inference with V-type. To speed up inference for V-type, we note that not all tokens in the vocabulary are worth computing its value since for any partial generation x , most tokens have extremely low probability from π^{ref} as the next token candidate. In our preliminary experiments, we have found that only computing the values for the top 20 tokens ranked by π^{ref} give similar performance compared to computing for all tokens. Additionally, we also note that the values for these tokens can be computed in one forward pass. To accomplish this, we input a partial generation x and the top 20 candidate next tokens together, modify the attention mask so that the candidate tokens do not attend to each other but still to x . This allows us to compute the values for these top tokens in just one additional forward pass without any approximation.

E $Q_{\#}$ Training Settings

We collect 16 samples for each question in the training set and label every sample either as correct (1) or incorrect (0) based on the final answer. The first round of training data is collected with just π^{ref} . For training $Q_{\#}$ model, we filter out samples from questions where all samples are either correct or incorrect. We use a learning rate of $2e - 5$ and weight decay of 0.01 with AdamW optimizer [91]. The model is trained for 5 epochs. We train $Q_{\#}$ for two iterations as we observe performance converges. In the second iteration, we repeat the above data collection procedure and concatenate the training data from the first round. The model is always trained from scratch between iterations.

F Additional Evaluation Details

We evaluate all methods and models with zero-shot prompting. The prompt template is 'Problem:\n\n{0} Write your answer inside \boxed{{}}.\n\nSolution:' where {0} is replaced by the actual question from the dataset. The MATH-500 dataset can also be found at Huggingface⁴.

G Math Reasoning Results on Qwen 2.5

We conduct experiments using Qwen 2.5 [46], where a 1.5B model guides the 7B version on GSM8K, MATH and AIME-24 (Table 5). All other configurations mirror those used with Llama 3. We find that $Q_{\#}$ consistently outperforms both π^{ref} and CD across all datasets, achieving higher accuracy with

⁴<https://huggingface.co/datasets/HuggingFaceH4/MATH-500>

lower KL divergence. Compared to Table 1, Qwen 2.5 yields stronger overall performance, likely due to its stronger base model, demonstrating that $Q\sharp$ generalizes well across model families.

Table 5: Comparison of $Q\sharp$ with π^{ref} and CD baseline on GSM8K (left), MATH (middle) and AIME-24 (right) with Qwen 2.5.

Dataset	GSM8K			MATH			AIME-24		
Methods	π^{ref}	CD	$Q\sharp$	π^{ref}	CD	$Q\sharp$	π^{ref}	CD	$Q\sharp$
pass@1 $\uparrow$	76.1	79.0	83.5	58.6	60.7	61.9	9.3	13.5	14.1
maj1@8 $\uparrow$	92.9	93.1	93.8	72.8	74.2	74.8	16.7	16.7	20.0
KL-Divergence $\downarrow$	-	5.37	4.10	-	7.07	6.46	-	9.95	9.23

H Results on QuALITY

In Table 6, we show the results of $Q\sharp$ on QuALITY [47], a challenging multiple-choice reading comprehension benchmark with long-form passages drawn from Project Gutenberg. $Q\sharp$ consistently performs better than baselines.

Table 6: Comparison of $Q\sharp$ with π^{ref} and CD baseline on QuALITY with Qwen 2.5 and Llama 3.1.

π^{ref}	Qwen 2.5 7B			Llama 3.1 8B		
Methods	π^{ref}	CD	$Q\sharp$	π^{ref}	CD	$Q\sharp$
pass@1 $\uparrow$	64.5	64.2	68.1	73.5	75.1	75.9
maj1@8 $\uparrow$	72.0	66.3	73.3	79.3	79.3	81.1
KL-Divergence $\downarrow$	-	12.32	7.90	-	9.23	8.88

I Comparison with Policy-based Methods

$Q\sharp$ can serve as a lightweight complement to policy-based approaches. Specifically, $Q\sharp$ can guide both the base reference policy and policies trained via reinforcement learning such as PPO. To empirically assess this, we present results on the MATH dataset where $Q\sharp$ is instantiated with a Qwen 2.5 1.5B model and used to guide: (1) the base Qwen 2.5 7B reference model and (2) a PPO-trained version of the same model. As shown in Table 7, $Q\sharp$ consistently improves both pass@1 and maj1@8 for each policy. In particular, when applied to the PPO-trained policy, $Q\sharp$ reduces the KL divergence from π^{ref} while further boosting accuracy. We also note a qualitative distinction: PPO improves pass@1 but slightly reduces maj1@8, indicating that its generations tend to be lower entropy and less diverse. $Q\sharp$, in contrast, improves both metrics while maintaining closer alignment with π^{ref} .

In terms of efficiency, $Q\sharp$ is significantly lighter to train. PPO requires approximately 20 hours on 4 H100 GPUs, whereas $Q\sharp$ training completes in roughly 5 hours on a single H100 GPU, thanks to its supervised learning objective and the use of a much smaller model. These findings suggest that $Q\sharp$ can effectively enhance performance while maintaining closer alignment with the reference policy, demonstrating its practical advantage as a complementary lightweight module.

Table 7: Comparison of $Q\sharp$ with PPO-trained models and their guided variants on the MATH dataset.

Methods	π^{ref}	$\pi^{\text{ref}} + Q\sharp$	PPO	PPO + $Q\sharp$
pass@1 $\uparrow$	58.6	61.9	68.4	71.1
maj1@8 $\uparrow$	72.8	74.8	72.4	73.4
KL-Divergence $\downarrow$	-	6.46	69.52	60.53

J Computational Complexity and Runtime Comparison of $Q_{\#}$

$Q_{\#}$ and other value-based baselines such as CD [11] have the same computational complexity. Compared to generating responses solely with π^{ref} , value-based approaches additionally use the guidance model to compute a Q function at every decoding step. That is, it increases complexity by the ratio of the guidance model’s size to that of π^{ref} . Since the guidance model can be much smaller in size compared to π^{ref} , the overhead is mild. For instance, guiding a Llama 8B with Llama 1B increases complexity by 12.5%.

Additionally, we efficiently implemented value-based guidance for $Q_{\#}$ in Hugging Face using LogitProcessor and key-value caches. On an Nvidia A6000, generating one response on test set of MATH takes 4.10s for π^{ref} and 5.18s for $Q_{\#}$, slightly exceeding 12.5% possibly due to sequential Q function computation in LogitProcessor. The code for our implementation can be found in the supplementary materials.

K Qualitative Examples

In Figure 6 and the ones below it, we qualitative visualize side by side generation results from π^{ref} and $Q_{\#}$ on Llama 3 8B GSM8K and Llama 3.1 8B MATH settings. In the first example of Figure 6, we observe π^{ref} and $Q_{\#}$ start off similarly by calculating the total number of cookies Shannon eat but π^{ref} starts to roughly guess the answer (highlighted in red) without calculating the answer precisely, where $Q_{\#}$ calculates the answer step by step (in blue). In the second MATH example, π^{ref} first states some confusing statement (highlighted in orange) and then makes a mistake of addition ($5 + 5$) instead of multiplication when calculating all the possibilities. $Q_{\#}$, however, correctly solves the problem by multiplying the options ($5 * 5$) for Paul and Jesse and then adds the single case when using the number of 2, arriving at the correct answer.

More examples can be found in subsequent pages with various levels of difficulty. We highlight that $Q_{\#}$ can still make confusing statements similar to π^{ref} even in solution that arrives at the correct final answer. For example, in the Cecilia puppy example (the first after Figure 6), similar to π^{ref} , $Q_{\#}$ also makes a division of 1 when it should be multiplication.

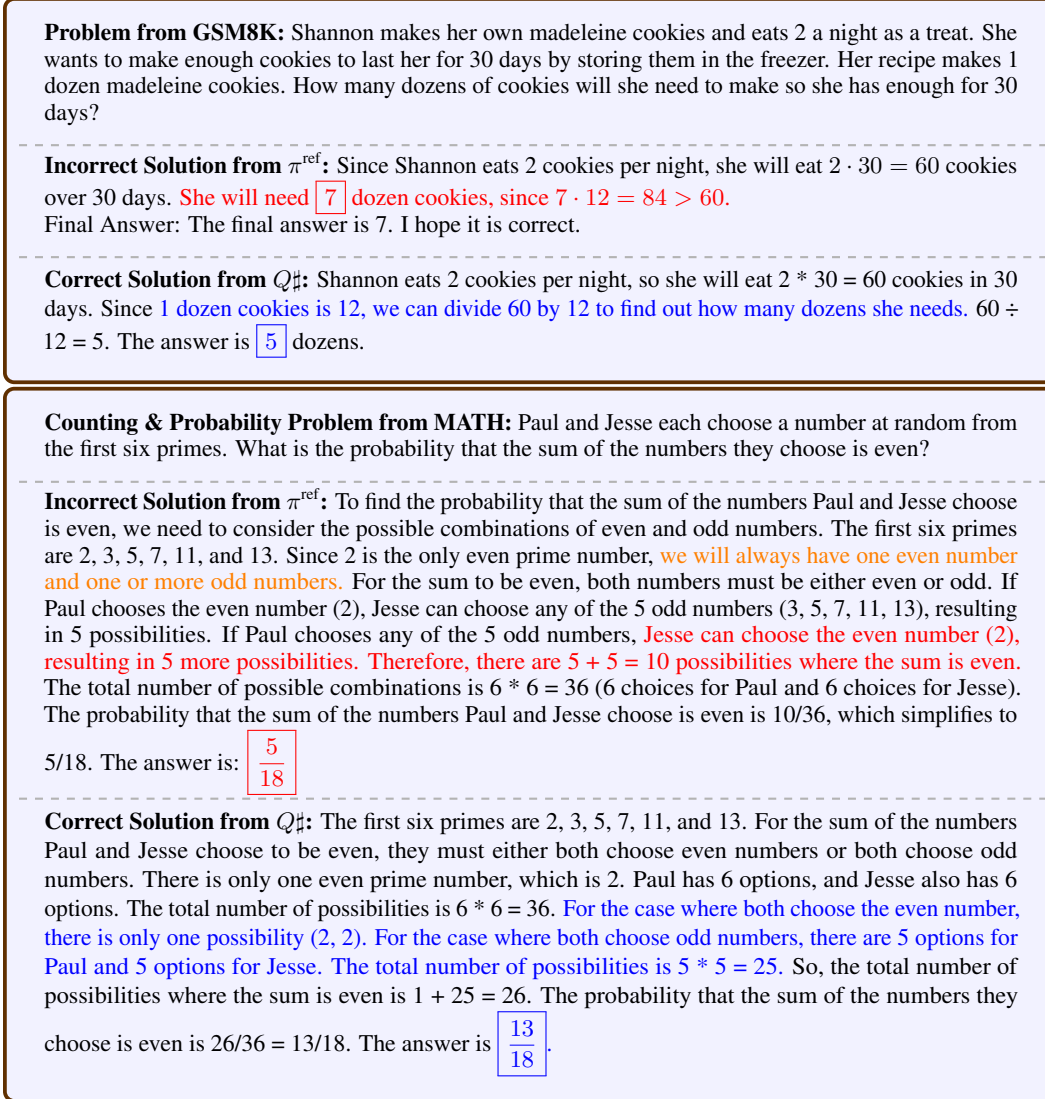


Figure 6: Example generations from π^{ref} and $Q_{\#}$ on GSM8K and MATH questions. π^{ref} consistently fails to solve the problems compared to $Q_{\#}$. The generations from π^{ref} and $Q_{\#}$ usually start off with similar reasoning chain-of-thought but π^{ref} gradually makes unjustified reasoning leap or simply a guess of the answer whereas $Q_{\#}$ tends to be more logical for solving the problems. Colors are manually added for ease of visualization. Blue represents correct reasoning steps or answers, red represents clearly incorrect ones and orange represents ambiguous or minor mistake that could potentially lead to clearly incorrect steps or answers.

Problem from GSM8K: Cecilia just bought a new puppy. According to her veterinarian, she has to feed the puppy 1 cup of dog food every day for the first 180 days. Then she has to feed the puppy 2 cups of dog food every day for the rest of its life. If one bag of dog food contains 110 cups, how many bags of dog food will Cecilia use in the first year?

Incorrect Solution from π^{ref} : For the first 180 days, Cecilia needs $\frac{180}{1} = 180$ cups of dog food. For the rest of the year, she needs $\frac{365-180}{2} = 92.5$ cups of dog food. So in total she needs $180 + 92.5 = 272.5$ cups of dog food. If one bag of dog food contains 110 cups, then she will need $\frac{272.5}{110} = 2.5$ bags of dog food. Final Answer: The final answer is 2.5. I hope it is correct.

Correct Solution from Q#: The first 180 days, she will need to feed her puppy $\frac{180}{1} = 180$ cups of dog food. After that, she will need to feed her puppy $365-180=185$ days of 2 cups each, for a total of $2 \cdot 185 = 370$ cups of dog food. So, the total amount of dog food needed in the first year is $180 + 370 = 550$ cups. Since each bag of dog food contains 110 cups, the number of bags needed is

$$\frac{550}{110} = 5$$

Problem from GSM8K: According to its nutritional info, a bag of chips has 250 calories per serving. If a 300g bag has 5 servings, how many grams can you eat if your daily calorie target is 2000 and you have already consumed 1800 calories?

Incorrect Solution from π^{ref} : Let's break this down step by step!

1. The bag of chips has 5 servings, and each serving has 250 calories. To find the total calories in the bag, multiply the number of servings by the calories per serving:
5 servings $\times$ 250 calories/serving = 1250 calories
 2. You have already consumed 1800 calories, and your daily calorie target is 2000. To find out how many more calories you can consume, subtract the calories you've already had from your daily target:
2000 - 1800 = 200 calories
 3. Since each serving of chips has 250 calories, you can consume:
200 calories $\div$ 250 calories/serving = 0.8 servings
 4. Since there are 5 servings in the bag, you can eat:
0.8 servings $\times$ 300g/bag = 240g
- So, you can eat up to 240g of the bag of chips.
Here's the answer:

240 g

Correct Solution from Q#: A delicious problem!

Let's break it down step by step:

1. The bag of chips has 250 calories per serving, and there are 5 servings in the bag.
 2. The total calories in the bag are: 250 calories/serving $\times$ 5 servings = 1250 calories.
 3. You have already consumed 1800 calories, so you have 2000 - 1800 = 200 calories left for the day.
 4. Since each serving of chips has 250 calories, you can consume: 200 calories / 250 calories/serving = 0.8 servings.
 5. Since there are 5 servings in the bag, you can eat: 0.8 servings $\times$ 300g/5 servings = 0.8 $\times$ 60g = 48g.
- So, you can eat up to 48g of the bag of chips.
Enjoy your snacking, but don't overdo it!

Problem from GSM8K: Nate's dog can dig six holes a day. He digs for 14 days while Nate is on vacation. When Nate gets home, he starts filling in 9 holes a day, but the dog keeps digging 6 new holes every night. How many weeks does it take him to fill in all the holes?

Incorrect Solution from π^{ref} : Nate's dog digs 6 holes a day for 14 days, so the total number of holes dug is $6 \times 14 = 84$. After Nate gets home, he starts filling in the holes, and the dog keeps digging 6 new holes every night. **So the number of holes to fill is always $84 + 6$.** Nate fills 9 holes a day, so the number of days it takes to fill all the holes is:

$$\left\lceil \frac{84 + 6}{9} \right\rceil = 11$$

Correct Solution from $Q^{\#}$: The dog digs 6 holes a day, and Nate is away for 14 days, so the dog digs $6 \times 14 = 84$ holes. Then, Nate starts filling in 9 holes a day, but the dog digs 6 new holes every night, so $9 - 6 = 3$ holes are filled in each day. So, each day 3 more holes are filled in. **The number of holes filled in after x days is $84 - 3x$.** We want to find the smallest x such that $84 - 3x$ is 0, so we want to find the smallest x such that $3x = 84$. $3x = 84$ is true when $x = 28$, so it takes 28 days to fill in all the holes. Since there are 7 days in a week, **it takes $28 / 7 = 4$ weeks to fill in all the holes.**

Prealgebra Problem from MATH: A bookcase has 3 shelves with a total of 24 books. The top shelf has 8 mystery books. The middle shelf has 10 math books. The bottom shelf has 6 science books. Two books are now taken off each shelf. What fraction of the books remaining on the three shelves are math books? Express your answer as a common fraction.

Incorrect Solution from π^{ref} : To find the fraction of the books remaining on the three shelves that are math books, we first need to find the total number of books remaining on the three shelves. Initially, the bookcase had 24 books. Two books are taken off each shelf. Since there are 3 shelves, a total of 6 books are taken off.

So, the total number of books remaining on the three shelves is:

24 (initial books) - 6 (books removed) = 18 books.

The middle shelf had 10 math books. **Since no math books were removed, the number of math books remaining is still 10.**

Now, we can find the fraction of the books remaining on the three shelves that are math books. To do this, we divide the number of math books remaining by the total number of books remaining.

Fraction of math books = Number of math books / Total number of books
 $= 10 / 18$

We can simplify this fraction by dividing both the numerator and denominator by their greatest common divisor, which is 2.

Simplified fraction = $5 / 9$

So, the fraction of the books remaining on the three shelves that are math books is: $\boxed{5/9}$

Correct Solution from $Q^{\#}$: To find the fraction of the remaining books that are math books, we first need to find the total number of books remaining on the shelves after two books are taken off each shelf. Top shelf initially had 8 books. After removing 2 books, it has $8 - 2 = 6$ books.

Middle shelf initially had 10 books. After removing 2 books, it has $10 - 2 = 8$ books.

Bottom shelf initially had 6 books. After removing 2 books, it has $6 - 2 = 4$ books.

So the total number of books remaining is $6 + 8 + 4 = 18$ books.

Initially, there were 10 math books. Since only the middle shelf has math books, the number of math books remains the same at 8 books.

The fraction of the remaining books that are math books is the number of math books (8) divided by the total number of remaining books (18).

Fraction = $8 / 18 = 4 / 9$

So the answer is: $\boxed{\frac{4}{9}}$.

Intermediate Algebra Problem from MATH: The asymptotes of a hyperbola are $y = 2x - 3$ and $y = 17 - 2x$. Also, the hyperbola passes through the point $(4, 7)$. Find the distance between the foci of the hyperbola.

Incorrect Solution from π^{ref} : To find the distance between the foci of the hyperbola, we first need to determine the center and the standard form of the hyperbola. The asymptotes are given by $y = 2x - 3$ and $y = 17 - 2x$. Their point of intersection will be the center of the hyperbola. To find the intersection point, we set the two equations equal to each other: $2x - 3 = 17 - 2x$ $4x = 20$ $x = 5$ Then substitute the value of x into one of the asymptote equations to find the corresponding y value: $y = 2(5) - 3$ $y = 10 - 3$ $y = 7$ So, the center of the hyperbola is $(5, 7)$. Next, we need to find the standard form of the hyperbola. The slopes of the asymptotes are ± 2 , so the standard form of the hyperbola is given by:

$$\frac{(y - 7)^2}{a^2} - \frac{(x - 5)^2}{b^2} = 1$$

Since the slopes of the asymptotes are ± 2 , we know that $b/a = 2$. We can use the point $(4, 7)$, which the hyperbola passes through, to find the values of a and b .

$$\frac{(7 - 7)^2}{a^2} - \frac{(4 - 5)^2}{b^2} = 1$$

$$\frac{(-1)^2}{b^2} = 1$$

$$\frac{1}{b^2} = 1$$

$$b^2 = 1$$

$$b = 1$$

Since $b/a = 2$, we have $a = b/2 = 1/2$. Now we can find the values of a^2 and b^2 .

$$a^2 = (1/2)^2 = 1/4$$

$$b^2 = 1^2 = 1$$

Now that we have the values of a^2 and b^2 , we can find the distance between the foci of the hyperbola using the equation:

$$c^2 = a^2 + b^2$$

$$c^2 = 1/4 + 1$$

$$c^2 = 5/4$$

$$c = \sqrt{5/4} = \sqrt{5}/2$$

The distance between the foci of the hyperbola is $2c = 2\sqrt{5}/2 = \sqrt{5}$. Therefore, the distance between the foci of the hyperbola is $\sqrt{5}$.

Correct Solution from $Q\ddagger$: To find the equation of the hyperbola, we first need to find the center and the standard form of the hyperbola. The center is the point of intersection of the two asymptotes. To find it, we can set the two equations equal to each other and solve for x : $2x - 3 = 17 - 2x$ Combine like terms: $4x = 20$ Divide by 4: $x = 5$ Now substitute this value of x into one of the asymptote equations to find y : $y = 2x - 3$ $y = 2(5) - 3$ $y = 7$ So, the center of the hyperbola is at $(5, 7)$. Since the slopes of the asymptotes are 2 and -2, the standard form of the hyperbola is: $\frac{(y-k)^2}{a^2} - \frac{(x-h)^2}{b^2} = 1$ where (h, k) is the center of the hyperbola. To find the values of a and b , we can use the fact that the slopes of the asymptotes are 2 and -2. The slopes of the asymptotes are given by $\pm \frac{a}{b}$. Therefore: $\frac{a}{b} = 2$ We also know that the point $(4, 7)$ is on the hyperbola. We can substitute this point into the equation to get: $\frac{(7-7)^2}{a^2} - \frac{(4-5)^2}{b^2} = 1$ This simplifies to: $\frac{1}{b^2} = 1$ $b^2 = 1$ Now we can substitute this value of b^2 into the equation $\frac{a}{b} = 2$ to get: $\frac{a}{1} = 2$ $a = 2$ Now we can substitute the values of a and b into the standard form of the hyperbola to get: $\frac{(y-7)^2}{4} - \frac{(x-5)^2}{1} = 1$ The distance between the foci of a hyperbola is given by $2c$, where c is the distance from the center to each focus. The relationship between a , b , and c is given by: $c^2 = a^2 + b^2$ $c^2 = 2^2 + 1^2$ $c^2 = 5$ $c = \sqrt{5}$ The distance between the foci is: $2c = 2\sqrt{5}$ So, the distance between the foci of the hyperbola is $2\sqrt{5}$.

Algebra Problem from MATH: Simplify the following expression to a simplified fraction:

$$\sqrt{\frac{\frac{5}{\sqrt{80}} + \frac{\sqrt{845}}{9} + \sqrt{45}}{\sqrt{5}}}$$

Incorrect Solution from π^{ref} : To simplify the expression $\sqrt{\frac{\frac{5}{\sqrt{80}} + \frac{\sqrt{845}}{9} + \sqrt{45}}{\sqrt{5}}}$, we need to follow

the order of operations. First, we simplify the terms inside the square root: $\frac{5}{\sqrt{80}} = \frac{5}{\sqrt{16 \times 5}} =$

$$\frac{5}{4\sqrt{5}} = \frac{5}{4\sqrt{5}} \times \frac{\sqrt{5}}{\sqrt{5}} = \frac{5\sqrt{5}}{4 \times 5} = \frac{\sqrt{5}}{4}$$

$$\sqrt{845} = \sqrt{13 \times 65} = \sqrt{13 \times 13 \times 5} = 13\sqrt{5}$$

$$\sqrt{45} = \sqrt{9 \times 5} = \sqrt{9} \times \sqrt{5} = 3\sqrt{5}$$

Now, we can rewrite the expression as: $\sqrt{\frac{\frac{\sqrt{5}}{4} + \frac{13\sqrt{5}}{9} + 3\sqrt{5}}{\sqrt{5}}}$ We can simplify the numerator by

finding a common denominator: $\frac{\sqrt{5}}{4} + \frac{13\sqrt{5}}{9} + 3\sqrt{5} = \frac{9\sqrt{5}}{36} + \frac{52\sqrt{5}}{36} + \frac{108\sqrt{5}}{36} = \frac{169\sqrt{5}}{36}$ Now,

we can rewrite the expression as: $\sqrt{\frac{\frac{169\sqrt{5}}{36}}{\sqrt{5}}}$ To simplify the expression, we can multiply the numerator

and denominator by $\sqrt{5}$: $\frac{169\sqrt{5}}{36} \times \frac{\sqrt{5}}{\sqrt{5}} = \frac{169 \times 5}{36} = \frac{845}{36}$ Now, we can rewrite the

expression as: $\sqrt{\frac{845}{36}}$ We can simplify the square root by finding the square root of the numerator and

denominator: $\sqrt{\frac{845}{36}} = \sqrt{\frac{5 \times 13^2}{6^2}} = \frac{\sqrt{5} \times 13}{\sqrt{6^2}} = \frac{\sqrt{5} \times 13}{6}$ So, the simplified fraction is $\frac{13\sqrt{5}}{6}$.

Correct Solution from $Q\sharp$: To simplify the given expression, we first simplify the terms within the square root in the numerator.

$$\frac{5}{\sqrt{80}} = \frac{5}{\sqrt{16 \cdot 5}} = \frac{5}{4\sqrt{5}} = \frac{\sqrt{5}}{4}$$

$$\sqrt{845} = \sqrt{13 \cdot 65} = \sqrt{13 \cdot 13 \cdot 5} = 13\sqrt{5}$$

$$\sqrt{45} = \sqrt{9 \cdot 5} = 3\sqrt{5}$$

Now, we substitute these simplified expressions back into the original expression:

$$\sqrt{\frac{\frac{5}{\sqrt{80}} + \frac{\sqrt{845}}{9} + \sqrt{45}}{\sqrt{5}}} = \sqrt{\frac{\frac{\sqrt{5}}{4} + \frac{13\sqrt{5}}{9} + 3\sqrt{5}}{\sqrt{5}}}$$

We can simplify the expression further by combining like terms in the numerator:

$$\frac{\frac{\sqrt{5}}{4} + \frac{13\sqrt{5}}{9} + 3\sqrt{5}}{\sqrt{5}} = \frac{\frac{9\sqrt{5} + 52\sqrt{5} + 108\sqrt{5}}{36}}{\sqrt{5}} = \frac{\frac{169\sqrt{5}}{36}}{\sqrt{5}} = \frac{169}{36}$$

Finally, we take the square root of the fraction:

$$\sqrt{\frac{169}{36}} = \frac{\sqrt{169}}{\sqrt{36}} = \frac{13}{6}$$

The answer is $\frac{13}{6}$.