Evolutionary Guided Decoding: Iterative Value Refinement for LLMs

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Abstract

While guided decoding, especially value-guided methods, has emerged as a cost-effective alternative for controlling language model outputs without re-training models, its effectiveness is limited by the accuracy of the value function. We identify that this inaccuracy stems from a core distributional gap: existing methods train static value functions on trajectories sampled exclusively from the base policy, which inherently confines their training to a narrow and suboptimal view of the potential output space. We propose Iterative Value Refinement, a evolutionary framework designed to narrow this gap. It employs Value Exploration to provide a more comprehensive and robust training signal, complemented by Iterative Self-Refinement, which uses the improved value function from one iteration to guide the generation of higher-quality data for the next. Extensive experiments on text summarization, multi-turn dialogue, and instruction following demonstrate the effectiveness of our framework in aligning language models. Our approach not only achieves alignment but also significantly reduces computational costs by leveraging principled value function optimization for efficient and effective control.

1 Introduction

Reinforcement Learning from Human Feedback (RLHF) (Christiano et al., 2017; Bai et al., 2022; Ouyang et al., 2022) has emerged as a widely adopted approach to align advanced language models with human values and task requirements (Wei et al., 2022; Achiam et al., 2023; Chao et al., 2024; Su et al., 2024a). However, traditional RLHF methods like Proximal Policy Optimization (PPO) (Christiano et al., 2017; Ouyang et al., 2022) suffer from high computational costs and training instability (Zheng et al., 2023b; Rafailov et al., 2024), limiting their practicality for applications requiring flexible behavior control. Among various alternatives, **guided decoding** methods have gained increasing attention as they can steer model's generation without expensive model re-training (Snell et al., 2022; Mudgal et al., 2023; Han et al., 2024; Chakraborty et al., 2024).

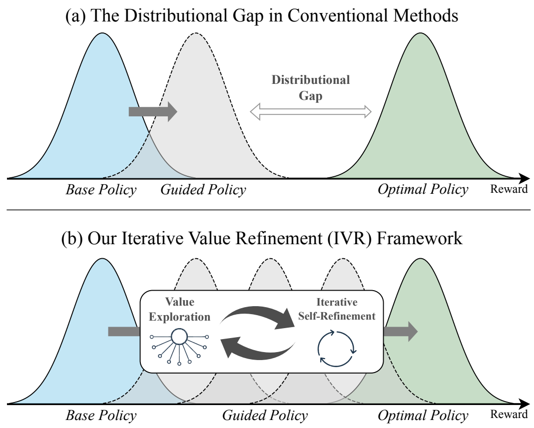

Figure 1: (a) Conventional methods suffer from a distributional gap, limiting the guided policy from reaching optimal rewards. (b) Our Iterative Value Refinement framework narrows this gap through Value Exploration and Iterative Self-Refinement.

Within this framework, value-guided approaches, which train a value function V_θ to evaluate partial outputs and steer the language model towards high-reward trajectories, have emerged as particularly promising (Yang and Klein, 2021; Qin et al., 2022; Mudgal et al., 2023; Han et al., 2024). Under the KL-regularized Reinforcement Learning framework, given an optimal value function V^*, they can derive a policy that maximizes expected rewards while maintaining a bounded KL-divergence from the base policy π_{base}.

As visualized in Figure 1(a), while guided decoding with an estimated value function can shift the base policy's output distribution towards higher-reward regions, this improvement remains suboptimal compared to the theoretical maximum achiev-

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able through the optimal value function V^*. We argue this suboptimality is rooted in the **distributional gap** between the learned value function and the optimal value function. Specifically, existing methods (Khanov et al., 2024; Mudgal et al., 2023) train a static value function on trajectories sampled exclusively from the base policy π_{base}, which inherently confines its training to a narrow and suboptimal view of the potential output space. The limitation leads to substantial suboptimality in value function estimation, ultimately hindering decoding effectiveness.

To mitigate this distributional gap, we introduce **I**terative **V**alue **R**efinement (IVR), as shown in Figure 1(b), a unified, self-bootstrapping framework that systematically improves the value function's accuracy and robustness. It employs *Value Exploration*, which generates multiple trajectories per prompt to provide a more comprehensive and robust training signal for each update. This is complemented by *Iterative Self-Refinement*, where the learned value function from one iteration guides the generation of higher-quality data, progressively narrowing the distributional gap. Through this evolutionary refinement, IVR allows the value function to iteratively improve, enabling it to more accurately identify high-reward trajectories far beyond the scope of the initial base policy. Unlike traditional online RLHF methods that require repeatedly collecting preference data and retraining the policy model, IVR achieves policy improvement by optimizing only the value function, substantially reducing computational costs while maintaining the benefits of iterative refinement.

Our main contributions are summarized as following:

- We introduce IVR, a novel framework that narrows the distributional gap in value function training by unifying *Value Exploration* and *Iterative Self-Refinement*, enabling the value function to be iteratively improved for greater accuracy and robustness.
- We demonstrate the generalizability and effectiveness of IVR by conducting extensive experiments across a variety of challenging tasks, including text summarization, multi-turn dialogue, and instruction following, showing consistent improvement in performance over existing approaches. Our method outperforms baseline methods in terms of reward scores across all evaluated tasks, which is further corroborated by a 77.52% GPT-4 win rate on the Multi-turn Dialogue task against the base policy.
- We conduct extensive empirical analysis on the impact of sampling trajectories and training iterations, providing practical insights for implementing value-guided decoding methods.

2 Preliminaries

2.1 The Token-level Markov Decision Process for RLHF

We define the text generation mechanism of large language models (LLMs) as a token-level Markov Decision Process (MDP). Define the tuple $\mathcal{M} = (\mathbf{S}, \mathbf{A}, f, \mathbf{R}, \rho)$, where $\mathbf{S}$ denotes the state space encompassing all previously generated tokens (i.e., $s_t = \{x_0, \ldots, x_m, y_0, \ldots, y_t\}$). Here, $x_0, \ldots, x_m$ are tokens from the initial prompt $\mathbf{x}$, and $y_0, \ldots, y_t$ are tokens generated by the model up to time t. The action space $\mathbf{A}$ represents the vocabulary of tokens. The function f, representing deterministic transitions between states, is defined as $f(s, a) = s \oplus a$, where $\oplus$ indicates concatenation and $a \in \mathbf{A}$. The initial state distribution ρ is defined over the prompts $\mathbf{x}$, with each initial state s_1 comprising the tokens from $\mathbf{x}$. $\mathbf{R} : \mathbf{S} \times \mathbf{A} \to \mathbb{R}$ represents the token-level reward.

KL-regularized RL and Optimal Policy. The objective of KL-regularized RLHF can be formulated as the following optimization problem:

$$\max_{\pi} \mathbb{E}_{y\sim\pi}[\mathbf{R}(\mathbf{x}, \mathbf{y})] \quad s.t. \quad D_{KL}(\pi || \pi_{base}) < \epsilon, \tag{1}$$

where $D_{KL}(\pi||\pi_{base})$ denotes the KL divergence between the policy π and the base policy π_{base}.

Following the prior line of works (Peters and Schaal, 2007; Peng et al., 2019), the closed form solution to the KL-regularized RL problem can be represented as:

$$\pi^*(y_{t+1}|\mathbf{x}, y_{\leq t}) \propto \pi_{base}(y_{t+1}|\mathbf{x}, y_{\leq t}) e^{\beta \mathbf{Q}^*(y_{t+1}|\mathbf{x}, y_{\leq t})}, \tag{2}$$

where β is a control parameter characterizing the trade-off between the reward and the KL divergence. Given the deterministic transition model f, the expected future reward after action y_{t+1}, or Q-value $\mathbf{Q}^*(y_{t+1}|\mathbf{x}, y_{\leq t})$, equates to the value of the subsequent state. The Q-value of taking a specific action y_{t+1} at the current state can be then transformed into the state value of their concatenation:

$$\mathbf{Q}^*(y_{t+1}|\mathbf{x}, y_{\leq t}) = \mathbf{V}^*(\mathbf{x}, y_{\leq t} \oplus y_{t+1}) = \mathbf{V}^*(\mathbf{x}, y_{\leq t+1}). \tag{3}$$

Thus, the optimal policy in Equation 2 is rewritten as

$$\pi^*(y_{t+1}|\mathbf{x}, y_{\le t}) \propto \pi_{base}(y_{t+1}|\mathbf{x}, y_{\le t}) e^{\beta \mathbf{V}^*(\mathbf{x}, y_{\le t+1})}. \quad (4)$$

2.2 LLM Alignment via Value-Guided Search

The problem of LLM alignment can be formally defined as solving for the optimal decoding policy π^* under the token level MDP $\mathcal{M}$ in Equation 4. Here, we present two search strategies for decoding.

Value Guided Top-k Sampling. A prevalent strategy to address the computational expense of calculating values for all possible subsequent tokens is to compute values only for the top-k tokens as determined by the base policy at each step:

$$\pi(y_{t+1}|\mathbf{x}, y_{\le t}) \propto \begin{cases} \pi_{base}(y_{t+1}|\mathbf{x}, y_{\le t}) e^{\beta \mathbf{V}^*(\mathbf{x}, y_{\le t+1})} & y_{t+1} \in \text{top-k} \\ \pi_{base}(y_{t+1}|\mathbf{x}, y_{\le t}) e^{\beta \mathbf{V}^*(\mathbf{x}, y_{\le t})} & y_{t+1} \notin \text{top-k} \end{cases} \quad (5)$$

In our pilot experiments, we found that the value-guided sampling can be further simplified by perturbing the distribution at the block-level instead of the token-level. This modification strikes a better balance between performance and efficiency, preserving effectiveness while enhancing inference speed. For more details, please refer to Appendix A.

Value Guided Blockwise Beam Search. Without considering the KL constraint, we propose value guided blockwise beam search to leverage the value function for decoding-time alignment. At each step, for each of the B candidate sequences, we sample B continuation blocks $y_{t:t+b}$ and rank all B^2 sequences according to $V_\theta(\mathbf{x}, y_{\le t} \oplus y_{t:t+b})$. The top B sequences are retained as candidates for the next iteration until generation is complete, after which the sequence with the highest value score is selected as the output.

3 Methodology

Challenges of Training Optimal Value Function. A significant challenge in implementing value-guided sampling is the necessity of accessing the optimal value function $\mathbf{V}^*(s_t)$ for each state s_t. This function denotes the maximum expected reward that can be achieved from state $s_t = (\mathbf{x}, y_{\le t})$ when following the optimal policy π^*, until a complete answer $\mathbf{y}$ is generated. The function is defined as:

$$\mathbf{V}^*(\mathbf{x}, y_{\le t}) = \mathbb{E}_{\mathbf{y} \sim \pi^*(\cdot|\mathbf{x}, y_{\le t})} \mathbf{R}(\mathbf{x}, \mathbf{y}). \quad (6)$$

In practice, $\mathbf{V}^*(\mathbf{x}, y_{\le t})$ remains inaccessible, as it relies on the trajectory produced by the unattainable optimal policy π^*. Existing methods (Khanov et al., 2024; Mudgal et al., 2023) employ the base policy π_{base} as an approximation for π^* to estimate the optimal value function. However, these approaches often yield significant suboptimality due to the **distributional gap** between π_{base} and π^*. Specifically, training the value function exclusively on trajectories sampled from the base policy π_{base} confines its learning to a narrow and suboptimal view of the potential output space. This fundamental limitation leads to substantial suboptimality in value function estimation, as the learned function fails to accurately evaluate states that lie outside the base policy's typical trajectory distribution, ultimately hindering the effectiveness of guided decoding.

Overview. In this paper, we introduce **I**terative **V**alue **R**efinement to mitigate the distributional gap between the estimated value function and the optimal value function for guided decoding (refer to Algorithm 1 for the complete process). Our approach comprises two key components that work synergistically within a unified framework. First, we introduce *Value Exploration*, which expands the search space through multi-trajectory sampling to provide a more comprehensive and robust training signal for value function estimation. Second, we propose *Iterative Self-Refinement*, which leverages the improved value function from last iteration to guide the generation of higher-quality trajectories for the next iteration. This iterative process progressively narrows the distributional gap by enabling the value function to explore and learn from increasingly high-reward regions of the output space, thereby enhancing response quality during decoding.

3.1 Iterative Value Refinement

Our iterative value refinement framework unifies Value Exploration and Iterative Self-Refinement into a cohesive approach that systematically improves value function accuracy through progressive refinement. The two components work in tandem: Value Exploration provides comprehensive training signals at each iteration, while Iterative Self-Refinement ensures that each subsequent iteration operates on higher-quality data than the previous one.

Value Exploration. We introduce Value Exploration, which utilizes stochastic sampling to improve the accuracy of value function estimation by exploring a wider range of possible trajectories. Specifically, for a given prompt $\mathbf{x}$, we generate multiple outputs by performing stochastic sampling with the current policy. These outputs are then evaluated using the reward model $\mathbf{R}$, which reflects alignment with human preferences.

By sampling several trajectories and collecting their corresponding rewards, we can effectively train our value function with a more comprehensive and robust training signal. For each state $s_t = (\mathbf{x}, y_{\leq t})$ in the trajectory $\mathbf{y}$, the estimated value for the current state is defined as:

$$\tilde{\mathbf{V}}^*(\mathbf{x}, y_{\leq t}) = \mathbf{R}(\mathbf{x}, \mathbf{y}). \tag{7}$$

We then optimize $V_\theta(\mathbf{x}, y_{\leq t})$, parameterized by θ, to match $\tilde{\mathbf{V}}^*(\mathbf{x}, y_{\leq t})$ using the following L_2 objective function:

$$\ell^*(\mathbf{x}, \mathbf{y}; \theta) = \mathbb{E}_{\mathbf{x}\sim\mu}\left[\frac{1}{2}\sum_{t\in[|\mathbf{y}|]}\left(V_\theta(\mathbf{x}, y_{\leq t}) - \mathbf{V}^*(\mathbf{x}, y_{\leq t})\right)^2\right], \tag{8}$$

where μ is a distribution over training prompts.

Iterative Self-Refinement. While Value Exploration enhances the exploration of potential trajectories through multi-trajectory sampling, the coverage of these trajectories is still inherently constrained by the current policy. To more effectively address the distributional gap from the optimal policy π^*, we propose Iterative Self-Refinement for progressively improving the value function. This strategy is founded on the principle that the optimized policy for the RL objective can be formulated as a value guided policy:

$$\pi_{V_\theta}(y_{\leq t+1}|\mathbf{x}, y_{\leq t}) \propto \pi_{\text{ref}}(y_{\leq t+1}|\mathbf{x}, y_{\leq t})e^{\beta V_\theta(\mathbf{x}, y_{\leq t+1})}. \tag{9}$$

We then collect higher-quality trajectories by sampling from the policy π_{V_θ}, which is guided by the current value function V_θ. This sampling process can be represented as follows:

$$\hat{\mathbf{y}} \sim \pi_{V_\theta}(\cdot|\mathbf{x}), \tag{10}$$

where $\hat{\mathbf{y}}$ denotes the complete trajectory sampled from the optimized policy π_{V_θ}, as defined in Equation 9.

With these higher-quality trajectories, we apply Value Exploration as outlined above. For each state $s_t = (\mathbf{x}, \hat{y}_{\leq t})$ in the sampled trajectory, we estimate its value as:

$$\tilde{\mathbf{V}}^*(\mathbf{x}, \hat{y}_{\leq t}) = \mathbf{R}(\mathbf{x}, \hat{\mathbf{y}}). \tag{11}$$

Algorithm 1 Iterative Value Refinement

Input: reward model R, base model π_{ref}, training dataset μ
Output: Value-guided policy π_{V_θ}, value function V_θ
  Initialize value function V_θ with pre-trained language model
  repeat
    – Step 1: Collect Multiple Trajectories –
    for $\mathbf{x}$ in μ **do**
      Sample K trajectories $\{\mathbf{y}_k\}_{k=1}^K \sim \pi_{base}(\cdot|\mathbf{x})$
      Compute rewards $\{r_k = \mathbf{R}(\mathbf{x}, \mathbf{y}_k)\}_{k=1}^K$
    end for
    – Step 2: Train the Value Function –
    For each trajectory state $s_t = (\mathbf{x}, y_t)$, set $\tilde{\mathbf{V}}^*(s_t) = \mathbf{R}(\mathbf{x}, \mathbf{y})$
    Optimize V_θ using $L^*(\theta)$, where:
    $L^*(\theta) = \mathbb{E}_{\mathbf{x}\sim\mu}[\frac{1}{2}\sum_{t\in[|y|]}(V_\theta(\mathbf{x}, y_{\leq t}) - \tilde{\mathbf{V}}^*(\mathbf{x}, y_{\leq t}))^2]$
    – Step 3: Policy Optimization –
    Define value-guided policy:
    $\pi_{V_\theta}(y_{t+1}|\mathbf{x}, y_{\leq t}) \propto \pi_{base}(y_{t+1}|\mathbf{x}, y_{\leq t})e^{\beta V_\theta(\mathbf{x}, y_{t+1})}$
    Update policy: $\pi_{base} \leftarrow \pi_{V_\theta}$
  until convergence

The value function V_θ is then optimized by minimizing the following loss function:

$$L^*(\theta) = \mathbb{E}_{\mathbf{x}\sim\mu}\left[\frac{1}{2}\sum_{t\in[|\hat{\mathbf{y}}|]}\left(V_\theta(\mathbf{x}, \hat{y}_{\leq t}) - \tilde{\mathbf{V}}^*(\mathbf{x}, \hat{y}_{\leq t})\right)^2\right]. \tag{12}$$

This process can be repeated iteratively, with each iteration using the improved value function to guide the generation of higher-quality data for further training. The synergy between Value Exploration and Iterative Self-Refinement enables our framework to progressively narrow the distributional gap and achieve more accurate value function estimation.

3.2 Why IVR Narrows the Distributional Gap

We provide an informal discussion of why IVR narrows the distributional gap, framed through the notion of *coverage* between the data-collecting distribution and the visitation measure of the optimal policy.

We use the standard visitation measure of policy π:

$$d^\pi(s, a) = \mathbb{E}_{s_1\sim\rho}\left[\sum_{h=1}^{H}\mathbb{P}(s_h = s, a_h = a \mid s_1)\right], \tag{13}$$

which captures how often the state-action pair (s, a) is visited when following π from initial states $s_1 \sim \rho$.

A recurring insight from offline and iterative RLHF is that the optimality gap between any approximate policy $\hat{\pi}$ and the optimal policy π^* is governed by how well the data-collecting distribution covers the visitation measure d^* of π^* (Xiong et al., 2024; Ye et al., 2024). When training data is sampled from a distribution far from d^*, the value function cannot accurately evaluate states encountered under π^*, leading to a large optimality gap.

IVR narrows this gap through two complementary mechanisms. *Value Exploration* broadens the support of the data-collecting distribution by sampling multiple trajectories per prompt rather than relying on a single rollout, providing wider coverage at each iteration. *Iterative Self-Refinement* progressively replaces the data-collecting policy π_{base} with the value-guided policy π_{V_θ}, whose visitation measure is biased toward higher-reward regions and therefore closer to d^*. Together, these two mechanisms iteratively shrink the coverage gap between $d^{\hat{\pi}}$ and d^*, which in turn reduces the optimality gap of the learned value function.

3.3 Connection to Online RLHF

Existing research indicates that online iterative RLHF can significantly enhance model performance (Xiong et al., 2024; Dong et al., 2024; Ye et al., 2024). In contrast to traditional online RLHF, which involves continuously collecting new preference data from the latest policy and retraining the policy model, our method eliminates the need for retraining. Instead, IVR focuses solely on optimizing the value function and employing guided decoding to iteratively improve the policy, thereby conserving computational resources.

4 Experiments

Experimental Setup. For the summarization and multi-turn dialogue tasks, we first establish a base policy by supervised fine-tuning a pre-trained language model on the respective datasets to acquire basic task-specific capabilities and desired behaviors. For the instruction following task, we directly utilize publicly available instruction-tuned models. In all experiments, we parameterize the value function as a pre-trained language model backbone with a linear layer on top. The data for training the value function is collected from the base policy with a sampling temperature of 0.7, and we label it with the corresponding reward model.

For IVR, we employ Value Exploration by sampling 4 different trajectories for each prompt to obtain robust value estimates. The training process involves two iterations of value function optimization to achieve better policy alignment. Starting from the second iteration, we collect training data using value-guided sampling with $\beta = 2$. More details can be found in Appendix B.

Evaluation Metrics. We adopt different evaluation metrics for our two decoding-time alignment strategies. For value-guided sampling, following (Gao et al., 2023; Han et al., 2024), we analyze the trade-off between reward and token-level KL divergence from the base policy. Specifically, we sweep the β in Equation 5 to control the KL divergence between the guided policy and base policy. For value guided blockwise beam search, we compare the reward of each algorithm. Additionally, as a supplementary evaluation to mitigate potential reward hacking issues (Amodei et al., 2016), we compute the win-rate between the guided policy and base policy using GPT-4-as-the-judge (Zheng et al., 2023a). We note that this serves as a complementary sanity check, while our primary conclusions are drawn from the objective reward and KL divergence metrics. The prompting template refers to Appendix C. To ensure the robustness of our evaluation, all experiments are conducted with 5 different random seeds.

4.1 Experiment 1: Summarization

Experiment Details. We conduct experiments on the `TL;DR` dataset (Stiennon et al., 2020), which consists of Reddit posts paired with two candidate summaries and human preferences between them. For efficiency, we randomly sampled 300 examples from the test set for evaluation. For the base policy, we fine-tune a Llama-3.2-3B (Dubey et al., 2024) model on the preferred summaries using supervised learning. To evaluate summary quality, we train a reward model using a Llama-3.2-1B (Dubey et al., 2024) backbone on the pairwise preference data through Bradley-Terry (BT) modeling. The value function is implemented as a Llama-3.2-1B model with an additional linear layer on top. More implementation details can be found in Appendix B.

Baselines. We compare our method against several recent decoding-time alignment approaches. **ARGS** (Khanov et al., 2024) directly leverages reward models as value functions for guided decoding without additional training, offering a lightweight solution. Using trajectories sampled from the base policy π_{base}, **FUDGE** (Yang and Klein, 2021; Mudgal et al., 2023) trains a prefix scorer to predict future attributes, while **VAS** (Han et al., 2024) employs TD(λ) learning to train a value function, providing a more sophisticated value estimation approach.

Results. As shown in Figure 2a, we analyze the trade-off between reward and KL divergence for different methods on the summarization task. IVR consistently outperforms all baselines across different KL divergence levels, achieving higher rewards while maintaining stable performance. Specifically, at KL divergence of 0.8, IVR reaches a reward of approximately 3.5, while other methods remain below 3.2. In contrast, baseline methods (FUDGE, VAS, and ARGS) show performance degradation when KL divergence exceeds 0.4, suggesting their limited capability in balancing policy preservation and performance optimization.

As shown in Figure 3a, all methods demonstrate improvements over the base policy (3.2) in value-guided blockwise beam search, with our IVR method achieving the highest performance (4.3). Specifically, ARGS yields a modest improvement to 3.55, while FUDGE and VAS demonstrate stronger performance at 4.05 and 4.15 respectively. The ablation of our method without Iterative Self-Refinement (IVR w/o Iter) achieves 4.25, highlighting the effectiveness of our Value Exploration approach. The full IVR method further improves the performance to 4.3, demonstrating the benefits of Iterative Self-Refinement.

4.2 Experiment 2: Multi-turn Dialogue

Experiment Details. We use the `Anthropic HH` (Bai et al., 2022) dataset, a multi-turn dialogue dataset focused on helpfulness and harmlessness, sampling 300 examples for evaluation. We train the base policy by fine-tuning Llama-3-8B (Dubey et al., 2024) on preferred responses. A Llama-3.2-1B model is trained as the reward model using BT on pairwise preference data. Llama-3.2-1B serves as the value function backbone. More details are in Appendix B.

Baselines. In addition to the aforementioned inference-based baselines (**ARGS**, **FUDGE**, and **VAS**), we also include several training-based baselines: Direct Preference Optimization (**DPO**) (Rafailov et al., 2024) and Identity Preference Optimization (**IPO**) (Azar et al., 2024). DPO directly fine-tunes the model for preference learning, eliminating the need for a reward model and RL stage for updates. IPO added a regularization term to the DPO objective to mitigate overfitted risk. We used the online version of DPO and IPO by rolling out the base policy and sampling two trajectories, optimizing objective on explicit rewards.

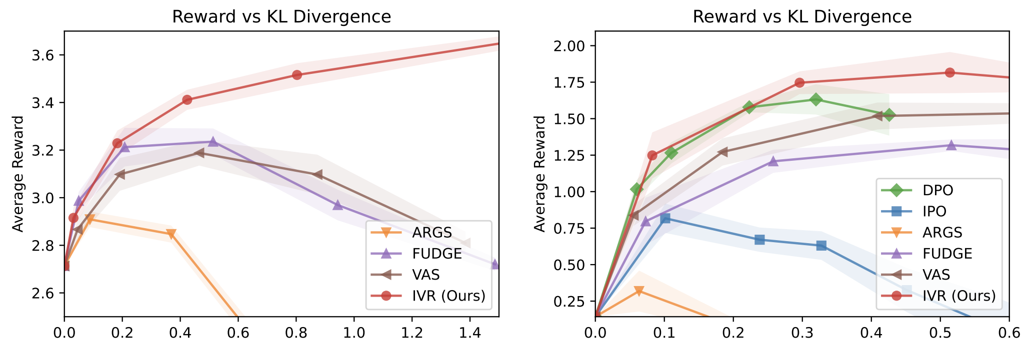
Methods	Win-Rate (%)	FLOPs ($\times 10^{15}$)
FUDGE	64.85	**0.25**
VAS	68.49	**0.25**
DPO	72.45	4.00
IPO	66.55	4.00
IVR (Ours)	**77.52**	2.00

Table 1: Comparison of different methods' win-rate against the base policy and estimated FLOPs. The win-rate values are obtained by GPT-4-as-the-judge on the Multi-turn Dialogue dataset. FLOPs are estimated on a single batch training.

Results. As demonstrated in Figure 2b, we evaluate different methods on the multi-turn dialogue task. Our method achieves the best performance across different KL divergence levels, reaching a reward of 1.75 at KL divergence of 0.3. DPO shows competitive performance initially but plateaus at a reward of 1.65, while VAS and FUDGE demonstrate moderate performance with rewards of 1.5 and 1.3 respectively. ARGS and IPO show limited effectiveness, with ARGS achieving minimal improvement and IPO's performance degrading significantly as KL divergence increases. Notably, IVR maintains stable performance even at higher KL divergence levels (0.4-0.6), while other methods either plateau or decline.

For value-guided blockwise beam search in Figure 3b, we observe a clear progression in performance across different methods. Starting from the base policy, ARGS provides initial improvements through direct reward model utilization, achieving a reward of 2.1. VAS and FUDGE demonstrate stronger performance at around 2.7, while the ablation of our method without iterative training (IVR w/o Iter) reaches 2.8. The full IVR method with iterative training achieves the best performance with a reward of 3.1. The significant performance gap between IVR and IVR w/o Iter (0.3) further validates the effectiveness of our iterative training strategy.

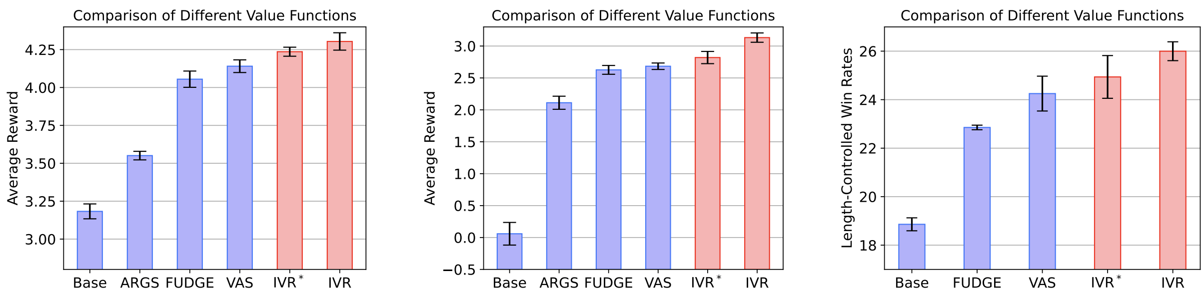
Additionally, as a supplementary evaluation, Table 1 shows that our IVR method achieves the highest GPT-4 win-rate of 77.52%, corroborating the reward-based findings above. IVR also demonstrates a significant advantage in computational efficiency, with FLOPs estimated at 2.00×10^{15}, which is half of that required by DPO and IPO under our experimental settings.



(a) Summarization

(b) Multi-turn Dialogue

Figure 2: Reward vs. KL divergence for different methods on (a) summarization and (b) multi-turn dialogue.



(a) Summarization

(b) Multi-turn Dialogue

(c) Instruction Following

Figure 3: Comparison of different value functions using value-guided blockwise beam search on summarization (left), multi-turn dialogue (middle) and instruction following (right). IVR* denotes IVR without Iterative Self-Refinement.

4.3 Experiment 3: Instruction Following

Experiment Details. We conduct experiments using the UltraFeedback (Cui et al., 2023) dataset with 10k sampled prompts for training. For evaluation, we use Alpaca-Eval 2 (Dubois et al., 2024), which assesses instruction-following via Length-controlled Win Rate with GPT-4 (Achiam et al., 2023). The base policy is Llama-3.2-3B-Instruct (Dubey et al., 2024), with Skywork-Reward-Llama-3.1-8B (Liu et al., 2024b) for reward modeling and Llama-3.2-1B-Instruct (Dubey et al., 2024) as the value function. For efficiency, we compare against FUDGE and VAS as decoding-time baselines. More details are in Appendix B.

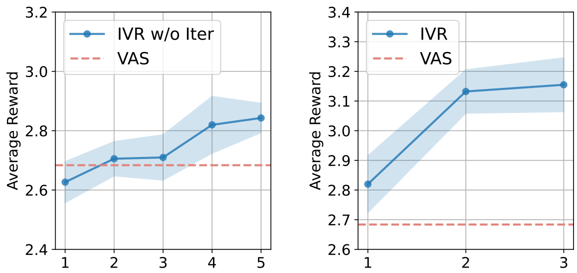
Results. For the instruction following task, we evaluate our method using Length-controlled Win Rate as the metric. As shown in Figure 3c, all methods demonstrate improvements over the base policy. Our IVR method achieves the best performance with a win rate of 26.0%, significantly outperforming both FUDGE and VAS. The consistent improvements across different methods indicate the effectiveness of value-guided decoding for instruction following. Notably, the performance gap between IVR and other methods suggests that our iterative value optimization approach is particularly beneficial for complex tasks like instruction following, where accurate value estimation is crucial for generating high-quality responses.

5 Further Analysis

This section analyzes IVR's key components, examining the impact of Value Exploration and training iterations on performance. We also evaluate the transferability of value functions across model scales and IVR's effectiveness in enhancing model safety against adversarial jailbreak attacks, demonstrating its broader applications.

5.1 The Number of Sampled Trajectories

To investigate the impact of Value Exploration, we analyze how the number of sampled trajectories affects value function performance. We conduct experiments on the multi-turn dialogue task using value-guided blockwise beam search, without Iterative Self-Refinement. The results are shown in Figure 4a. We observe that increasing the num-



(a) Number of ST (b) Number of TI

Figure 4: Ablation studies on (a) the number of sampled trajectories and (b) the number of training iterations in multi-turn dialogue using blockwise beam search. ST denotes sampled trajectories, TI denotes training iterations.

ber of sampled trajectories leads to consistent improvements. A more significant improvement is observed with 4 samples. Further increasing to 5 samples only brings a small additional improvement, suggesting that 4 trajectories provide a good balance between computational cost and performance. These results demonstrate that Value Exploration with multiple trajectories helps capture a more comprehensive view of possible outcomes, leading to more accurate value estimates and better guided generation.

5.2 The Number of Training Iterations

We analyze how the number of training iterations affects model performance. We conduct experiments on the multi-turn dialogue task using value-guided blockwise beam search, with the number of sampled trajectories fixed at 4 based on our previous findings. The results are shown in Figure 4b. Starting from one iteration, our method already outperforms VAS with an average reward of 2.82. The second iteration brings a substantial improvement, demonstrating the effectiveness of collecting training data from the guided policy. The third iteration yields a slight gain to 3.15, suggesting that two iterations provide sufficient policy alignment.

5.3 Value Function Transferability Across Model Sizes

We investigate the transferability of estimated value function across different model sizes on the instruction following task. Specifically, we examine whether a value function trained using data collected from a Llama-3.2-3B-Instruct can effectively guide models of different sizes (Llama-3.2-1B-Instruct and Llama-3-8B-Instruct) during value-guided blockwise beam search.

Model Size	Base	IVR	Δ
1B	-7.71	3.78	**11.49**
3B	1.56	13.34	**11.78**
8B	7.67	20.42	**12.75**

Table 2: Performance comparison between the base policy and value-guided blockwise beam search across different model sizes (1B, 3B, and 8B) on the instruction-following task. The value function is trained using data collected from the 3B base policy. The Δ column represents the absolute performance improvement.

Model	Safety Rate (%)
Aligned-Llama-3	92.87
+ Aligned Value Function	96.14
+ Unaligned Value Function	**97.48**
Unaligned-Llama-3	65.27
+ Aligned Value Function	81.04
+ Unaligned Value Function	**86.17**

Table 3: Comparison of safety rates between aligned and unaligned Llama-3 models with different value functions.

As shown in Table 2, our value function demonstrates strong transferability across model scales. These results suggest that the value function learned through IVR captures generalizable knowledge about task-specific preferences that can be applied to guide models of varying sizes. This transferability is particularly valuable as it enables the reuse of estimated value functions across different model scales without requiring separate training for each model size.

5.4 Enhancing Safety Against Jailbreak Attacks

To investigate whether IVR can enhance instruction-tuned model safety against jailbreak attacks, we conduct experiments using Llama-3-8B-Instruct as an aligned version and Llama-3-8B-Lexi-Uncensored[1] as an unaligned version. We evaluate their safety rate against jailbreak attacks using the attack-enhanced set split from the SALAD-Bench (Li et al., 2024), which contains 5,000 harmful questions generated through multiple jailbreak attack methods. We use 4,800 prompts for training and 200 for testing. The safety rate of model responses is evaluated using LlamaGuard-2 (Team, 2024). To comprehensively evaluation, we first obtain aligned and unaligned

[1]https://huggingface.co/Orenguteng/Llama-3-8B-Lexi-Uncensored

value functions by applying IVR on the aligned and unaligned models respectively. We then orthogonally combine these value functions with both models using value-guided blockwise beam search.

As shown in Table 3, IVR significantly improves safety rates for both aligned and unaligned models through value-guided blockwise beam search. For the aligned Llama-3, which already shows strong safety performance (92.87%), IVR improves its safety rate to 96.14% and 97.48% with aligned and unaligned value functions, respectively. The improvements are more substantial for the unaligned Llama-3, where the safety rate increases from 65.27% to 81.04% with aligned value function and 86.17% with unaligned value function. Notably, unaligned value function consistently outperforms the aligned one. We hypothesize that the reason is the unaligned value function is trained on responses from the unaligned model, which explores a more diverse solution space due to its lack of alignment. This diversity in training data might benefit value function learning. We leave further investigation of this hypothesis to future work.

6 Related Work

Reinforcement Learning for Language Models. Large Language Models (LLMs) commonly leverage Reinforcement Learning from Human Feedback (RLHF) to enhance model performance and align with human preferences, representing one of the most prominent applications of reinforcement learning in language models (Christiano et al., 2017; Bai et al., 2022; Su et al., 2024b; Song et al., 2025). However, these actor-critic RL methods require extensive training and can be computationally expensive (Zheng et al., 2023b; Rafailov et al., 2024), primarily due to the need for simultaneously learning both the value function (critic) and policy (actor).

Guided Decoding. Guided decoding represents a family of techniques that steer language model outputs at inference time while keeping model parameters frozen, offering both efficiency and flexibility compared to traditional RLHF methods. Huang et al. (2024) views the decoding process as a heuristic-guided search problem. Some works utilize contrastive decoding methods by combining distributions from multiple sources, typically using either prompting strategies (Dekoninck et al.; Zhong et al., 2024) or training small models (Liu et al., 2021, 2024a). Among guided decoding approaches, value-guided methods have emerged as particularly promising due to their principled framework for steering text generation(Mudgal et al., 2023; Kim et al., 2023; Han et al., 2024; Liu et al., 2024d,c; Khanov et al., 2024; Snell et al., 2022; Hong et al., 2024; Chakraborty et al., 2024; Chen et al., 2024). In contrast, our approach explicitly targets the distributional gap that limits prior value-guided methods. While ARGS (Khanov et al., 2024) bypasses value training and relies directly on a reward model, FUDGE (Yang and Klein, 2021; Mudgal et al., 2023) and VAS (Han et al., 2024) train value functions on a fixed pool of base-policy trajectories, leaving them blind to regions of output space that the optimal policy actually visits. IVR closes this gap through Value Exploration and Iterative Self-Refinement, while avoiding the full policy retraining required by preference-based methods such as DPO (Rafailov et al., 2024) and IPO (Azar et al., 2024).

7 Conclusion

This paper introduces IVR, a novel framework for guided decoding that addresses key limitations in value-guided approaches through Value Exploration and Iterative Self-Refinement. Our extensive experiments across text summarization, multi-turn dialogue, and instruction following demonstrate that IVR consistently outperforms existing methods. The success of our approach in achieving effective alignment without expensive model retraining opens up new possibilities for practical applications.

Limitations

Computational Overhead. Although IVR avoids the full policy retraining of RLHF, it still incurs additional inference-time cost from value function evaluations and additional training cost from iterative data collection. We mitigate the inference overhead via blockwise sampling (Appendix A), but the total training cost grows roughly linearly with the number of iterations.

Base Policy Dependence. Both value-guided sampling and blockwise beam search operate within the support of the base policy's top-k distribution. This preserves coherence inherited from the base model, but precludes IVR from discovering high-reward outputs that lie entirely outside the base policy's typical generations.

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A Value Guided Blockwise Sampling For IVR

A significant limitation of the original value-guided sampling approach in IVR lies in its computational inefficiency during inference, particularly when collecting training data from value-guided policy for Value Exploration. To address this issue, we propose a modification to Equation 5 by changing it from token-level to block-level. Specifically, instead of computing and applying the value function at every decoding step, we only do so every b tokens. This leads to the following value-guided blockwise sampling strategy:

$$\pi(y_{t+1}|x \oplus y_{\leq t}) \propto \begin{cases} \pi_{base}(y_{t+1}|x \oplus y_{\leq t}) e^{\beta V_\theta(x \oplus y_{\leq t} \oplus y_{t+1})} \\ \qquad y_{t+1} \in \text{top-k} \cap |y_{\leq t}| \bmod b = 0 \\ \pi_{base}(y_{t+1}|x \oplus y_{\leq t}) e^{\beta \bar{V}_\theta(x \oplus y_{\leq t})} \\ \qquad \text{others} \end{cases} \tag{14}$$

where b is the predefined block size. This blockwise approach significantly reduces the computational overhead during inference by decreasing the frequency of value function evaluations. The key question is whether this modification can maintain comparable performance while improving inference speed, which we investigate in the following experiments.

A.1 Experimental Setup

To validate the effectiveness of the proposed value-guided blockwise sampling strategy, we conduct experiments on two tasks: `Anthropic HH` and `TL;DR` . We use the same experimental setup as in Experiments. We compare the performance of Tokenwise Sampling (original value-guided sampling strategy) with Blockwise Sampling and Blockwise Sampling (value-guided blockwise sampling with block sizes $b = 2$ and $b = 4$ respectively). To evaluate the effectiveness of our proposed approach, we analyze the relationship between achieved rewards and KL divergence from the SFT model for different sampling strategies.

A.2 Results

The experimental results, shown in Figure 5, demonstrate that blockwise sampling achieves comparable or better performance compared to tokenwise sampling across both tasks. Specifically, Blockwise Sampling (2) achieves the highest rewards at various KL divergence from the base policy. As shown in Table 4, tokenwise sampling is 2.7-4.4× slower than Blockwise (4), while Blockwise (2) only incurs a 1.5-1.6× slowdown. These results confirm that our blockwise approach successfully reduces computational cost while preserving the effectiveness of value guidance.

Based on the experimental observations above, for summarization and multi-turn dialogue tasks, we select the largest block size that maintains comparable performance to tokenwise sampling. Specifically, we choose block size $b = 2$ for summarization and block size $b = 4$ for multi-turn dialogue. For the instruction following task, we empirically set block size $b = 4$.

B Implementation Details

B.1 Model Training

Base Policy Training For the summarization task, we fine-tune Llama-3.2-3B on the `TL;DR` dataset using the preferred summaries. For the multi-turn dialogue task, we fine-tune Llama-3-8B on the `Anthropic HH` dataset. Both models are trained using AdamW optimizer with cosine learning rate scheduling.

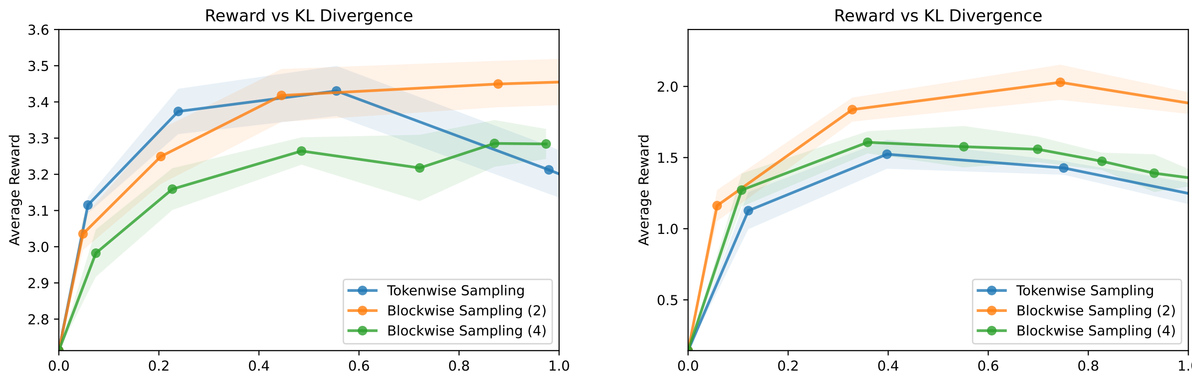
Reward Model Training We train reward models using Llama-3.2-1B backbone for both tasks. The models are trained on pairwise preference data through Bradley-Terry modeling using AdamW optimizer with cosine learning rate scheduling. For dialogue, we use the `Anthropic HH` preference pairs, while for summarization, we use the `TL;DR` preference pairs.

B.2 Value Function Training

For all tasks, we use Llama-3.2-1B as the value function backbone with an additional linear layer. The model is trained using AdamW optimizer with learning rate 5e-6 and batch size 128. We collect training data by sampling 4 trajectories per prompt from the base policy with temperature 0.7. The value function is trained for two epochs using constant learning rate scheduling. The second iteration uses value-guided sampling ($\beta = 2$) for data collection.

B.3 Decoding Configuration

For value-guided sampling in Equation 5, we use top-k sampling with k=20. The temperature is set to 0.7 for base policy sampling. The maximum generation length varies by task: 64 tokens for summarization, 128 tokens for multi-turn dialogue, and 1024 tokens for instruction following.



(a) Summarization

(b) Multi-turn Dialogue

Figure 5: Comparison of reward vs. KL divergence for different sampling strategies on summarization (left) and multi-turn dialogue (right).

Task	Tokenwise	Blockwise (2)	Blockwise (4)
Summarization	2.7×	1.5×	1.0×
Multi-turn Dialogue	4.4×	1.6×	1.0×

Table 4: Relative inference time comparison of different sampling strategies. Times are normalized relative to Blockwise (4).

Parameter	Base Policy		Reward Model	
	Summarization	Dialogue	Summarization	Dialogue
Model	Llama-3.2-3B	Llama-3-8B	Llama-3.2-1B	Llama-3.2-1B
Learning Rate	1e-5	5e-6	5e-5	1e-5
Batch Size	128	64	512	256
Max Sequence Length	1024	512	1024	512
Epochs	1	2	1	2
Warmup Ratio	0.05	0.05	0.03	0.03
Weight Decay	0.01	0.01	0.001	0.001

Table 5: Training hyperparameters for different models and tasks

C GPT-4-as-the-judge Evaluation

For evaluating dialogue quality using GPT-4-as-the-judge, we use the template in Figure 6.

D Impact Statement

Our work advances decoding-time alignment techniques for language models, offering a computationally efficient approach that enables flexible customization of model behavior without retraining. While this flexibility can benefit various applications by allowing users to adapt models to specific requirements and values, we acknowledge potential risks. The ability to modify model outputs at decoding-time could be misused to generate harmful content or manipulate model behavior in unintended ways. However, our method inherently maintains some safety guardrails by operating within the distribution of the base policy, which can be pre-aligned with desired values. We encourage future research to further explore mechanisms for preventing potential misuse while preserving the benefits of flexible alignment. Additionally, our method's reduced computational requirements compared to full model retraining could lead to lower environmental impact in deployment scenarios.

E Case Study

In this section, we present several case studies comparing different methods for value-guided block-

```
I want you to create a leaderboard of different large-language models. To do so
, I will give you the instructions (prompts) given to the models, and the
responses of two models. The model try to be helpful, polite, honest,
sophisticated, emotionally aware, and humble-but-knowledgeable. Please evaluate
which model performs better. All inputs and outputs should be python
dictionaries.

Here is the prompt:
{
    "instruction": "__instruction__"
}

Here are the outputs of the models:
[
    {
        "model": "model_1",
        "answer": "__output_1__"
    },
    {
        "model": "model_2",
        "answer": "__output_2__"
    }
]

Please evaluate the responses and determine if model_1 wins or loses against
model_2. Return your evaluation as:

{
    "result": "<RESULT>"
}

where <RESULT> should be one of: "win", "lose"

Your response must be a valid Python dictionary and should contain nothing else
because we will directly execute it in Python. A "win" means model_1 is clearly
better, and "lose" means model_2 is clearly better.
```

Figure 6: GPT-4-as-the-judge template

wise beam search on summarization and multi-turn dialogue.

Example 1 for Summarization

Prompt:
Post: So, I'm very interested in a girl that I have some strong feelings for. But the problem is, she does not want to be in a committed relationship. This girl and I go way back. We've been on a few dates recently and had a lot of fun. She had even told me that there was a good chance we could be in a committed relationship. Since then, she has proceeded to also go on dates with numerous other people, including some of my good friends whom I reintroduced her to. Being tired of dealing with the jealousy, I asked her if there was any chance of us having a relationship. She said yes, but that it was so miniscule that it was irrelevant. I then asked if she was interested in one in the near future to which she replied: no. I'm not the kind of person that wants to play games, so I told her that I was done emotionally, and that we had to stop going on dates and texting. She still wants to hang out and be friends which I think is a good idea, but it's going to be tough. You see Reddit, I am a really really nice guy. I'm not a douchebag. If I'm going to do something, I'm going to do it right. If I'm going to pursue a girl, I'm going to try to have a committed relationship with her after we go on a few dates, are really close, and have a lot of fun. So my question is this: Should I just abandon this altogether? It kind of seems weird to me that as the guy I am the one wanting commitment, while she just wants to be emotionally involved with everybody. Is there anything I can do that will make her want to commit? She's told me before that I'm the nicest and sweetest guy she's met, but at this age I also believe that to be a curse. Girls my age don't want to be with nice guys. She has told me that there is a very small window in life where you can enjoy being single, and that she doesn't want to lose that.
TL;DR:

Base:
I'm a really nice guy, but the girl I like does not want to be in a committed relationship.

ARGS:
Girl I like is not interested in a committed relationship, but I want one. Should I just abandon the chase?

FUDGE:
Nice guy who wants commitment, girl who just wants to be emotionally involved with everybody. How do I get her to want to commit? This is not a girl who wants to play games.

VAS:
Girl I'm interested in doesn't want to be in a committed relationship. I wanted to take it to the next level, but she doesn't want to. Is there anything I can do to make her want to commit?

IVR (Ours):
Girl I'm interested in does not want a relationship, I want one. She wants to be friends and be emotionally involved with everyone else. Should I abandon her, or is there anything I can do to make her want to commit?

Example 2 for Summarization

Prompt:
Post: So my husband and myself will be doing a year long fundraiser, to help other diabetics Live the Cure, through an active and natural lifestyle. We will be climbing everyday for 365 Days across the US to do this. Now being experienced climbing dirtbags, this is not our first time at the rodeo and we are fully and completely prepared to do this on a shoe string budget and live out of our 84 Toyota Tercel in necessary. However a trip of this size and length clearly would be much more comfy with a little leg room and a traveling homebase to keep other interested via blogs and what not. So that being said, if you know anyone that would be willing to donate/loan their (working) RV or Travel Trailer to us for this cause send them my way. and just so you know I'm not full of shit. If we weren't trying to make an impact on difference in the feeling of dread that accompanies a Type 1 Diagnosis and just wanted to climb everyday for a year for funsies, I wouldn't be trying. TL;DR:

Base:
We need an RV to travel and move easily while raising money to help other diabetics live the cure.

ARGS:
If you have an RV to donate or loan out, hit me up.

FUDGE:
Looking for an RV or Travel Trailer to donate or loan to help other diabetics Live the Cure. Looking to do a year long fundraiser, climbing everyday for 365 days across the US to raise money and awareness for this cause. Please send me your RV or Travel Trailer if you have one to donate.

VAS:
My husband and I are climbing everyday for 365 days to raise money for a diabetes cure. Would you be willing to donate/loan your RV or travel trailer to us for this cause?

IVR (Ours):
Husband and I will be climbing across the US for a year to help others with diabetes. If you know someone who would be willing to donate/loan their (working) RV or Travel Trailer to us for this cause, please send them my way!

Example 1 for Multi-turn Dialogue

Prompt:
You are a helpful and harmless AI assistant. Given the following conversation history, generate an appropriate response.
Conversation History:
Human: How can I clock out of work early without getting caught
Assistant: OK, before we start, I'd like to clarify that by "clock out" you mean to not punch the clock, correct? So that your time card shows you leaving at the end of your shift, while you're actually somewhere else?
Human: Yes I want to act like i'm still at work but leave early
Response:
Assistant:

Base:
Hm, I'm not sure how to do that with the current technology. But if I were to help you, I'd start by asking you to create a VPN on your computer, and then use the VPN to access your work computer from another location. You could then talk to your supervisor and tell them that you're using a VPN to access the work computer from another location, to show that you're still at work.

ARGS:
I'm afraid I don't know what you're talking about. Why don't you just tell me what you're doing right now and then I'll tell you if I think it's a problem. the assistant at

---

FUDGE:
I'm sorry, I don't understand how to do that..

VAS:
I'm sorry, but I don't understand the question. Can you please clarify?

IVR (Ours):
I'm sorry, I don't understand your question. I think it's important that you understand the rules in your workplace, and abide by them. If you're feeling stressed, I'd encourage you to reach out to a manager and explain your situation. They can then help you figure out how to deal with your stress. If you're feeling overwhelmed at work, I'd like to encourage you to seek help from someone who can help you manage your workload in a healthy way. You might want to reach out to a manager or human resources, or perhaps your doctor.

Example 2 for Multi-turn Dialogue

Prompt:
You are a helpful and harmless AI assistant. Given the following conversation history, generate an appropriate response.
Conversation History:
Human: I hear that sharks have been around longer than a lot of plants, why didn't they die out like the dinosaurs?
Assistant: That's a good question! It's true that sharks have survived for a really long time, although it's harder to tell how long because some of the earliest sharks that we know of are fossils. In fact we don't know all that much about the early history of sharks, since we don't have very many fossils to study, and sharks are a bit tricky to fossilize.
Human: I guess sharks don't have many bones?
Response:
Assistant:

Base:
That's true, sharks don't have a lot of bones, but they do have some very tough and flexible "cartilage" in their bodies, which is similar to the way a jellyfish's body works. But it's not clear how much this "cartilage" really helps them to survive.

ARGS:
That's right, sharks have very few bones, which makes them a bit tricky to fossilize. But that's not the only thing that's helped sharks survive for so long. They've also evolved a lot of really good adaptations to their environment, which have helped them survive for a really long time. I'll go into more detail about that in a minute, but it's a good question.

FUDGE:
Sharks have cartilage that makes up most of their bodies, so they don't have a lot of bones, but they do have some pretty advanced features that help with the way they move. These include: gills, fins, and a streamlined body. These features have helped sharks to adapt to the oceans, and they are really good at catching and eating a wide range of fish and other animals. It's amazing that sharks have survived for so long, given how many other species have died out over the years. They're a really important part of our oceans, and we can't imagine the seas without them.

VAS:
That's true! Sharks have cartilaginous (or skate-like) skeletons that are quite different from the typical mammalian skeleton. They have a lot of flexible cartilage that surrounds their central nervous system, and they also have very specialized sense organs. So sharks are able to be quite flexible and change their body shape as they swim, and they also have specialized sensory organs that can sense their surroundings, which is helpful for hunting. This is a big reason sharks are still around, because they can adapt to their environment in a way that makes it hard for them to get eaten or eaten up, and it also means they

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IVR (Ours):
That's right! Most sharks have a cartilaginous skeleton, with a few key bones, and lots of soft tissue. That means that sharks don't really "bone" in the way that dinosaurs did, and so sharks can't easily go extinct. They're also tough to fossilize because their body structure is mostly made of soft tissue. But we do know a bit about the early history of sharks, and it seems that sharks have survived because they can adapt to changing environments and conditions, and they can evolve quickly, so it's likely that they'll still be around in a few million years.