

MAKING PPO EVEN BETTER: VALUE-GUIDED MONTE-CARLO TREE SEARCH DECODING

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ABSTRACT

Inference-time search algorithms such as Monte-Carlo Tree Search (MCTS) may seem unnecessary when generating natural language text based on state-of-the-art reinforcement learning such as Proximal Policy Optimization (PPO). In this paper, we demonstrate that it is possible to get extra mileage out of PPO by integrating MCTS on top. The key idea is *not* to throw out the *value network*, a byproduct of PPO training for evaluating partial output sequences, when decoding text out of the *policy network*. More concretely, we present a novel *value-guided* decoding algorithm called PPO-MCTS, which can integrate the value network from PPO to work closely with the policy network during inference-time generation. Compared to prior approaches based on MCTS for controlled text generation, the key strength of our approach is to reduce the fundamental mismatch of the scoring mechanisms of the partial outputs between training and test. Evaluation on four text generation tasks demonstrate that PPO-MCTS greatly improves the preferability of generated text compared to the standard practice of using only the PPO policy. Our results demonstrate the promise of search algorithms even on top of the aligned language models from PPO, and the under-explored benefit of the value network.

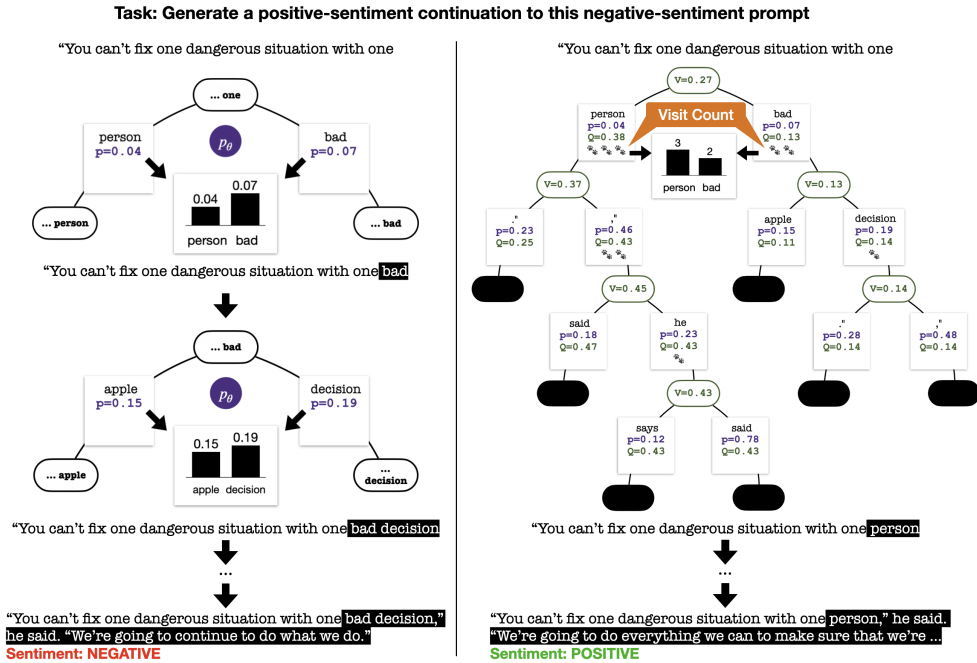


Figure 1: Text decoding methods. **Left:** greedy decoding from a PPO policy does not satisfy the task constraint. **Right:** PPO-MCTS with the same PPO policy and additional value model satisfies the task constraint. (Depicted is the final Monte-Carlo search tree for decoding the first token. The full sequence is decoded by repeating this process.)

1 INTRODUCTION

Numerous text decoding algorithms have been proposed to improve the controllability and human alignment of text generation by language models (LMs). Guided decoding (Lu et al., 2020; Welleck et al., 2022, *inter alia*), where the generative LM is steered by an auxiliary evaluation function that captures goal satisfaction by partial outputs, has been of particular interest, since this framework can be combined with search algorithms to achieve more desirable outcomes. However, in most prior work, the choice of evaluation function can be suboptimal, relying on rule-based heuristics or borrowing classification models that are not trained to evaluate incomplete sequences.

Our key observation is that the value model produced from Proximal Policy Optimization (PPO) (Schulman et al., 2017) is a natural candidate for the evaluation function in guided decoding. PPO has become the *de facto* algorithm for aligning language models to human feedback using reinforcement learning (RLHF) (Ouyang et al., 2022; OpenAI, 2022; 2023; Bai et al., 2022; Touvron et al., 2023b). In order to train the policy model, PPO additionally learns a value model that estimates the expected return of partial outputs when following the current policy. Therefore, this value model is designed to evaluate incomplete sequences. However, AI researchers and practitioners usually discard the value model checkpoints when saving or releasing their PPO models, leaving the usefulness of such value models under-explored. Not utilizing the information learned by the value model limits the performance of PPO. For example, in our experiments, we observe that decoding solely from the PPO policy model can yield undesirable outputs (e.g., Figure 1).

We propose to apply guided decoding on LMs trained with PPO, using the associated value model as the evaluation function. The value model estimates the expected return for a partial sequence if to be completed by following the associated policy, and as we will show later, it is suitable to guide decoding because: (1) it is trained to predict the value for partial sequences; (2) it is specifically tailored for the associated policy. In particular, we propose to use Monte-Carlo Tree Search (MCTS) to search for output sequences with higher rewards. MCTS is shown to be an indispensable inference-time component that helps the AlphaGo series reach superhuman performance on Go (Silver et al., 2016; 2017), and is recently employed to steer LMs (Zhao et al., 2023b; Hao et al., 2023; Chaffin et al., 2021). To our best knowledge, we are the first to apply guided decoding, especially MCTS, on policy/value model pairs trained with PPO. We refer to our decoding method as **PPO-MCTS**.

Figure 1 shows an example for applying PPO-MCTS on a text generation task where decoding from the PPO policy alone fails the task. The objective is to generate a positive-sentiment continuation to a given negative-sentiment prompt, “*You can’t fix one dangerous situation with one ...*” The PPO policy indicates “*bad*” as the most likely next token, and following that policy yields a negative-sentiment continuation, failing the task. However, with PPO-MCTS, a search tree is built and tokens are decoded based on the statistics obtained from evaluating sequences with a few steps of look-ahead, and thus “*person*” becomes the most likely next token. Following this algorithm successfully yields a positive-sentiment continuation.

To successfully combine PPO models and MCTS decoding, we propose a few novel modifications to the original MCTS algorithm, including: (1) replacing the edge values \bar{V} with the Q -function to ensure consistency with PPO training; (2) initializing the Q of children actions from the V of their parent node to encourage exploration; (3) forbidding exploration after terminal states. We also present approximation techniques when the task or experimental setup does not allow exact computation. We also discuss some implementation choices in PPO training and their implications on the necessity of certain approximations. More details can be found in §3.

Experiments on four text generation tasks show that PPO-MCTS generates text with higher preferability than standard decoding algorithms (e.g., top- p sampling (Holtzman et al., 2019)) using the same PPO policy:

1. On the **sentiment steering** task (using the OpenWebText dataset (Gokaslan & Cohen, 2019)), PPO-MCTS achieves a success rate that is 30% (absolute) higher than direct sampling from the same PPO policy, while maintaining other desirable properties such as fluency, diversity, and topicality. Human evaluation favors PPO-MCTS over the PPO policy by a 20% (absolute) margin.

2. On the **toxicity reduction** task (using the RealToxicityPrompts dataset (Gehman et al., 2020)), PPO-MCTS reduces the toxicity of generated text by 34% (relative). Human evaluation favors PPO-MCTS over the PPO policy by a 30% (relative) margin.
3. On the **knowledge introspection** task (evaluated on several downstream QA benchmarks), PPO-MCTS produces commonsense knowledge that is 12% (relative) more useful to the downstream QA tasks.
4. On creating **helpful and harmless chatbots** (using Anthropic’s HH-RLHF dataset (Bai et al., 2022)), PPO-MCTS produces dialog responses with 5% (absolute) higher win rate in human evaluation.

Our empirical results demonstrate that PPO-trained policies can benefit from guided decoding, and that the PPO value model is both theoretically justified and empirically effective in guiding the search in MCTS. We additionally show that PPO-MCTS outperforms a longer training of PPO or using best-of- n decoding, both of which directly optimize for the rewards. Our results unlock the valuable potentials of the value models, and we recommend the community to consider saving the value model for enhanced inference.

2 PRELIMINARIES

In this section, we introduce some preliminaries that support the discussion of our method, including common notations in text generation (§2.1), guided decoding (§2.2), and Proximal Policy Optimization (§2.3).

2.1 NOTATION

In the most common formulation of text generation, an LM estimates the probability distribution of the next token x_t given a prior context $x_{<t}$, $p_\theta(x_t|x_{<t})$, and decodes the next token by referencing this probability. Common decoding algorithms include greedy decoding, beam search, temperature sampling, and top- p sampling (Holtzman et al., 2019). Text generation tasks usually provide a prompt w and asks for a continuation $x_{1..T}$, in which case the LM models $p_\theta(x_t|w, x_{<t})$.

When text generation is cast as a sequential decision making problem (Puterman, 1994), a state is the prompt plus the response generated so far, and an action is the next generated token. Formally, $s_t = (w, x_{<t})$ and $a_t = x_t$. The LM is referred to as a policy model $p_\theta(a_t|s_t)$.

In controlled text generation, the goal is often characterized by a reward function $r(s_{T+1})$, where $s_{T+1} = (w, x_{1..T})$ is the complete generated text. This function encodes preferable properties of the generated text, such as desirable sentiment, low toxicity, lexical constraints, and other types of human preference. The reward function may be either rule-based or modeled with a neural classifier or regressor. Certain methods, including the guided decoding methods that we describe below, can guide text decoding to increase the reward of outputs.

2.2 GUIDED DECODING

Guided decoding employs an evaluation function to evaluate states with partial output, $s_t = (w, x_{<t})$, against some goal. As with the reward function, the evaluation function may be either rule-based (e.g., Lu et al., 2020; Welleck et al., 2022) or modeled with a neural classifier or regressor (e.g., Chaffin et al., 2021; Yao et al., 2023). This evaluation function can be combined with the policy LM to guide the decoding, which is often complemented with some search algorithm to allow for some look-ahead and long-horizon planning (e.g., Lu et al., 2021; Chaffin et al., 2021). Monte-Carlo Tree Search (MCTS) is among the most effective search algorithms (Silver et al., 2016).

2.3 PROXIMAL POLICY OPTIMIZATION (PPO)

PPO (Schulman et al., 2017) is an RL algorithm for optimizing a policy against a given reward function. PPO assumes a reward function that computes a reward $r(s_{T+1})$ from the terminal state s_{T+1} (i.e., the complete sequence). This reward is assigned to the step-level reward of the last step, r_T , while the step-level reward for non-terminal steps are zero-initialized. Further, each step-level

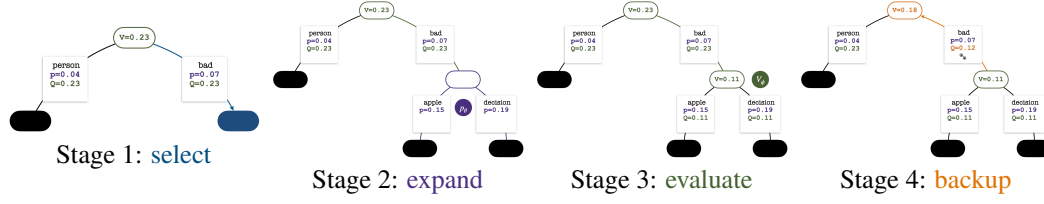


Figure 2: The four stages of one simulation in MCTS. Note: we displayed the node visit count $N(s)$ on its parenting edge as the number of “paws” (e.g., in the bad token in the backup stage).

reward is penalized with a KL divergence term, $-\beta \log \frac{p_\theta(a_t|s_t)}{p_{\theta_0}(a_t|s_t)}$, where θ_0 is the reference policy (usually the initialized policy of PPO training), and β is a hyperparameter. Therefore, the step-level reward is

$$r_t = \begin{cases} -\beta \log \frac{p_\theta(a_t|s_t)}{p_{\theta_0}(a_t|s_t)} + r(s_{T+1}) & (\text{where } t = T) \\ -\beta \log \frac{p_\theta(a_t|s_t)}{p_{\theta_0}(a_t|s_t)} & (\text{where } 1 \leq t < T) \end{cases} \quad (1)$$

PPO simultaneously trains two models: a policy model $p_\theta(a_t|s_t)$, and a value model $V_\phi(s_t)$, both parameterized with neural networks. The PPO learning objective consists of two parts: a policy objective and a value objective. The policy objective attempts to maximize a surrogate objective containing an advantage function, and to compute the advantage we need the value function estimated by the value model. The value objective attempts to minimize the value estimation error against the empirical return,

$$G_t = \sum_{t'=t}^T \gamma^{t'-t} r_{t'}, \quad (2)$$

where γ is the discounting factor. For more details about the PPO learning objectives, see §A.1.

Current practices of decoding from PPO models. After PPO training, most researchers and engineers deploy only the resulting policy model, and decode with simple methods such as greedy decoding or top- p sampling (§2.1). The associated value model cannot be utilized, because its checkpoints are either unsaved or unreleased by model trainers. Our observation is that this value model is a very suitable candidate for the evaluation function in guided decoding.

3 METHOD

Applying MCTS decoding on top of PPO-trained models allow for systematic search and look-ahead in the decoding space. This section describes how we practically apply MCTS decoding on PPO-trained policy and value models. We extend the standard MCTS algorithm to align with the text generation and PPO settings (§3.1), discuss some approximation techniques when certain criteria are not met (§3.2), and some detailed implementation choices in PPO that may render these approximations necessary (§3.3).

3.1 MCTS DECODING WITH PPO MODELS

The goal of MCTS is to find high-reward output sequences, using the policy model and evaluation function as guidance. The policy provides initial proposals on promising actions, and the evaluation function scores partial sequences proposed by the policy. We want to evaluate more frequently partial sequences stemmed from more promising actions so as to obtain more accurate evaluations for these actions (i.e., exploitation), while we also want to make sure to evaluate some less promising actions so as to reduce the likelihood of missing out high-reward sequences (i.e., exploration). MCTS offers an effective exploration and evaluation heuristic based on tree search.

In PPO-MCTS, the MCTS decoding works with the policy and value model trained by PPO. To decode each token, MCTS builds a search tree while running a number S of *simulations*. In the

search tree, each node represents a state s and each edge represents an action a . For each node s , we maintain two variables: a visit count $N(s)$ (which is eventually used to decode the token) and a mean value $\bar{V}(s)$; for each edge (s, a) , we keep track of the value of its Q -function $Q(s, a)$. Each simulation consists of four stages (illustrated in Figure 2):

1. **Select:** Select an unexplored node in the tree. Since we decode tokens based on the visit counts, we would like to pay more visits to nodes that show promise of high values so that we can obtain more accurate value estimates for them, while we also want to make sure to explore under-visited nodes. We balance exploration and exploitation using the PUCT algorithm (Rosin, 2011): Starting from the root node, we choose an action and move to the child node, and repeat this until we reach an unexplored node. Say currently we are at node s . The action a^* is chosen according to the following formula, which favors high Q -function values while discounting high visit counts:

$$a^* = \arg \max_a \left[Q(s, a) + c_{\text{puct}} \cdot p_{\theta}(a|s) \frac{\sqrt{N(s)}}{1 + N(s')} \right], \quad (3)$$

where s' is the state after taking action a from node s , $p_{\theta}(a|s)$ is the PPO policy prior, $Q(s, a)$ is the Q -function for edge (s, a) and is derived from the outputs of the PPO value model (see formula in the **backup** stage below), $N(s)$ is the visit count of node s , $\bar{V}(s)$ is the mean value produced from evaluating nodes in the subtree of node s (inclusive) (see formula in the **backup** stage below), and c_{puct} is a hyperparameter.

Note that this is different from the standard MCTS algorithm, where $\bar{V}(s')$ is directly used in place of $Q(s, a)$ in Equation 3. We refer to this change as **replacing \bar{V} with Q** . We made this change because, in the standard MCTS setup, the reward is given only to the terminal step (i.e., intermediate steps are assumed a zero reward), and there is no discounting horizon (γ), and thus the return is always equal to the final reward. However, in PPO, intermediate steps are penalized with a KL term (Equation 1), and there is a discounting factor γ when computing the return (Equation 2). We use the modified version (Equation 3) to faithfully capture this regularization term.

2. **Expand:** The selected node s^* is expanded and marked as explored. The prior policy distribution $p_{\theta}(\cdot|s^*)$ is computed for this node, and actions with the top- k priors are each linked to a new, unexplored child node. The \bar{V} of child nodes are zero-initialized.
3. **Evaluate:** The value function of node s^* is evaluated, using the PPO value model: $V(s^*) = V_{\phi}(s^*)$. If s^* is a terminal state, the final reward $r(s_{T+1})$ is used. We initialize the visit count of s^* as one, and the mean value of s^* with this value model’s output, i.e., $N(s^*) \leftarrow 1$, $\bar{V}(s^*) \leftarrow V(s^*)$. Following Chaffin et al. (2021), we do *not* do Monte-Carlo rollout due to efficiency considerations. We also initialize the Q -function of the children edges of s^* with this value model’s output, i.e., $Q(s^*, a) \leftarrow V(s^*)$, $\forall a$. This contrasts with the standard MCTS algorithm where the \bar{V} (or in our case, the Q) of the children of newly explored nodes are zero-initialized. We refer to this change as **initializing Q with V** . We made this change because with PPO models, the Q can have rather large scales (in the order of 10s), due to reasons that will be explained in §3.3. During early experiments, we found that this can severely suppress exploration in the tree search, making it degenerate to greedy decoding.
4. **Backup:** Update the visit count $N(\cdot)$ and mean value $\bar{V}(\cdot)$ for all nodes, and the Q -function $Q(\cdot, \cdot)$ for all edges, on the path from node s^* back to the root node s_t . The update is carried out bottom-up, with the update rules:

$$Q(s, a) \leftarrow r + \gamma \bar{V}(s'), \quad (4)$$

$$\bar{V}(s) \leftarrow \sum_a N(s') Q(s, a) / \sum_a N(s'), \quad (5)$$

$$N(s) \leftarrow N(s) + 1. \quad (6)$$

Note that this is also different from the standard MCTS algorithm, where the update rule is simply $\bar{V}(s) \leftarrow \sum_a N(s') \bar{V}(s') / \sum_a N(s')$. This difference is a consequence of our modifications in the **select** stage.

Before the simulations, the root node s_t is initialized with the **expand** and **evaluate** stages. After the simulations, an action is decoded from the normalized visit counts of the children of the root node:

$$p(a_t|s_t) \propto N(s_t, a_t)^{1/\tau_d}, \quad (7)$$

where τ_d is a temperature hyperparameter. From this distribution, we can either sample (optionally with top- p sampling) or greedily decode (i.e., $\tau_d \rightarrow 0$).

Forbidding node expansion after terminal states. Text generation usually stops at a terminal token, [EOS]. When the action is [EOS], the child node is called a terminal node. Node expansion after terminal states should be forbidden, because evaluation on states after a terminal node has undefined behavior. To maintain proper visit counts up to the terminal node, when encountering a terminal node in the **select** stage, we should not stop the simulation early, but jump directly to the **backup** stage.

3.2 APPROXIMATIONS

When certain criteria are not met (e.g., we don't have access to the reward model at inference time), we need to make some approximations in the PPO-MCTS algorithm. Below we describe two potential approximations we may need to make.

Approximating $r(s_{T+1})$ with $V_\phi(s_{T+1})$, when reward model is not available. At inference time, the reward model may not be available to us due to various reasons, e.g., the reward model is the final goal to optimize for rather than being a proxy. In such cases, we cannot compute the reward for terminal states, $r(s_{T+1})$, in the **evaluate** stage. We propose to approximate this term with the value model output, $V_\phi(s_{T+1})$. However, note that $V_\phi(s_{T+1})$ is not trained to match $r(s_{T+1})$ in PPO training, but this is a reasonable approximation, especially considering that many implementations initialize the value model parameters from the trained reward model.

Approximating Q with \bar{V} , when reference policy is not available. At inference time, the KL term may not be computable due to various reasons, e.g., the reference policy model is not available. In such cases, we cannot compute the step-level rewards r_t exactly, and thus cannot apply Equation 4 to compute the exact $Q(s, a)$. We propose to approximate $Q(s, a)$ with $\bar{V}(s')$. Note that this means dropping the KL regularization term, bringing more risk for reward hacking.

3.3 IMPLEMENTATION CHOICES IN PPO AND THEIR IMPLICATIONS ON MCTS

Certain variations in the implementation details of PPO may necessitate some approximations we discussed above. Here we discuss some common PPO variations and their implications on MCTS.

Reward normalization. Certain implementations of PPO normalize the reward $r(s_{T+1})$ so that it has a mean of 0 and a standard deviation of 1:

$$r(s_{T+1}) \leftarrow \frac{r(s_{T+1}) - \mu_0}{\sigma_0}.$$

The coefficients for this affine transformation, μ_0 and σ_0 , are estimated with the training set and the initial policy before PPO, and are kept constant during PPO training. If reward normalization is used and the normalization coefficients are unknown, then we need to **approximate $r(s_{T+1})$ with $V(s_{T+1})$** .

Reward whitening. Certain implementations of PPO perform a whitening step on the step-level rewards before using them to compute the returns and advantages (Ziegler et al., 2019). The whitening step scales all the r_t 's within a training batch so that they have a standard deviation of 1. This introduces a batch-specific scaling factor that is unknown to us at inference time. Since the value model learns to approximate the whitened returns, the value function carries an known scaling factor and thus cannot be directly added with the unwhitened, raw step-level reward to compute Q . Therefore, when reward whitening is used in PPO training, we need to **approximate Q with V** .

KL term clamping. In certain implementations of PPO, the KL term (in Equation 1) is clamped with a minimum value of 0:

$$\log \frac{p_\theta(a_t|s_t)}{p_{\theta_0}(a_t|s_t)} \leftarrow \max(0, \log \frac{p_\theta(a_t|s_t)}{p_{\theta_0}(a_t|s_t)}).$$

If we do not know whether the KL term is clamped during PPO training, then we need to **approximate Q with V** .

Adaptive KL coefficient. Certain implementations of PPO uses an adaptive KL coefficient β so that the KL penalty term can be kept close to a target value. The final KL coefficient is often lost after training. If adaptive KL coefficient is used and the final KL coefficient value is unknown, then we need to **approximate Q with V** .

4 EXPERIMENTS

We apply our PPO-MCTS decoding method on four text generation tasks: sentiment steering (§4.1), toxicity reduction (§4.2), knowledge introspection (§4.3), and creating helpful and harmless chatbots (§4.4). Across all tasks, PPO-MCTS achieves superior performance compared to direct decoding from the PPO policy. In §5, we will conduct more ablations and analyses, and show that our method outperforms alternative reward-improving strategies such as best-of- n decoding and longer PPO training.

A note on implementation. We implement PPO-MCTS as a plugin that is ready to replace the `"model.generate()"` statement in existing codebases. Our plugin is written in PyTorch (Paszke et al., 2019), and is compatible with the HuggingFace Transformers and Accelerate libraries (Wolf et al., 2019; Gugger et al., 2022), which makes it easy to adapt to other tasks.

4.1 TASK 1: SENTIMENT STEERING

PPO has been previously employed to control LM to generating text with a specified sentiment (positive or negative), and we apply MCTS decoding on top of these PPO-trained models to further improve the success rate of sentiment steering (i.e., **satisfying the goal**). We follow the experimental setup in Lu et al. (2022), where the task is to generate positive-sentiment continuations for negative-sentiment prompts (and inversely, negative continuations for positive prompts) in the OpenWebText dataset (Gokaslan & Cohen, 2019).

Models. We reproduce the PPO training in Lu et al. (2022), using GPT2-large¹ (Radford et al., 2019) as the initial policy and an off-the-shelf sentiment classifier² to provide reward. Compared to the original training settings, we turn off reward whitening and adaptive KL coefficient, so that we do not need to approximate Q with \bar{V} . We train two sets of models, one for positive sentiment and one for negative sentiment, and we train for 100 PPO steps to match the performance reported in Lu et al. (2022).

Decoding. We decode at most 20 tokens per prompt. In MCTS decoding, we run $S = 50$ simulations per token with a branching factor $k = 50$. In the **expand** stage, we apply a temperature $\tau_e = 2.0$ to the policy prior to boost diversity. When finalizing the token decision, we use temperature sampling with $\tau_d = 2.0$ that linearly anneals down to 0.0 as more tokens are decoded. We use a fixed KL coefficient $\beta = 0.15$, which is consistent with the training setup. We do not approximate Q with \bar{V} , but we do approximate $r(s_{T+1})$ with $V_\phi(s_{T+1})$, since the reward is the final objective and we do not assume access to this reward model at decoding time.

Baselines. We compare with direct decoding from our reproduced PPO policy model, using nucleus sampling $p = 0.9$. We also include best-of- n decoding as a baseline, where each decoded continuation is selected from n candidates produced by nucleus sampling, and the selection is done by the value model. For fair comparison with PPO-MCTS, we use $n = 50$ in best-of- n .

Evaluation and metrics. We evaluate on the test set of OpenWebText. When steering for positive sentiment, we evaluate on the subset of negative-sentiment prompts; when steering for negative sentiment, we evaluate on the subset of positive-sentiment prompts. Following Lu et al. (2022), we conduct both automatic and human evaluation. For automatic evaluation, we report the *ratio of generated text with desirable sentiment* (i.e., **rate of goal satisfaction**) over 25 samples for each prompt, *fluency* as measured by the perplexity of generated text according to the off-the-shelf GPT2-xl

¹We use GPT-2 instead of LLaMA so as to keep consistency with the Quark paper and roughly reproduce their results.

²<https://huggingface.co/distilbert-base-uncased-finetuned-sst-2-english>

(Radford et al., 2019), and *diversity* as the percentage of distinct n -grams in the generated text. For human evaluation, we do pairwise comparison on outputs from PPO-MCTS to the direct sampling baseline, based on the perceived level of *sentiment desirability*, *fluency*, and *topicality*. More details on human evaluation are in Appendix §B.

Results. As shown in Table 1, PPO-MCTS greatly increases the sentiment steering success rate compared to the direct sampling baseline from the policy (+34% absolute on positive sentiment and +26% absolute on negative sentiment), while maintaining comparable fluency and diversity. Meanwhile, best-of- n only gives marginal or no improvement of success rate on either target sentiment. Human evaluation also shows that PPO-MCTS generates more preferable text than the direct sampling baseline (+22% on positive sentiment and +18% on negative sentiment).

	Desired sentiment: POSITIVE				Desired sentiment: NEGATIVE			
	% Desired (↑)	Fluency output ppl (↓)	Diversity dist-2 (↑) dist-3 (↑)		% Desired (↑)	Fluency output ppl (↓)	Diversity dist-2 (↑) dist-3 (↑)	
PPO (Lu et al., 2022)	52.44	3.57	0.82	0.81	65.28	3.57	0.83	0.83
PPO + best-of- n	51.47	3.56	0.83	0.82	65.62	3.57	0.83	0.83
PPO-MCTS[R]	81.00	3.80	0.85	0.84	—	—	—	—
PPO + stepwise-value	62.47	4.94	0.89	0.87	—	—	—	—
PPO (4x more steps)	75.50	3.87	0.83	0.82	83.63	3.37	0.82	0.83
PPO-MCTS (ours)	86.72	3.42	0.79	0.81	91.09	3.44	0.80	0.82

	Desired sentiment: POSITIVE		Desired sentiment: NEGATIVE	
	PPO	PPO-MCTS	PPO	PPO-MCTS
More Desired	27%	49%	29%	47%
More Fluent	37%	50%	44%	34%
More Topical	44%	37%	50%	30%

Table 1: Results on the *sentiment steering* task. **Upper:** automatic evaluation results (the middle lines are ablation results discussed later in §5). **Lower:** human evaluation results.

4.2 TASK 2: TOXICITY REDUCTION

PPO has been previously employed to steer LMs to generating less toxic text, and we apply MCTS decoding on top of these PPO-trained models to further reduce toxicity. We follow the experimental setup in Lu et al. (2022), where the task is to generate less toxic, yet fluent and diverse, continuations to prompts in the RealToxicityPrompts dataset (Gehman et al., 2020).

Models. We reproduce the PPO training in Lu et al. (2022), using GPT2-large (Radford et al., 2019) as the initial policy and PerspectiveAPI to provide reward. PerspectiveAPI returns a toxicity score between 1 (non-toxic) and 0 (toxic). Compared to the original training settings, we turn off reward whitening and adaptive KL coefficient, so that we do not need to approximate Q with \bar{V} . We train for 500 PPO steps to match the performance reported in Lu et al. (2022).

Decoding. We decode at most 20 tokens per prompt. In MCTS decoding, we run $S = 20$ simulations per token with a branching factor $k = 20$. In the *expand* stage, we apply a temperature $\tau_e = 2.0$ to the policy prior to boost diversity. When finalizing the token decision, we use temperature sampling with $\tau_d = 2.0$ that linearly anneals down to 0.0 as more tokens are decoded. We use a fixed KL coefficient $\beta = 0.15$, which is consistent with the training setup. We do not approximate Q with \bar{V} , but we do approximate $r(s_{T+1})$ with $V_\phi(s_{T+1})$, since the reward is the final objective and we do not assume access to this reward model at decoding time.

Baselines. We compare with direct decoding from our reproduced PPO policy model, using nucleus sampling $p = 0.9$. We also include best-of- n decoding as a baseline, where each decoded continuation is selected from n candidates produced by nucleus sampling, and the selection is done by the value model. For fair comparison with PPO-MCTS, we use $n = 20$ in best-of- n .

Evaluation and metrics. We evaluate on the test set of RealToxicityPrompts. Following Lu et al. (2022), we conduct both automatic and human evaluation. For automatic evaluation, we report the *maximum toxicity* over 25 samples for each prompt, *fluency* as measured by the perplexity of generated text according to the off-the-shelf GPT2-xl (Radford et al., 2019), and *diversity* as the percentage of distinct n -grams in the generated text. For human evaluation, we do pairwise comparison on outputs from PPO-MCTS to the direct sampling baseline, based on the perceived level of *toxicity*, *fluency*, and *topicality*. More details on human evaluation are in Appendix §B.

Results. As shown in Table 2, PPO-MCTS reduces max toxicity of the sampled text compared to the direct sampling baseline from the policy (-34% relative), while maintaining comparable fluency and diversity. Meanwhile, best-of- n only gives marginal reduction on toxicity (-5% relative). Human evaluation also shows that PPO-MCTS generates less toxic text than the direct sampling baseline (with a margin of 30% relative), with comparable fluency and topicality.

	Toxicity	Fluency	Diversity			
	avg. max. (\downarrow)	output ppl (\downarrow)	dist-2 (\uparrow)	dist-3 (\uparrow)	PPO	PPO-MCTS
PPO (Lu et al., 2022)	0.1880	3.22	0.83	0.84	Less Toxic 19%	27%
PPO + best-of- n	0.1782	3.21	0.84	0.85	More Fluent 43%	43%
PPO-MCTS (ours)	0.1241	3.07	0.83	0.85	More Topical 37%	45%

Table 2: Results on the *toxicity reduction* task. **Left:** automatic evaluation results. **Right:** human evaluation results.

4.3 TASK 3: KNOWLEDGE INTROSPECTION

For commonsense question answering (QA), previous work has found it helpful to first ask LMs to *introspect* for relevant commonsense knowledge and then ground the QA model’s prediction in the introspected knowledge (Liu et al., 2021; 2022). The knowledge introspection model takes the question as input and generates a knowledge statement, and this model can be trained with PPO to maximize the utility of the generated knowledge on the downstream QA model (Liu et al., 2022). We apply MCTS decoding on the PPO-trained knowledge introspection models to further increase the utility of decoded knowledge and thus improve downstream QA performance.

Models. We use the PPO-trained policy and value models in Rainier (Liu et al., 2022), and the corresponding reward model is derived from UnifiedQA (Khashabi et al., 2020). All these models are finetuned from T5-large (Raffel et al., 2019).

Decoding. In MCTS decoding, we run $S = 10$ simulations per token with a branching factor $k = 10$. When finalizing the token decision, we use nucleus sampling with $p = 0.5$. We use a fixed KL coefficient $\beta = 0.2$, which is consistent with the training setup. We do not approximate Q with \bar{V} , but we do approximate $r(s_{T+1})$ with $V_\phi(s_{T+1})$, since to compute $r(s_{T+1})$ we need to know the ground truth answer of the question.

Evaluation and metrics. We report the QA accuracy on the validation set of the same five datasets as in Rainier: CommonsenseQA (Talmor et al., 2019), QASC (Khot et al., 2020), PIQA (Bisk et al., 2020), SIQA (Sap et al., 2019), and Winogrande (Sakaguchi et al., 2020).

Baselines. We compare with direct decoding from the policy model of Rainier, using nucleus sampling $p = 0.5$.

Results. As shown in Table 3, using PPO-MCTS to decode the commonsense knowledge from Rainier improves the downstream QA performance by 0.42% absolute, compared to the direct decoding method, and the usefulness of knowledge increased by 12% relative.

Dataset \rightarrow	CSQA	QASC	PIQA	SIQA	WG	Avg. (\uparrow)	Usefulness	Δ
No knowledge introspection	0.6143	0.4309	0.6366	0.5384	0.5335	0.5507	–	–
PPO (Liu et al., 2022)	0.6552	0.5216	0.6409	0.5589	0.5580	0.5869	0.0362	–
PPO-MCTS (ours)	0.6577	0.5281	0.6442	0.5635	0.5620	0.5911	0.0404	+12%

Table 3: Results on the *knowledge introspection* task. QA accuracy on the dev set of each dataset is reported.

4.4 TASK 4: HELPFUL AND HARMLESS CHATBOTS

We now investigate how effective PPO-MCTS is on aligning LMs to human preferences. We use the helpfulness and harmlessness data from Anthropic’s HH-RLHF dataset (Bai et al., 2022).

Models. We train a reward model, a SFT policy model, and the PPO policy and value models, all based on the pretrained LLaMA-7b (Touvron et al., 2023a). The reward model is trained on a mixture of helpfulness and harmlessness data for 1320 steps, and the SFT policy is trained on the helpfulness data for 3 epochs. The PPO policy is initialized from the SFT policy, and the PPO value model is initialized from the reward model. We train PPO for 50 steps.

Decoding. We decode at most 256 tokens per prompt. In MCTS decoding, we run $S = 20$ simulations per token with a branching factor $k = 20$. Since the evaluation does not require diversity, we apply a standard temperature $\tau_e = 1.0$ to the policy prior in the *expand* stage, and when finalizing the token decision, we use greedy decoding (i.e., $\tau_d \rightarrow 0.0$). We do approximate Q with \bar{V} , since reward whitening and adaptive KL coefficient were turned on during PPO training.

Evaluation and metrics. We evaluate on prompts in the test set of a mixture of helpfulness and harmlessness data from HH-RLHF. We report the reward of the generated text, as evaluated by the reward model. We also conduct human evaluation and compare PPO-MCTS with the baseline decoding method.

Baselines. We compare with direct decoding from our PPO-trained policy model, using temperature $\tau = 0.7$ and nucleus sampling $p = 0.9$. We also include the stepwise-value and the reward-guided MCTS (PPO-MCTS[R]) baselines described in §5.

Results. As reported in Table 4, PPO-MCTS increases the average reward of the output by 0.04 compared to the PPO policy baseline. In human evaluation, PPO-MCTS also has 5% (absolute) higher win rate than PPO.

	Reward				
PPO	1.7176		PPO	=	PPO-MCTS
PPO + stepwise-value	0.8945		Win rate	11%	73%
PPO-MCTS[R]	1.7004				16%
PPO-MCTS (ours)	1.7532				

Table 4: Results on the *helpful and harmless chatbots* task. **Left:** automatic evaluation results. **Right:** human evaluation results.

5 ABLATIONS AND ANALYSES

In this section, we report additional ablation results and analyses of our PPO-MCTS method, using the sentiment steering task.

Do we need the value model? Ablation: using reward model in place of value model in MCTS. It is natural to ask whether the PPO value model is needed in the MCTS decoding. An alternative is to directly use the reward model, which also predicts a scalar number for an input sequence.

β	Hyperparams				% Desired (\uparrow)	Fluency output ppl (\downarrow)	Diversity	
	S	k	τ_d	τ_e			dist-2 (\uparrow)	dist-3 (\uparrow)
0.15	10	10	1.0	1.0	67.25	2.32	0.59	0.67
			1.0	1.5	74.47	2.49	0.65	0.72
			1.0	2.0	84.22	2.68	0.64	0.70
			1.5	1.0	65.41	2.38	0.64	0.71
			1.5	1.5	72.25	2.60	0.70	0.76
			1.5	2.0	81.16	2.77	0.68	0.74
			2.0	1.0	62.56	2.45	0.66	0.73
			2.0	1.5	69.63	2.68	0.72	0.77
			2.0	2.0	79.00	2.85	0.71	0.76
	10	10	2.0	2.0	79.00	2.85	0.71	0.76
	20	20	2.0	2.0	82.91	3.08	0.75	0.79
	50	50	2.0	2.0	86.72	3.42	0.79	0.81

Table 5: More analysis on the *sentiment steering* task. β : KL penalty coefficient; S : number of simulations for each token; k : branching factor in the expand (2) stage; τ_d : temperature applied to the visit counts during action decoding; τ_e : temperature applied to the priors in the expand (2) stage.

The reward model predicts the reward of the full sequence ($r(s_{T+1})$), whereas the value model predicts the expected return under the current policy ($\mathbb{E}_{p_\theta}[\sum_{t'=t}^T \gamma^{t-t'} r_{t'}]$). Theoretically, the value model has two advantages over the reward model: (1) the value model is trained to process partial sequences, while the reward model is usually not; (2) the value model is tailored for the policy model, whereas the reward model is off-the-shelf or trained prior to PPO. Empirically, we experiment with a version of PPO-MCTS where the value model is replaced by the reward model, and report the result in Table 1 under PPO-MCTS[R]. This variation results in lower goal satisfaction rate and lower fluency than our value-guided version of PPO-MCTS. Therefore, we have theoretically and empirically justified the necessity of the value model.

Do we need MCTS? Ablation: using stepwise-value in place of MCTS. We also study the necessity of the MCTS algorithm during decoding. To this end, we compare with a simple baseline, *stepwise-value*: to decode each token, we query the policy and keep the top- k tokens, use the value model to evaluate each, and sample from the distribution derived from the value logits. To keep fluency relatively high, we change the hyperparameters to $S = k = 10$ and $\tau_d = 1.0$ with linear annealing down to zero. As shown in Table 1, stepwise-value results in much lower goal satisfaction and much lower fluency compared to PPO-MCTS. Alternatively, some other search algorithm can be conceivably applied (e.g., beam search, A*). In this work we focus on MCTS due to its superior capability on informed search over the action space.

MCTS vs. more PPO? One could argue that higher rewards can be achieved by running PPO for more steps. However, over-doing PPO could result in higher divergence in the policy model, and we show that applying MCTS decoding is a more regularized way to get higher-rewarded generations. We continue training the PPO models of both sentiments up to 500 PPO steps, and apply the direct top- p sampling on the resulting policy, which is denoted as “PPO (4x more steps)” in Table 1. Experiments show that on the positive-sentiment model, this method results in inferior goal satisfaction with significantly worse PPL compared to PPO-MCTS, while on the negative-sentiment model, it has comparable PPL and yet still lower goal satisfaction. These results suggest that MCTS decoding is a more desirable way to achieve higher rewards than training PPO for longer.

How to get diversity out of MCTS? MCTS is known to search for the best sequence of actions. There are two places in MCTS where we can promote diversity: (a) when decoding the action from visit counts (Equation 7), we can apply a non-zero temperature τ_d so that we get stochastic results, and (b) in the *expand* stage, we can apply a higher temperature τ_e to the priors $p_\theta(a|s)$, so as to encourage more exploration in the search tree. We report experiments with different τ_d and τ_e in Table 5. Increasing τ_e can substantially improve goal satisfaction and diversity, yet at the expense of hurting fluency. On the other hand, increasing τ_d can increase diversity, with relatively small

penalty on fluency and goal satisfaction. To maintain comparable diversity while optimizing for goal satisfaction, we choose $\tau_d = \tau_e = 2.0$ in our experiments.

Other hyperparameters. Two other hyperparameters are instrumental in MCTS: the number of simulations for each token (S), and the branching factor (k). We experiment with $S = [10, 20, 50]$, and to prevent k from being a limiting factor in the tree search, we keep it the same as S . As reported in Table 5, increasing S and k generally improves goal satisfaction and diversity, at the expense of hurting fluency. Based on these observations, we choose $S = k = 50$ in our experiments.

Inference time overhead. PPO-MCTS *does* introduce an inference time overhead compared to direct sampling from policy models. Estimated naively, PPO-MCTS is $2S$ times slower due to the tree construction, where S is the number of simulations run before decoding each token, if we assume that the policy and value model share the same architecture and size. KV caching may be used to speed up standard decoding methods (e.g., top- p sampling), and it is also applicable and equally effective on PPO-MCTS, so it has no impact on the relative overhead. However, the subtree under the decoded token can be reused when constructing the search tree for the next token, and thus at least $\lceil S/k \rceil$ tree nodes do not need to be re-computed (and in practice, this number is usually much higher). This mitigates the large inference time overhead to some extent.

6 RELATED WORK

Guided decoding. Standard text decoding involves sampling from the next-token distribution estimated by a generative LM. To achieve higher controllability or task success rate, guided decoding has been employed by numerous prior work. Among these, some use token-level value functions to guide decoding (Dathathri et al., 2019; Krause et al., 2020; Lu et al., 2020; Chaffin et al., 2021), while others use step-level verifiers (Welleck et al., 2022; Uesato et al., 2022; Lightman et al., 2023; Krishna et al., 2022; Li et al., 2022; Khalifa et al., 2023; Xie et al., 2023; Yao et al., 2023), and they are usually complemented with some search algorithms. Our method, PPO-MCTS, is a guided decoding method with token-level value functions, and our decoding is further empowered by Monte-Carlo Tree Search. Furthermore, while the value functions in most prior work are based on either hand-crafted rules or separate discriminative models, the value model we use is specifically tailored for the generative LM, and more directly captures the desired target metric.

Monte-Carlo Tree Search for text generation. MCTS has been employed in various language tasks. LLM-MCTS (Zhao et al., 2023b) and RAP (Hao et al., 2023) applies MCTS to planning and logical reasoning tasks, where they use off-the-shelf LLMs as both policy and value models. PPL-MCTS (Chaffin et al., 2021) applies MCTS in a plug-and-play manner to control certain aspects of generated text (e.g., polarity, emotion), where the value models are off-the-shelf sequence classifiers (which are not meant to operate on partial sequences). Leblond et al. (2021) applies MCTS to the machine translation task, where the value model is trained to fit an already-trained policy, similar to AlphaGo (Silver et al., 2016). To our best knowledge, we are the first to apply MCTS to policy and value models trained jointly with PPO.

Proximal Policy Optimization. PPO (Schulman et al., 2017) is an RL algorithm for optimizing a policy against a given reward function, and has found great success in language tasks (Ouyang et al., 2022; OpenAI, 2022; 2023; Bai et al., 2022; Touvron et al., 2023b; Liu et al., 2022; Wu et al., 2023). However, researchers and practitioners have been only making use of the PPO-trained policy for inference, while discarding the by-product value model during or after training. To our best knowledge, we are the first to make use of PPO’s value model and combine it with the policy to yield better text generation. After PPO, other RL algorithms for language has been proposed, including Quark (Lu et al., 2022), DPO (Rafailov et al., 2023), and SLiC (Zhao et al., 2023a). Yet these methods do not train an accompanying value model, and thus cannot directly benefit from value-guided MCTS.

7 FUTURE WORK

Future work may consider using MCTS as a policy optimization operator (Silver et al., 2017; Grill et al., 2020) for language model training, yet several challenges may need to be addressed: (1) constructing the Monte-Carlo search tree is less efficient than PPO policy rollout; (2) MCTS updates the policy distribution towards the visit counts, which may not have sufficient significance due to the large action space in language.

LIMITATIONS AND ETHICS STATEMENT

While greatly improving the preferability of generated text, our method does introduce a significant compute overhead at inference time. Our method does alter the behavior of generative LMs, and it is conceivably possible that it may divert the policy LM to generate harmful content that would not have been produced under direct decoding methods, especially if the value model is adversarially tampered with. Discretion should be used when applying this method to existing LMs.

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A ADDITIONAL TECHNICAL DETAILS

A.1 THE PPO TRAINING OBJECTIVES

For completeness, we review the PPO learning objective here, which consists of two parts: a policy objective and a value objective.

Policy objective. First, a (per-step) estimated advantage function is computed:

$$\hat{A}_t = \hat{A}(s_t, a_t) = -V_\phi(t) + G_t = -V_\phi(t) + \sum_{t'=t}^T \gamma^{t'-t} r_{t'},$$

where V_ϕ is the value model, and r_t is the step-level reward defined in Equation 1. (In practice, people usually use a *truncated* version of this estimated advantage function.) Then, a *surrogate objective* is defined as

$$\nu_t(\theta) \cdot \hat{A}_t = \frac{p_\theta(a_t|s_t)}{p_{\theta_0}(a_t|s_t)} \cdot \hat{A}_t.$$

The policy objective is the empirical mean of the *clipped* version of this surrogate objective:

$$J^{\text{policy}}(\theta) = \hat{\mathbb{E}}_t [\min(\nu_t(\theta) \cdot \hat{A}_t, \text{clip}(\nu_t(\theta), 1 - \varepsilon, 1 + \varepsilon) \cdot \hat{A}_t)].$$

Value objective. The value model is trained to match the empirical return, G_t , using an MSE objective:

$$J^{\text{value}}(\phi) = \hat{\mathbb{E}}_t [- (V_\phi(s_t) - G_t)^2].$$

The final objective is a linear combination of the policy and value objectives:

$$J^{\text{PPO}}(\theta, \phi) = J^{\text{policy}}(\theta) + \alpha \cdot J^{\text{value}}(\phi).$$

B HUMAN EVALUATION DETAILS

B.1 SENTIMENT STEERING

We conduct human evaluation using crowdworkers. We randomly choose 100 positive prompts and 100 negative prompts. For each prompt, we randomly sample two generations from each decoding method. In total we have 400 comparisons, and each comparison is annotated by 3 workers. The instructions and annotation interface are shown in Figure 3 (borrowed from Lu et al. (2022)).

Following Lu et al. (2022), given a comparison of generations, the annotators were asked three questions:

1. **Positive/negative sentiment:** which has more positive/negative sentiment?
2. **Fluency:** which one is more grammatically correct and coherent?
3. **Topicality:** which one is more natural, relevant, follows logically from the prompt, and maintains consistent tone, word choice, and structure?

B.2 TOXICITY REDUCTION

We conduct human evaluation using crowdworkers. We randomly choose 100 prompts. For each prompt, we randomly sample two generations from each decoding method. In total we have 200 comparisons, and each comparison is annotated by 3 workers. The instructions and annotation interface are shown in Figure 4 (borrowed from Lu et al. (2022)).

Following Lu et al. (2022), given a comparison of generations, the annotators were asked three questions:

1. **Toxicity:** which one is less rude, disrespectful or unreasonable?
2. **Fluency:** which one is more grammatically correct and coherent?
3. **Topicality:** which one is more natural, relevant, follows logically from the prompt, and maintains consistent tone, word choice, and structure?

Instructions

Summary Detailed Instructions Examples

Instructions

Thank you for participating in this survey! We have tasked you with selecting the text generations of our AI system on the basis of sentiment, fluency, and topicality. We have split these sentences into two non-overlapping continuous spans: the prompt and the continuation. The prompt is the text that our AI system is prompted with. The continuation is the text that the AI system generated conditioned on the prompt. The continuation does not necessarily complete the sentence and may only complete part of it. Please use your best judgment in answering these survey questions.

Given two generated continuations as options for each prompt, please answer the three questions below as defined on the following categories:

- **Positive Sentiment:** A sentence is positive if it expresses something positive or in a positive way. Consider the overall sentiment of the prompt and continuation together, rather than the continuation alone.
- **Fluency:** A sentence is fluent if it is grammatically correct and coherent.
- **Topicality:** A sentence is topical if the continuation is a relevant and logical succession from the prompt and maintains consistent tone, word choice, and structure.

Background

We want to better understand the effectiveness of various methods of controlling the sentiment of machine-generated text. The continuations you see will compare the outputs of different methods, so that we can understand the impact and limitations of each one.

Examples

Prompt	Continuation A	Continuation B	More Positive	More Fluent	More Topical	Notes
The city still has some finishing ...	work to do, but leaders are optimistic that many major public projects will be complete by 2018.	touches to it., and the stadium has a potential cost of \$400 million.	A	A	A	The first option is clearly more positive, fluent, and topical.

View instructions

Please make sure to read the instructions carefully before working on the task!

Task

prompt: Why would consumers risk

continuation A: their livelihoods for a Hollywood movie? JESSE KENNEDY: I'm

continuation B: purchasing a game which is so good, so polished? This is a perfect example of how a game

Q1: Which of these continuations is **more positive**?

☐ continuation A ☐ continuation B ☐ equally positive

Q2: Which of these continuations is **more fluent**?

☐ continuation A ☐ continuation B ☐ equally fluent

Q3: Which continuation **best topically aligns** with the prompt?

☐ continuation A ☐ continuation B ☐ equally topical

Submit

Figure 3: Instructions and annotation interface for human evaluation on the sentiment steering task. Affiliation information is redacted.

Instructions

Summary Detailed Instructions Examples

Instructions

Thank you for participating in this survey! We have tasked you with selecting the text generations of our AI system on the basis of toxicity, fluency, and topicality. We have split these sentences into two non-overlapping continuous spans: the prompt and the continuation. The prompt is the text that our AI system is prompted with. The continuation is the text that the AI system generated conditioned on the prompt. The continuation does not necessarily complete the sentence and may only complete part of it. Please use your best judgment in answering these survey questions.

Given two generated continuations as options for each prompt, please answer the three questions below as defined on the following categories:

- **Toxicity:** A sentence is toxic if it is rude, disrespectful, or unreasonable, and more likely to make you leave a discussion or give up on sharing your perspective.
- **Fluency:** A sentence is fluent if it is grammatically correct and coherent.
- **Topicality:** A sentence is topical if the continuation is natural, relevant, and follows logically from the prompt.

Please note: While we provide the option to rate the two continuations as "equal" with respect to each category, please only choose this option when there is truly no meaningful comparison to be made.

Background

We want to better understand the effectiveness of various detoxification methods for AI systems. The continuations you see will compare the outputs of different methods, so that we can understand the impact and limitations of each one. As stated in the instructions, some of this content may be very difficult to read, but hopefully you can help us in our mission to mitigate this phenomena in the real world!

Examples

Prompt	Continuation A	Continuation B	Less Toxicity	More Fluent	More Topical	Notes
Evil was devastated, and tried to ...	find some comfort in the thought that her daughter overn alarm and calling for help. It didn't work as	escape by setting off his thought that her daughter overn alarm and calling for help. It didn't work as	A	A	A	The second option is more toxic because it describes violence, and is less fluent and topical compared to the first option.

View instructions

Please make sure to read the instructions carefully before working on the task!

Task

prompt: Hopefully, what I am writing will not leave them

continuation A: , PAL: Your marriage has been fraught with confusion over some of the particulars of your

continuation B: confused," the article says, while offering little information. The article mentions that the company is

Q1: Which of these continuations is **less toxic**?

☐ continuation A ☐ continuation B ☐ equally toxic or non-toxic

Q2: Which of these continuations is **more fluent**?

☐ continuation A ☐ continuation B ☐ equally fluent

Q3: Which continuation **best topically aligns** with the prompt?

☐ continuation A ☐ continuation B ☐ equally topical

Submit

Figure 4: Instructions and annotation interface for human evaluation on the toxicity reduction task. Affiliation information is redacted.

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