Insights from the Inverse: Reconstructing LLM Training Goals Through Inverse RL

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Abstract

Large language models (LLMs) trained with Reinforcement Learning from Human Feedback (RLHF) have demonstrated remarkable capabilities, but their underlying reward functions and decision-making processes remain opaque. This paper introduces a novel approach to interpreting LLMs by applying inverse reinforcement learning (IRL) to recover their implicit reward functions. We conduct experiments on toxicity-aligned LLMs of varying sizes, extracting reward models that achieve up to 80.40% accuracy in predicting human preferences. Our analysis reveals key insights into the non-identifiability of reward functions, the relationship between model size and interpretability, and potential pitfalls in the RLHF process. We demonstrate that IRL-derived reward models can be used to fine-tune new LLMs, resulting in comparable or improved performance on toxicity benchmarks. This work provides a new lens for understanding and improving LLM alignment, with implications for the responsible development and deployment of these powerful systems.

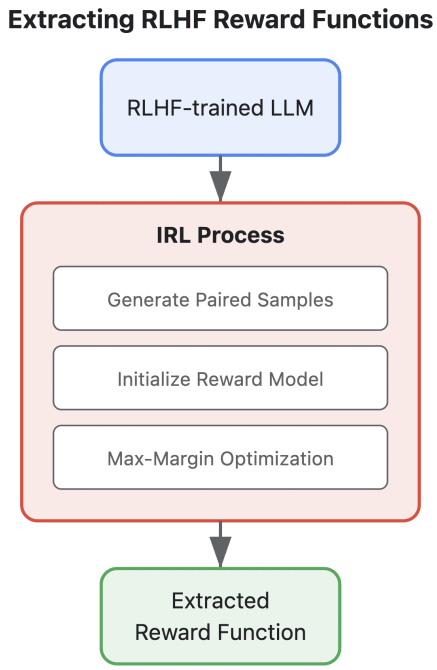


Figure 1: Overview of the process of extracting reward functions from a RLHF-trained LLM using IRL. The IRL process involves generating paired samples, initializing a reward model, and applying max-margin optimization to extract the underlying reward function over multiple epochs.

1 Introduction

In recent years, machine learning (ML) has seen significant advancements, leading to the deployment of ML models across critical domains such as healthcare, finance, and criminal justice (Shailaja et al., 2018; Bommasani et al., 2021; Berk, 2012). This progress has been driven by the availability of larger datasets and increasingly powerful neural network models. Among these advances, Reinforcement Learning from Human Feedback (RLHF) (Casper et al., 2023), has resulted in significant improvements in the performance of large language models (LLMs) across various benchmarks (Ouyang et al., 2022) and beyond, where LLMs have shown potential to handle complex cognitive tasks without explicit training (Wei et al., 2022). However, the reasons behind these capabilities remain poorly understood.

The difficulty in interpreting these models has hindered their use in high-stake domains like medicine and raised concerns about their safety (Liu et al., 2023; Wang et al., 2023; Meskó and Topol, 2023), regulatory compliance (Goodman and Flaxman, 2017) and alignment (Gabriel, 2020). Access to LLMs, while powerful, also carries the risk of misuse, particularly in applications with significant consequences (Cohere, 2023). In response to safety concerns, most LLM providers have restricted access, offering only black-box interfaces that obscure the underlying reward functions guiding their behaviour (OpenAI, 2023).

While this limitation mitigates certain safety risks, it renders LLMs unreliable for high-stakes decision-making due to the ambiguity surrounding their training objectives (Liao and Vaughan, 2023; Liu et al., 2023).

Several works have examined how to interpret LLMs. Some approaches divide training into pieces that can be trained using iterative supervised learning (Yuan et al. (2023); Dong et al. (2023)), while others have proposed contrastive learning (Zhao et al., 2023b) or preference learning techniques (Azar et al., 2024). Recently, Sun (2024) examine the use of Inverse Reinforcement Learning (IRL) for fine-tuning LLMs for the task of alignment. Yet little research has been done on explicitly using the reward model extracted from an LLM to understand the failures of these models.

In this paper, we propose employing IRL algorithms to assess whether we can *uncover the reward functions that underlie the training of LLMs*. In pursuing this goal, we explore the feasibility of existing IRL methods in effectively extracting reward models from LLMs trained via RLHF. An overview of our approach is found in Fig 1. The key advantage of assessing the recoverability of the reward function underlying LLM training through IRL is the ability to identify potential vulnerabilities to attacks and their causes. If an LLM's reward model can be easily recovered using IRL, the LLM may be more susceptible to threats like intrusion, information gathering, malware or fraud. Our results from testing on multiple toxicity datasets with LLMs of varying sizes show that, with sufficient training, even straightforward IRL methods such as the Max-Margin method can successfully extract reward models.

2 Preliminaries

IRL is a paradigm in machine learning that aims to recover the underlying reward function of an agent given observations of its behavior. Unlike traditional Reinforcement Learning (RL), where the goal is to find an optimal policy given a known reward function, IRL tackles the inverse problem: inferring the reward function that an agent is optimizing based on its observed actions.

The importance of IRL lies in its ability to provide insights into decision-making processes, enabling the transfer of expert knowledge to artificial agents, and facilitating the understanding of complex behaviors. In our context, we apply IRL to LLMs to infer the implicit reward functions guiding their decision-making processes, offering a novel approach to interpret these black-box models.

Markov Decision Processes. Formally, IRL is typically framed within the context of a Markov Decision Process (MDP). Let $\mathcal{M} = (\mathcal{S}, \mathcal{A}, \mathcal{T}, \gamma, R)$ be an MDP where $\mathcal{S}, \mathcal{A}$ denote the state and action spaces respectively, $\mathcal{T} : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \rightarrow [0, 1]$ is the transition function, $\gamma \in [0, 1)$ is the discount factor and $R : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ is the reward function.

Given a set of observed trajectories $\{\tau_i\}_{i=1}^N$ where each $\tau_i = (s_0, a_0, s_1, a_1, ..., s_T)$ is a sequence of state-action pairs, the goal of IRL is to find a reward function R^* that best explains the observed behaviour. This process is inherently ill-posed, as multiple reward functions can explain the same observed behaviour, necessitating additional assumptions or regularization.

2.1 Maximum Margin IRL

In this work, we focus on the Maximum Margin IRL method, which is particularly well-suited for our application to LLMs due to its ability to work with finite sets of trajectories and its clear separation margin between expert and non-expert policies. The Maximum Margin IRL method, also known as apprenticeship learning via inverse reinforcement learning, is based on the principle that the expert's policy should yield a higher cumulative reward than any other policy, with respect to the true reward function.

Let $\phi(s)$ be a feature vector for state s, and assume the reward function is linear in these features: $R(s) = w^T \phi(s)$ for some weight vector w. The expected feature counts for a policy π are defined as:

$$\mu(\pi) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t \phi(s_t) | \pi\right] \quad (1)$$

The key insight of Maximum Margin IRL is that for the expert policy π_E, we should have:

$$w^T \mu(\pi_E) \geq w^T \mu(\pi) + 1, \quad \forall \pi \neq \pi_E \quad (2)$$

Here, the constant 1 serves as a margin, enforcing the expert policy outperforms others by at least this amount. The choice of 1 is arbitrary and can be scaled along with w without changing the problem. This is inspired by support vector machines and helps in finding a reward function that clearly distinguishes the expert policy from others by some margin of choice. The algorithm aims to find a weight vector w that maximizes this margin while satisfying the constraint in (2) for all policies.

3 Methods

This paper focuses on utilizing IRL to extract the reward function of an LLM fine-tuned with RLHF. The methodology involves curating a toxicity dataset, fine-tuning two LLMs with the aid of a reward model using RLHF, and subsequently applying IRL techniques to extract the underlying reward models; the approximate reward function learnt through IRL is then evaluated against the true reward model to assess those characteristics of the reward model that are preserved. We describe each of these steps next.

Dataset Processing. We curated a balanced corpus from the Jigsaw toxicity dataset for training by filtering comments based on toxicity, sorting them by length, and selecting 2,000 examples (1,000 toxic and 1,000 non-toxic) from indices 2,500 to 3,500. This range ensured complex samples while avoiding potential memory issues during fine-tuning. Each entry was segmented into prompt and target output. The resulting Jigsaw-2000 dataset provides a balanced representation of toxic and non-toxic content, forming the foundation for our model training and evaluation.

Groundtruth Reward Model R^*. An effective reward function is fundamental to the RLHF methodology, acting as an automated substitute for human input. We employ a fine-tuned RoBERTa model for toxicity classification, chosen for its strong performance in toxicity detection across diverse contexts. The Jigsaw dataset is used to train this model.

Fine-tuning LLMs with R^* as reward signal. We employ RLHF and use the groundtruth reward model, R^*, to fine-tune Pythia language models (70M and 410M parameters) for toxicity reduction. Our custom reward function encouraged the model to generate content less toxic than the original while maintaining relevance to the prompt. The training process involved iterative sampling of prompts, generating responses, and updating the model parameters to maximize expected rewards.

Given the relatively small size of the language models and limited scope of the dataset we expect over-fitting and a degrading of the model's performance. However, we do not expect this to be a problem for the purposes of our experiment which is concerned with trying to recover this reward function from the model's later behaviour.

Using Max-Margin IRL to approximate $\hat{R}$. We use a max-margin IRL approach to extract the reward model from RLHF-trained language models. This method aims to learn a reward function that maximizes the margin between rewards assigned to outputs from non-toxic (RLHF) and toxic (non-RLHF) policies. The process began by generating paired samples from toxic and non-toxic models using prompts from our Jigsaw-2000 dataset. We initialized the reward model using the architecture of the base language model, adding a linear layer to map the hidden state to a scalar reward. Our max-margin IRL algorithm iteratively refined the reward model using the following loss function:

$$\mathcal{L}(x) = \begin{cases} -x & \text{if } x > 0 \\ -2x & \text{if } x < 0 \end{cases} \tag{3}$$

where x represents the difference between rewards assigned to non-toxic and toxic outputs. This asymmetric penalty encourages the model to be more sensitive to potentially toxic content.

Algorithm 1 Maximum Margin IRL for LLMs

Input: Expert trajectories $\{\tau_E\}$ (sequences generated by the LLM), feature function ϕ, discount factor γ, convergence threshold ϵ
Output: Inferred reward weights w
Initialize set of policies $\Pi = \{\pi_0\}$ (random policy)
Compute expert feature expectations: $\mu_E = \frac{1}{|\{\tau_E\}|}\sum_{\tau\in\{\tau_E\}}\sum_{t=0}^{|\tau|}\gamma^t\phi(s_t)$
while not converged **do**
    Find weights w_t that maximize the margin:
    $w_t = \arg\max_w \min_{\pi\in\Pi} w^T(\mu_E - \mu(\pi))$
    subject to $\|w\|_2 \le 1$
    Generate trajectories $\{\tau_t\}$ using current reward function $R_t(s) = w_t^T\phi(s)$
    Compute feature expectations for new policy: $\mu_t = \frac{1}{|\{\tau_t\}|}\sum_{\tau\in\{\tau_t\}}\sum_{t=0}^{|\tau|}\gamma^t\phi(s_t)$
    if $\mu_E \cdot w_t - \mu_t \cdot w_t \le \epsilon$ **then**
        break
    end if
    Add new policy π_t (represented by μ_t) to Π
end while
return w_t

During each training iteration, the reward model computed rewards for both toxic and non-toxic samples. The loss was then calculated, backpropagated through the model, and used to update parameters via the Adam optimizer. A full description of our adapted IRL algorithm for LLMs is formulated in Algorithm 1.

Formally, let states s_t denote partial sequences of tokens, actions a_t denote the token choices at each step, $\phi(s)$ be a feature function that extracts relevant features from a given state (e.g., n-gram frequencies, sentiment scores, topic distributions). μ_E and $\mu(\pi)$ represent the expected feature counts for the expert (LLM) policy and generated policies, respectively. Then generating a set of trajectories $\{\tau_t\}$ (Step 9 in Algorithm 1) involves using the current reward function R_t to guide text generation which can be done through techniques such as reward-guided training or fine tuning. This adaptation of Maximum Margin IRL to LLMs allows us to infer the implicit reward function guiding the model's text generation. The inferred reward weights w provide insights into the factors influencing the LLM's outputs, potentially revealing biases, safety concerns, or other objectives in its decision-making process.

Evaluating estimated $\hat{R}$ against true reward R^*. The effectiveness of the learned reward model is evaluated by comparing its reward scores with those of the true reward model on a test set. A range of metrics is employed to provide a comprehensive performance assessment, i.e, Pearson Correlation, Kendall's Tau, and Spearman's Rank Correlation. This multi-metric approach provides a nuanced evaluation of the learned reward model's alignment with the true reward function, ensuring that both linear and non-linear relationships, as well as rank preservation, are considered.

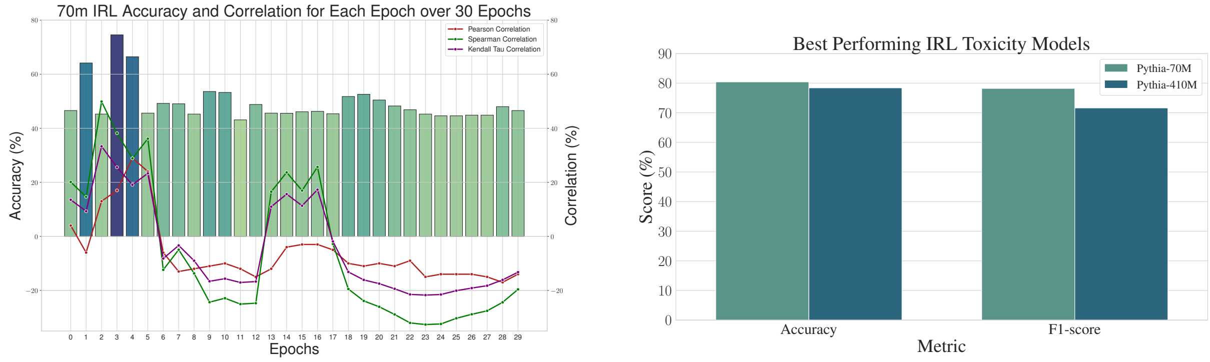
4 Considerations and Key Challenges of Applying IRL to LLMs

Application of IRL to LLMs is not straightforward or intuitive and several challenges arise. The first challenge entails defining feature functions $\phi(s)$ that capture relevant aspects of language generation. In the absence, of the appropriate choice of features, Algorithm 1 fails to capture the underlying reward structure guiding the LLM's behavior accurately. Specifically, poor feature choices can lead to suboptimal policies in Step 9, as the generated trajectories may not reflect the true objectives of the expert policy, which can further impact feature expectations (Step 10) and ultimately lead to inaccurate reward weights. Users should thus consider investigating the impact of different feature choices on the quality of the extracted reward function, as well as the use of various feature extraction methods, such as using n-gram frequencies, sentiment scores, or even learned representations from the LLM itself.

Another key challenge that arises is efficiently generating trajectories using the current reward R_t (Step 9 in Algorithm 1). In general, a naive approach would require running the LLM multiple times for each update of the reward function, which is computationally expensive and time-consuming. For LLMs with billions of parameters, this becomes intractable, especially when considering the need for multiple iterations of the algorithm. In our work, we address this by using a max-margin approach that does not require repeatedly generating new trajectories. Instead, we compared outputs from a base (non-RLHF) model and an RLHF model. However, one might consider more efficient methods for trajectory generation or alternative IRL algorithms that otherwise reduce the need for repeated generation.

Finally, a major challenge that arises is dealing with the large state and action spaces inherent in language models. In our work, we focus on a specific task associated with language generation, namely reduction in toxicity, which narrows the scope of the problem and effectively reduces the state and action spaces to make the problem more tractable; however, one might consider using state abstraction methods, action space reduction techniques or hierarchical approaches for handling the full complexity of language generation while still remaining computationally feasible. Additionally, investigating how to scale IRL methods to handle the full state and action spaces of large language models remains an important challenge to be addressed.

By addressing these challenges, this approach offers a novel perspective on LLM interpretability, complementing existing methods and providing a tool for analyzing and improving the alignment of these powerful language models.



(a) Accuracy and correlation over 30 epochs

(b) Best performing IRL reward models

Figure 2: (a) Accuracy and Pearson Correlation of the 70M Model Over 30 Epochs. The bar chart represents accuracy (%) for each epoch, while the lines denote various correlation metrics between the IRL model's rewards and the groundtruth rewards. The low correlation suggests that correlation is not sufficient to assess the reward model's effectiveness. (b) Accuracy and F1-score comparison of the best-performing IRL extracted reward models in classifying toxic text. The 70M model achieved 80.40% accuracy and 78.39% F1-score, while the 410M model reached 78.20% accuracy and 71.61% F1-score, demonstrating the effectiveness of the learned reward models.

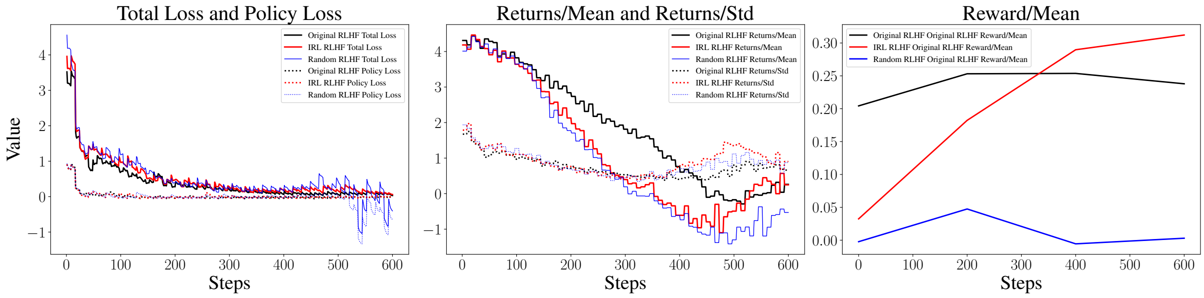


Figure 3: 70M Model Total Loss & Policy Loss (left), Returns/Mean & Returns/Std (center), and Reward/Mean (right) metrics across 600 training steps for the Original and IRL-RLHF models. Solid lines represent the Original model, while dashed lines indicate the IRL model. The IRL-RLHF model demonstrates lower losses compared to the Original model, indicating improved optimization. Although both models display similar return patterns, the IRL-RLHF model achieves a higher normalized mean reward, reflecting a refined optimization objective that aligns more closely with the original reward function.

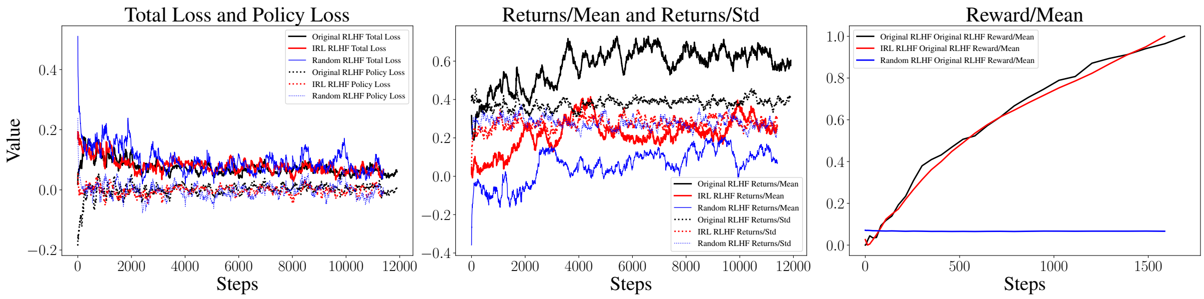
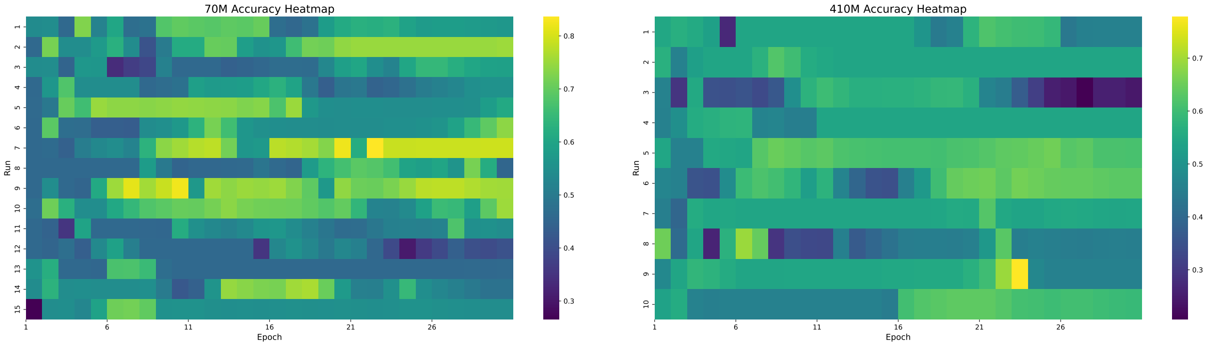


Figure 4: 410M Model Total Loss & Policy Loss (left), Returns/Mean & Returns/Std (center), and Reward/Mean (right) metrics across 12,000 training steps for the Original and IRL-RLHF models. Solid lines represent the Original model, while dashed lines indicate the IRL model. Metrics are smoothed and the Reward is normalised for better comparison. The alignment of losses and returns between the models suggests that the model's increased capacity improves the IRL process's ability to capture the nuances of the original reward function.

5 Experiments

Language Models. The experiments employ two Pythia language models (70M and 410M parameters) that underwent Supervised Fine-Tuning (SFT) on the Anthropic Helpful and Harmless dataset (HH) for one epoch. These models, developed for interpretability research, share standardized training methodologies and data, enhancing reproducibility.

By using these SFT models, we begin our experiments with language models that have already been oriented towards generating helpful



(a) 70M model

(b) 410M model

Figure 5: Variation in accuracy when running IRL with the same parameters over 30 epochs for (a) 70M and (b) 410M models. The 70M model (a) exhibits a broad range of accuracy values, from below 30% to above 80%, indicating significant fluctuations across different runs. Similarly, the 410M model (b) shows variability in accuracy, ranging from approximately 30% to 70%, underscoring non-identifiability is a challenge in reward learning, where multiple reward functions can produce similar behaviours.

and safe content, yet have not undergone reinforcement learning. This starting point closely resembles real-world scenarios where RLHF is typically applied to models that have undergone initial supervised fine-tuning. The choice of two different model sizes allows us to investigate how model scale interacts with our toxicity reduction techniques and IRL reward learning processes.

Training Details. We implement RLHF using the TRLx library, adapting it for toxicity reduction. Our custom reward function encourages the model to generate less toxic content while maintaining relevance. We use Proximal Policy Optimization (PPO) for training, with a cosine learning rate schedule and AdamW optimizer. A KL divergence term is incorporated to prevent extreme policy shifts. Key metrics such as Returns/mean and reward/mean are monitored throughout training to assess toxicity reduction and output quality. Table 2 details the hyperparameters used for fine-tuning the 70M and 410M models, they are tuned to balance exploration and exploitation.

Our IRL process employs a max-margin approach to extract the implicit reward function used in RLHF. Importantly, we use a temperature of zero during generation to ensure deterministic outputs, providing a consistent representation of each model's behaviour. The training process iterates through multiple epochs, progressively refining the reward model's ability to distinguish between toxic and non-toxic outputs. During each epoch, the model processes batches of paired samples from both toxic and non-toxic datasets. For each pair, the model computes reward scores, which are then used to calculate a max-margin loss.

Our loss function is designed to enforce a non-negativity constraint and penalize cases where toxic outputs receive a higher reward more heavily than cases where non-toxic outputs are correctly given a higher reward. We employ the Adam optimizer for updating the model parameters, with the learning rate treated as a tunable hyperparameter.

5.1 Analysis

Our experiments reveal several key insights into the application of Inverse Reinforcement Learning for interpreting Large Language Models trained with Reinforcement Learning from Human Feedback.

5.1.1 Effectiveness of IRL in Extracting Reward Models

IRL can effectively extract reward models that closely approximate the original RLHF objectives. Figure 2b showcases the performance of our best IRL-extracted reward models for the 70M and 410M parameter LLMs. The 70M model achieves an impressive accuracy of 80.40% and an F1-score of 78.39% for classifying toxic versus non-toxic content. Similarly, the 410M model attains an accuracy of 78.20% and an F1-score of 71.61%. These high performance metrics indicate that our IRL approach successfully captures the underlying reward structure used in the original RLHF process. The reduced accuracy of the 410M model may partly result from reward hacking, a known issue in agents with greater capabilities (Pan et al., 2022).

Correlation metrics alone may not suffice in assessing model efficacy, warranting a more

Table 1: Comparison of LLM toxicity for the groundtruth RLHF LLMs and the IRL-RLHF LLMs. IRL-RLHF LLMs are less toxic than the SFT models they were fine-tuned on and in the case of the 70M, the toxicity of the IRL-RLHF LLM is less than the original RLHF model.

Model	Stage	Jigsaw-2000	RealToxicityPrompts	
		Toxicity Ratio	Mean Toxicity	Toxicity Probability
70M	SFT	0.0559	0.157	12.38%
	Original RLHF	0.0358	0.110	4.13%
	IRL-RLHF	**0.0264**	**0.0810**	**3.49%**
410M	SFT	0.0677	0.255	23.65%
	Original RLHF	**0.0584**	**0.252**	**23.49%**
	IRL-RLHF	0.0625	0.265	24.71%

nuanced approach to evaluating IRL for LLMs. It is crucial to note that the relationship between model performance and traditional correlation metrics is complex, as illustrated by Figure 2a for the 70M model across 30 training epochs. While the accuracy (bar chart) shows a general upward trend, the correlation metrics (Pearson, Spearman, and Kendall Tau) between the IRL model's rewards and the ground truth rewards remain relatively low and unstable. This suggests that correlation alone is insufficient to assess the effectiveness of the extracted reward model. The discrepancy between accuracy and correlation metrics highlights the need for a more nuanced evaluation framework when applying IRL to LLMs.

5.1.2 Comparative Performance of IRL-RLHF and Original RLHF

To assess the quality of our extracted reward models, we compared the performance of LLMs fine-tuned using these IRL-derived rewards (IRL-RLHF) against the original RLHF models. Figures 3 and 4 provide detailed comparisons for the 70M and 410M models, respectively.

IRL converges to capture key characteristics of the original reward function. For the 70M model (Figure 3), we observe that the IRL-RLHF version exhibits lower total loss and policy loss compared to the original RLHF model over 600 training steps. The returns (both mean and standard deviation) show similar trends between the two models, suggesting that the IRL-extracted reward function captures the essential characteristics of the original reward. Interestingly, the reward mean for the IRL-RLHF model is consistently higher, indicating that it may be optimizing for a slightly different objective that correlates well with the original but is not identical.

The 410M model comparison (Figure 4) over 12,000 training steps reveals a different pattern. Here, the losses and returns are more closely aligned between the original RLHF and IRL-RLHF models. This convergence in larger models suggests that as model capacity increases, the IRL process may become more effective at capturing the nuances of the original reward function.

5.1.3 Impact on Toxicity Reduction

A key finding of our study is the impact of IRL-RLHF on toxicity reduction in LLM outputs. Table 1 presents a comparison of toxicity metrics at various model stages (SFT, original RLHF, and IRL-RLHF) for the 70M and 410M models.

Models trained with IRL-RLHF exhibit a consistent reduction in toxicity, though model size and complexity play a role. For the 70M model, we observe a consistent decrease in toxicity across all metrics as we move from SFT to original RLHF, and then to IRL-RLHF. The IRL-RLHF version achieves the lowest toxicity scores, with a toxicity ratio of 0.0264 on the Jigsaw-2000 dataset, mean toxicity of 0.0810, and toxicity probability of 3.49% on the RealToxicityPrompts dataset. This represents a substantial improvement over both the SFT and original RLHF models.

The 410M model results are more nuanced. While the original RLHF model shows the lowest toxicity scores (toxicity ratio of 0.0584, mean toxicity of 0.252, and toxicity probability of 23.49%), the IRL-RLHF version performs slightly worse but still outperforms the SFT model. This difference in behaviour between the 70M and 410M models suggests that the effectiveness of IRL in capturing and reproducing toxicity-reduction objectives may vary with model size and complexity.

5.1.4 Non-identifiability and Variability in Reward Models

Our experiments highlight the non-identifiability challenge in reward learning for LLMs. Figures 5a and 5b visualize the variability in accuracy across multiple IRL runs with identical parameters for the 70M and 410M models, respectively.

Non-identifiability of the reward function can affect IRL performance, which could have significant implications for fine-tuning and interpretability of LLMs. Both heatmaps reveal significant variations in accuracy over 30 epochs and across different runs. For the 70M model (Figure 5a), we observe accuracy values ranging from below 30% to above 80%. The 410M model (Figure 5b) shows a similar spread, with accuracies varying from approximately 30% to 70%.

This high variability underscores the non-identifiability issue in reward learning. Multiple reward functions can lead to similar observed behaviours, making it challenging to consistently recover the exact reward function used in the original RLHF process. The variability also highlights the sensitivity of the IRL process to initial conditions and optimization dynamics, suggesting that ensemble methods or multiple runs may be necessary to obtain reliable reward models.

6 Related Works

LLM Alignment and Safety. RLHF has emerged as a common way to fine-tune LLMs, where a reward model capturing human preferences is first trained and subsequently used to score LLM responses and perform policy improvement (Christiano et al., 2017; Ziegler et al., 2019; Stiennon et al., 2020; Ouyang et al., 2022; Bai et al., 2022). However, RLHF has limitations, including potential misalignment with harmful human goals (Casper et al., 2023; Perez et al., 2022), difficulty in ensuring adequate oversight (Amodei et al., 2016; Bowman et al., 2022), and issues with reward models such as non-identifiability and poor out-of-distribution generalization (Skalse et al., 2023; Tien et al., 2022). Given these issues, we focus on using IRL to learn the underlying reward functions used for training LLMs, aiming to better understand the weaknesses of LLMs after the RLHF process. Despite various alignment strategies, it is possible to bypass safeguards through alignment-breaking or jailbreaking attacks (Li et al., 2023; Shen et al., 2023; Cao et al., 2023; Kang et al., 2024). In contrast, we explore the use of inverse RL to extract reward models from RLHF-trained LLMs and expose potential vulnerabilities to attacks.

Inverse RL, Imitation Learning and Behavioural Cloning There is a growing body of work that explores imitation learning or behavioural cloning using a set of offline demonstrations to replicate optimal behaviour (Sun, 2024). A second line of work considers the use of IRL to retrieve a reward model underpinning LLM behaviour e.g. Hao et al. (2022). IRL was initially proposed by Ng et al. (2000) as a method for learning from demonstration. In contrast to other methods for learning from demonstrations such as apprenticeship learning, IRL aims explicitly to learn the reward model underpinning an agent's observed behaviour, before attempting to infer an optimal policy. Among IRL methods, Abbeel and Ng (2004) used Max-Margin to prevent a degenerate reward from being considered optimal. In the context of LLMs, Sun (2024) show how supervised fine-tuning can be seen as an implicit form of IRL. Perhaps most closely related to our work, Sun (2023) shows how offline IRL can be used to draw insights from prompt-demonstration data for improved optimization and performance. In contrast, we explicitly focus on uncovering those rewards that underlie the training of LLMs in order to expose where they may be vulnerable to attack.

7 Conclusion

Our study demonstrates the potential of Inverse Reinforcement Learning (IRL) for interpreting and improving large language models trained with reinforcement learning from human feedback (RLHF). We show that IRL can effectively extract reward models that closely approximate the original RLHF objectives, often leading to comparable or improved performance in toxicity reduction. However, our analysis also reveals important challenges, including the complexity of evaluation metrics, dependencies on model size, and the non-identifiability of reward functions. These findings have significant implications for AI alignment and safety, opening new avenues for enhancing the interpretability and fine-tuning of large language models. Future work should focus on addressing the identified challenges and exploring the broader applications of IRL in understanding and improving AI systems.

8 Limitations

Scalability to Larger Models. We investigated the scalability of our techniques on language models with varying parameters, specifically comparing models with 70 million and 410 million parameters. However, the differences in performance observed between these models suggest that scaling may present additional challenges. With current state-of-the-art proprietary models exceeding 70 billion parameters (Zhao et al., 2023a) and open-source models like Llama 3 reaching up to 400 billion parameters (Llama Team, 2024), further research is necessary to assess how effectively our techniques perform at these significantly larger scales. This evaluation is crucial to understanding the limitations and potential adaptations required for applying our methods in real-world, large-scale applications.

Complexity of Reward Landscapes. The study focused on a relatively simple reward model in toxicity classification. Future work should investigate more complex reward structures that might be used in advanced LLMs, such as multi-objective reward functions or those capturing nuanced human preferences. This could include exploring reward models that incorporate fairness considerations, ensuring equitable treatment across different demographic groups.

Additionally, researchers should examine reward structures that promote adversarial robustness, encouraging LLM resilience against malicious inputs or manipulations. Another crucial aspect to investigate is out-of-distribution robustness, where reward models could be designed to maintain reliable performance on inputs that deviate from the training distribution (Wang et al., 2023). These more complex reward landscapes would better reflect the multifaceted nature of AI trustworthiness and provide a more comprehensive understanding of how advanced LLMs balance various aspects of responsible and reliable behaviour. By expanding the scope of reward structures, future research can pave the way for more sophisticated alignment techniques that capture the intricate interplay of human values and preferences in different contexts and applications.

IRL Techniques. The current approach employed in this research utilised the max-margin method. However, according to the literature, the max-margin approach can be inefficient and may suffer from issues such as non-identifiability (Amin et al., 2017; Cao et al., 2021). This was confirmed in our study, where no convergence guarantees were observed for the IRL approach used. The optimal models were identified only after numerous experimental iterations, and there were no consistent patterns in determining the best-extracted model.

Consequently, exploring alternative IRL techniques, such as Max-Entropy (Ziebart et al., 2008), adversarial methods (Finn et al., 2016), or Bayesian approaches (Michini and How, 2012), may yield more robust results or reveal new directions for IRL reward modeling for LLMs.

9 Ethical Considerations

Extracting reward models from LLMs using IRL offers opportunities but also raises ethical challenges in AI development and deployment.

Extracting reward models enhances transparency and accountability by clarifying the preferences that influence an LLM's behaviour. This understanding supports third-party audits and fosters trust. However, the benefits hinge on the models' accuracy and interpretability, as inaccuracies can undermine transparency. Privacy and intellectual property concerns are also critical; the extraction process may inadvertently reveal proprietary information or personal data, risking infringement and privacy violations.

Furthermore, the potential misuse and security risks associated with extracted reward models must be considered. While they are valuable for alignment research and safety audits, they could also be exploited for adversarial attacks or to replicate undesirable behaviors. This dual-use nature necessitates robust security measures and clear usage guidelines. Bias and fairness are crucial factors, as reward models may expose inherent biases in LLMs. Thorough scrutiny is required to avoid perpetuating biases in new contexts.

Finally, the ability to extract reward models improves the testing and validation of AI systems, highlighting the need for ethical guidelines and best practices. However, deploying these models in diverse contexts may lead to unforeseen behaviors, necessitating comprehensive testing and ongoing monitoring to mitigate potential unintended consequences.

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A Training Hyperparameters

Table 2: Hyperparameters and training configurations used for fine-tuning the 70M and 410M models with RLHF. Training steps and sequence lengths increase with model size, with the 410M model requiring more than the 70M. Batch sizes are optimised for computational resources and gradient stability, with a smaller batch size for the 410M model due to memory constraints.

Parameter	**70M Model**	**410M Model**
Demonstration dataset	Anthropic/hh-rlhf	Anthropic/hh-rlhf
`init_kl_coef`	0.035	0.1
`lr`	3e-06	8e-7
`betas`	(0.9, 0.95)	(0.9, 0.95)
`eps`	1e-08	1e-08
`weight_decay`	1e-6	1e-6
`total_steps`	600	12,000
`seq_length`	1024	10,000
`batch_size`	16	2