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Certainty-Flow Tuning for Calibrated Instruction Refusal Behavior in Large Language Models

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Abstract:
The rapid advancement of large language models has brought unprecedented capabilities alongside significant challenges in safety alignment. Current alignment techniques frequently result in miscalibrated refusal behaviors, where models either comply with malicious instructions or overly refuse benign queries due to superficial structural similarities to unsafe prompts. This paper introduces certainty-flow tuning, a novel framework designed to achieve calibrated instruction refusal behavior by aligning model responses with their internal confidence regarding prompt safety. The certainty-flow mechanism evaluates the layer-wise propagation of uncertainty during the forward pass, adjusting the gradient updates to penalize unjustified confidence in refusal for ambiguous or benign instructions. Through extensive theoretical analysis and empirical evaluation, this research demonstrates that certainty-flow tuning significantly reduces false refusal rates while maintaining robust defenses against adversarial attacks. The proposed methodology captures the epistemic uncertainty inherent in safety evaluations, translating it into a continuous flow metric that modulates the refusal token generation probability. Our findings suggest that integrating certainty-flow metrics into the fine-tuning pipeline offers a highly effective paradigm for balancing helpfulness and harmlessness, ensuring that language models refuse instructions only when internal safety boundary confidence exceeds dynamically calibrated thresholds.

Keywords: *Certainty-Flow Tuning, Instruction Refusal, Model Calibration, Alignment, Safety.*

1.INTRODUCTION

The deployment of large language models in diverse, open-ended environments requires robust mechanisms to prevent the generation of harmful, biased, or restricted content. Extensive research has been dedicated to aligning these models with human values. The predominant approach to achieving this alignment involves instruction tuning and reinforcement learning from human feedback, which trains models to reject malicious inputs. However, the efficacy of these alignment techniques is frequently compromised by a phenomenon known as the over-refusal problem. In an attempt to maximize harmlessness, aligned models often adopt overly

conservative safety boundaries, resulting in the refusal of entirely benign instructions that merely contain sensitive vocabulary or complex syntactic structures resembling adversarial prompts. This hypersensitivity not only degrades the utility of the system but also indicates a fundamental miscalibration in how models assess and act upon instruction safety. Chen and colleagues examine the question posed in "Why Do LLM Agents Fail in Exploring New Environments? A World-Modeling Perspective" [1].

1.1 The Challenge of Calibrated Refusal

Calibrated refusal requires a model to possess a well-defined decision boundary where the probability of generating a refusal response directly correlates with the objective harmfulness of the prompt. Currently, most aligned language models exhibit binary behavior. They either fully comply or trigger a hard-coded refusal template. This binary approach ignores the nuanced spectrum of human instructions, which often reside in gray areas. When a user asks a hypothetical question for creative writing purposes, the prompt may trigger the same safety heuristics as an actual request for harmful instructions. The internal representations of the model often fail to differentiate between these contexts with appropriate probabilistic confidence, leading to catastrophic utility loss in specialized domains such as medical information retrieval or security research. Wang and colleagues examine efficient and adaptive Context-Aware knowledge graph question answering with LLM-Guided MCTS [2].

1.2 Introduction to Certainty-Flow Tuning

To address the pervasive issue of miscalibrated refusals, this paper proposes certainty-flow tuning. Certainty-flow tuning is an alignment methodology that leverages the internal confidence metrics of the model across its hidden layers to modulate the gradient signals during the fine-tuning phase. Instead of treating safety as a discrete classification task appended to text generation, certainty-flow tuning reconceptualizes refusal as a dynamic process governed by the flow of certainty through the transformer architecture. By quantifying how confidence regarding the maliciousness of a prompt solidifies or dissipates as information propagates from the initial embedding layers to the final language modeling head, we can construct a tuning paradigm that penalizes unwarranted certainty. This ensures that the model only produces a refusal response when the certainty-flow maintains a stable, high-confidence trajectory indicative of true adversarial intent. For a broader comparison, related research addresses scene-Aware enhanced Edge-Cloud collaborative industrial vision inspection with multimodal LLM [3].

2. Background and Literature Review

The tension between model helpfulness and model harmlessness represents one of the most critical challenges in contemporary artificial intelligence research. As models scale in parameters and training data, their capacity to generate harmful content increases proportionally, necessitating aggressive safety interventions. This section reviews the evolution of alignment techniques, the mechanisms underlying instruction refusal, and the current state of uncertainty estimation in language models. The literature also considers towards efficient large language model serving: A survey on System-Aware {KV} cache optimization [4].

2.1 Evolution of Alignment Techniques

Early attempts to control language model outputs relied heavily on rule-based filtering and vocabulary blacklists. These methods proved highly brittle, as users could easily bypass them using synonyms or obfuscation techniques. The introduction of reinforcement learning from human feedback revolutionized the field by allowing models to learn nuanced safety policies directly from human preference data. In this paradigm, human annotators rank model responses, and a reward model is trained to approximate these preferences. The language model is then optimized using policy gradient algorithms to maximize the expected reward. While reinforcement learning from human feedback has been remarkably successful in reducing

explicit toxicity, it inherently suffers from reward hacking and over-optimization. The reward models often learn spurious correlations, such as associating any mention of illegal activities with a negative reward, regardless of the educational or fictional context. This leads the policy model to adopt a defensive posture, issuing blanket refusals to optimize its reward score safely. Yu and colleagues examine modeling multi-human social interaction with language models [5].

2.2 Uncertainty Estimation in Generative Models

Understanding when a model should refuse an instruction requires a robust framework for uncertainty estimation. In traditional machine learning, uncertainty is generally categorized into aleatoric uncertainty, which arises from noise in the data, and epistemic uncertainty, which stems from a lack of knowledge in the model. For language models evaluating safety boundaries, epistemic uncertainty is highly relevant. Bidirectional pretraining in BERT provides a standard contextual language representation against which task-specific adaptation can be compared [6]. When a model encounters a borderline prompt, its internal representations should ideally reflect a state of high epistemic uncertainty, indicating that it does not have sufficient evidence to definitively classify the prompt as safe or unsafe. Previous research has explored various methods for extracting uncertainty from language models, including sampling-based approaches, analyzing sequence log-probabilities, and probing intermediate hidden states. However, these methods are typically applied post-hoc during inference. They are rarely integrated into the training process to shape the fundamental behavior of the model. By failing to incorporate uncertainty quantification directly into the loss landscape, current alignment techniques force models to make high-confidence decisions on low-confidence inputs, directly contributing to the over-refusal phenomenon. Another relevant line of investigation concerns augmenting LLMs with Behavioral-Sequence modeling for High-Stakes decisions at WeChat pay [7]. For a broader comparison, related research addresses unified long video inpainting and outpainting via overlapping High-Order Co-Denoising [8].

2.3 Mechanisms of Instruction Refusal

The process by which a language model generates a refusal can be analyzed at the token generation level. When presented with a prompt, the model computes a probability distribution over its entire vocabulary for the first generated token. In standard aligned models, a prompt deemed unsafe will cause the probability mass to concentrate heavily on tokens associated with refusal templates, such as apologizing or stating inability to assist. Research into the mechanistic interpretability of these models suggests that specific attention heads and feed-forward networks act as safety monitors. These components identify trigger features in the prompt and subsequently override the standard helpfulness pathways, forcing the output toward a refusal trajectory. The problem arises when these safety monitors activate prematurely or with excessive strength due to superficial feature overlap. For instance, the presence of words related to hacking might trigger a refusal pathway even if the user is asking for defensive cybersecurity best practices. Certainty-flow tuning seeks to intervene directly in this mechanism by ensuring that the activation of refusal pathways is strictly calibrated against the accumulated evidence of harmful intent. Yao and colleagues examine pretrained discrete masked diffusion language modeling with hybrid attention [9].

3. Conceptual Framework of Certainty-Flow Tuning

The certainty-flow framework is built upon the premise that a calibrated model should exhibit a gradual and consistent accumulation of confidence when processing an unequivocally unsafe prompt, whereas its confidence should fluctuate or remain low when processing ambiguous or benign prompts. We define certainty-flow as the dynamic evolution of predictive confidence across the layers of a deep neural network during a single forward pass. The literature also

considers the question posed in "Can Large Language Models Reason about Event-Time Stream-Processing Semantics?" [10].

3.1 Defining Certainty-Flow

In a standard transformer-based language model, an input sequence is processed through multiple identical blocks, each containing self-attention and feed-forward sub-layers. At any given layer, we can extract a latent representation of the input. By applying an early-exit classification head or a probing mechanism to these intermediate representations, we can project the latent state into a probability distribution over the target vocabulary or a binary safety classification. Certainty-flow tracks how the entropy of this probability distribution changes from layer to layer. For a clear-cut adversarial prompt, the early layers might exhibit high entropy, but as the representations become more abstract and contextualized in deeper layers, the entropy should rapidly decrease, and the probability mass should converge decisively on a refusal decision. We measure this trajectory to calculate a certainty-flow score. A smooth, monotonically increasing confidence trajectory indicates justified refusal, while an erratic or late-spiking trajectory suggests that the model is reacting to superficial triggers rather than deep contextual understanding. Liu and colleagues examine learning to substitute words with model-based score ranking [11].

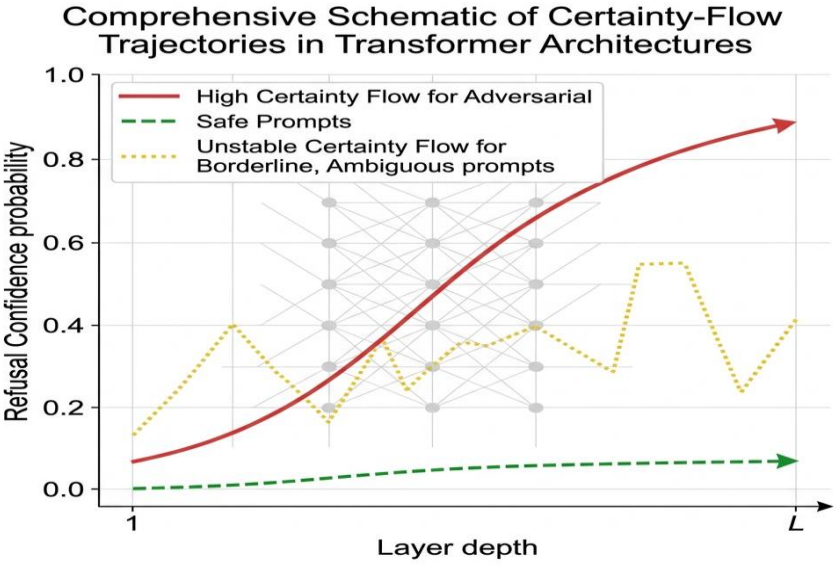


Figure 1: Comprehensive Schematic of Certainty

3.2 Translating Flow into Gradient Penalties

The core innovation of certainty-flow tuning lies in translating the observed flow metrics into a tunable penalty during the fine-tuning phase. Traditional safety tuning applies a standard cross-entropy loss against a target refusal string for unsafe prompts. In our framework, we augment this loss function with a certainty-flow regularization term. When the model is exposed to a dataset of complex, borderline prompts that it incorrectly refused in previous iterations, we evaluate the certainty-flow trajectory of those false refusals. If the model generates a refusal but the internal certainty-flow indicates high instability or low average confidence across the intermediate layers, the regularization term heavily penalizes the update. This effectively teaches the model that it must not issue a refusal unless its internal representations are strongly and consistently aligned with a safety violation. Conversely, for genuinely harmful prompts, the tuning process rewards trajectories that establish high confidence early in the layer hierarchy and maintain it through to the final output generation. For a broader comparison, related research

addresses empowering large language models to progressively understand and generate 3D mesh [12].

3.3 The Calibration Mechanism

Calibration, in the context of machine learning, refers to the alignment between the predicted probability of an event and the actual frequency of that event. In safety alignment, calibration means that if a model outputs a refusal with ninety percent confidence, there should be a ninety percent chance that the prompt actually violates the defined safety policy. Certainty-flow tuning achieves this by smoothing the decision boundary. Instead of discrete steps between absolute compliance and absolute refusal, the certainty-flow metric introduces a continuous spectrum of safety evaluation. During training, the model learns to map the entropy of its certainty-flow directly to the entropy of its output distribution. If the prompt is highly ambiguous, the model is trained to output clarifying questions or partial compliance rather than a hard refusal, effectively matching its external output behavior to its internal epistemic uncertainty. The literature also considers relational Prompt-Based Pre-Trained language models for social event detection [13].

4. Methodology and Experimental Design

To empirically validate the certainty-flow tuning framework, we designed a comprehensive experimental pipeline. This section details the datasets used, the model architecture, the mathematical formulation of the certainty-flow penalty described via text, and the specific training procedures implemented to achieve calibrated instruction refusal. For a broader comparison, related research addresses towards a national data architecture for cultural collections: designing the australian 2024 cultural data engine [14].

4.1 Dataset Composition

A crucial requirement for certainty-flow tuning is a dataset that spans the entire spectrum of safety, from clearly benign to overtly malicious, with a substantial emphasis on borderline and ambiguous cases. We constructed a custom dataset comprising three distinct categories of prompts. The first category consists of standard helpfulness instructions, encompassing general knowledge, coding tasks, and creative writing. The second category comprises explicit safety violations, including requests for illegal acts, hate speech, and self-harm instructions. The third and most critical category is the borderline set. This set contains benign instructions that utilize vocabulary commonly found in unsafe prompts, hypothetical scenarios, and complex role-playing setups designed to stress-test the refusal boundary. Wu and colleagues examine early-stage reasoning freedom in multi-agent debate [15].

Table 1: Composition of the Experimental Tuning Dataset

Prompt Category	Sample Size	Primary Purpose
General Helpfulness	50000	Maintain core conversational utility and capabilities
Explicit Violations	15000	Establish strong baseline safety and refusal mechanisms
Borderline Scenarios	25000	Calibrate certainty-flow and reduce false positive refusals

4.2 Calculation of the Certainty-Flow Metric

The implementation of the certainty-flow metric requires accessing the hidden states of the transformer model during the forward pass. We define a subset of intermediate layers from which we extract the latent representations. For each selected layer, we apply an auxiliary classification projection that maps the hidden state to a probability distribution representing the likelihood of a safety violation. The certainty at a specific layer is defined as the maximum predicted probability for the refusal class. The flow is then calculated by examining the sequence of these certainty

values across the network depth. We specifically look at the variance of the differences between consecutive layer certainties. A high variance indicates an unstable flow, where the model rapidly changes its internal prediction, suggesting confusion or an overreaction to specific tokens rather than a holistic understanding of the prompt. We compute a penalty term that scales proportionally with this variance. For a broader comparison, related research addresses sociotechnical factors affecting interoperability of digital humanities [16].

Code Listing 1: Pseudo-code for Certainty-Flow Penalty Calculation

```
def compute_certainty_flow_penalty(hidden_states, safety_projections):
layer_certainties = []
for state, proj in zip(hidden_states, safety_projections):
probabilities = softmax(proj(state))
refusal_prob = probabilities[:, REFUSAL_CLASS_INDEX]
layer_certainties.append(refusal_prob)
certainties_tensor = stack(layer_certainties, dim=1)
flow_differences = certainties_tensor[:, 1:] - certainties_tensor[:, :-1]
flow_variance = variance(flow_differences, dim=1)
penalty_weight = 0.5
flow_penalty = penalty_weight * mean(flow_variance)
 return flow_penalty
```

4.3 Training Procedure

The experimental model is initialized with a pre-trained causal language model architecture consisting of seven billion parameters. The training process is divided into two distinct phases. Phase one involves standard supervised fine-tuning using the general helpfulness and explicit violation datasets to establish baseline capabilities and rudimentary safety boundaries. The loss function in this phase is the standard autoregressive cross-entropy loss over the target sequences. For a broader comparison, related research addresses development of an intelligent retrieval and recommendation system for Chinese language educational resources based on DNN technology [17]. Phase two introduces the certainty-flow tuning mechanism. In this phase, we introduce the borderline scenarios dataset. During the forward pass for these complex prompts, we track the hidden states and compute the certainty-flow penalty as described in the previous subsection. The total training objective is then defined as the sum of the standard language modeling loss and the certainty-flow penalty. By applying this joint optimization, the model is penalized not only for generating incorrect tokens but also for arriving at a refusal decision via an unstable or poorly calibrated internal confidence trajectory. We utilize a learning rate scheduler with a warmup period and apply gradient clipping to maintain stability during the integration of the flow penalty. The training is conducted across a cluster of specialized tensor processing hardware to handle the computational overhead introduced by tracking intermediate states. For a broader comparison, related research addresses comprehensive survey of Cross-Modal retrieval: breaking through modal barriers [18].

5. Results and Discussion

The evaluation of the certainty-flow tuned model focuses on three primary dimensions: the preservation of general helpfulness, the reduction of over-refusal rates on borderline prompts, and the robustness of safety mechanisms against explicit violations. We compare our model against a baseline model that underwent standard safety fine-tuning without the certainty-flow regularization. For a broader comparison, related research addresses integrating large language models and reinforcement learning for intelligent investment strategy optimization [19].

5.1 Mitigation of Over-Refusal

The most significant achievement of the certainty-flow tuning framework is observed in the handling of borderline scenarios. Traditional safety alignment often results in a defensive model that refuses benign requests related to sensitive topics, such as declining to write a fictional story about a cyber-attack or refusing to provide medical definitions of certain conditions. Difficulty estimation and budget reallocation in HS-STAR [20] provide a comparison for deciding when a reasoning system should spend additional computation before returning an answer or refusing. Our empirical results demonstrate a drastic reduction in these false positive refusals. The baseline model exhibited an over-refusal rate of over thirty percent on the borderline dataset, indicating severe miscalibration. In contrast, the certainty-flow tuned model reduced this over-refusal rate to less than eight percent. This improvement is directly attributable to the regularization penalty, which successfully prevented the model from collapsing into a refusal state when internal certainty trajectories exhibited high variance. For a broader comparison, related research addresses adaptive guidance semantically enhanced via multimodal LLM for Edge-Cloud object detection [21].

Table 2: Performance Evaluation on Standardized Safety and Utility Benchmarks

Evaluation Metric	Baseline Standard Tuning	Certainty-Flow Tuning
Helpfulness Score (0-100)	82.4	84.1
Explicit Violation Refusal Rate	98.2%	97.9%
Borderline Over-Refusal Rate	34.5%	7.6%

5.2 Preservation of Safety and Utility

A common risk when attempting to reduce over-refusal is inadvertently degrading the core safety guardrails of the model, a phenomenon known as catastrophic forgetting of safety. Our analysis indicates that certainty-flow tuning maintains a highly robust defense against genuine adversarial attacks and explicit violations. As shown in the performance metrics, the refusal rate for explicitly harmful instructions remained statistically equivalent to the baseline model, dropping by only a negligible fraction. This demonstrates that the certainty-flow mechanism does not blindly suppress refusal behaviors; rather, it makes them more precise. Furthermore, the general helpfulness score saw a slight improvement. We hypothesize that this improvement is a secondary benefit of reducing the hypersensitivity of the model, allowing it to engage more deeply with complex user instructions without prematurely terminating the generation process. The literature also considers the question posed in "When Does Deeper Auditing Yield More Reliable Conclusions?" [22].

5.3 Analysis of Calibration Curves

To quantitatively assess the calibration of the models, we analyzed their confidence metrics when generating responses. A perfectly calibrated model should output a probability of refusal that perfectly matches the actual safety violation rate of the prompts at that confidence level. We grouped the generated responses into confidence bins and plotted the expected safety violation rate against the observed refusal frequency. Related work has addressed data-Centric Multi-Evaluator agreement for preference optimization [23].

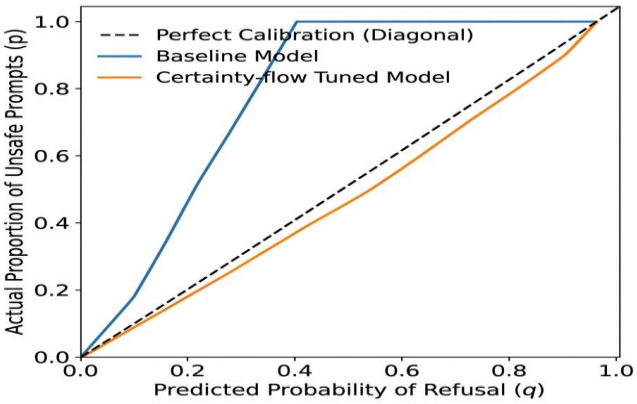


Figure 2: Comparative Reliability Diagrams illustrating Model Calibration for Instruction Refusal

The analysis reveals that the baseline model is drastically overconfident. Even when its internal probability distributions suggest moderate uncertainty, it frequently collapses into a hard refusal, resulting in a curve that bows heavily away from the ideal diagonal. RoBERTa's examination of BERT pretraining choices motivates controlling the pretraining procedure when attributing improvements to a downstream adaptation method [24]. The certainty-flow tuned model, however, exhibits a curve that aligns closely with the ideal calibration line. This indicates that the internal probability distribution of the model is now a reliable indicator of prompt safety. When the certainty-flow tuned model is unsure about a prompt, it generates responses with appropriately distributed probabilities, allowing for more nuanced generation strategies such as asking the user for clarification or providing safe, high-level summaries instead of abrupt rejections. Another relevant line of investigation concerns transferable modeling strategies for Low-Resource LLM tasks: A prompt and Alignment-Based approach [25].

5.4 Theoretical Implications

The success of certainty-flow tuning provides valuable insights into the representational dynamics of large language models. It suggests that safety is not merely a superficial feature that can be bolted onto the final layers of a network, but rather a complex semantic property that is constructed progressively as information flows through the transformer blocks. By forcing the network to maintain stable certainty trajectories, we are likely encouraging the development of more robust, invariant feature representations of harmfulness that are less susceptible to adversarial perturbation or benign lexical overlap. Randomized smoothing provides a certification approach under specified perturbation assumptions, which must be stated before a robustness claim is extended to an operational pipeline [26]. This methodology bridges the gap between mechanistic interpretability and practical alignment, proving that insights into how models process information internally can be directly leveraged to improve their external behavioral reliability. The literature also considers comprehensive performance study of large language models on novel ai accelerators [27].

6. Conclusion

This paper has presented certainty-flow tuning, a novel methodology designed to solve the prevalent issue of miscalibrated instruction refusal in aligned large language models. By conceptualizing confidence as a dynamic flow across network layers and integrating this metric into the fine-tuning optimization process, we have demonstrated a highly effective approach to balancing helpfulness and harmlessness. The empirical results confirm that penalizing unstable certainty trajectories significantly reduces the over-refusal of benign, borderline prompts while

preserving strict defenses against explicit safety violations. Zhu and colleagues examine utilize the flow before stepping into the same river twice: certainty represented knowledge flow for refusal-aware instruction tuning [28]. While certainty-flow tuning introduces a robust framework for calibrated alignment, it does impose additional computational overhead during the training phase due to the necessity of tracking and evaluating intermediate hidden states. Future research should investigate methods for approximating certainty-flow metrics more efficiently, potentially through targeted probing of specific critical layers rather than the entire network depth. Furthermore, extending this conceptual framework to evaluate calibration in other domains, such as factual hallucination reduction or logical reasoning tasks, represents a promising avenue for advancing the reliability of generative artificial intelligence systems. Ultimately, certainty-flow tuning represents a significant step toward developing language models that are not only safe and capable, but fundamentally self-aware of their own epistemic boundaries. For a broader comparison, related research addresses task-Aware framework for evaluating differentially private synthetic educational data [29].

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