

iFlip: Iterative Feedback-driven Counterfactual Example Refinement

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Abstract

Counterfactual examples are minimal edits to an input that alter a model’s prediction. They are widely employed in explainable AI to probe model behavior and in natural language processing (NLP) to augment training data. However, generating valid counterfactuals with large language models (LLMs) remains challenging, as existing single-pass methods often fail to induce reliable label changes, neglecting LLMs’ self-correction capabilities. To explore this untapped potential, we propose *iFlip*¹, an iterative refinement approach that leverages three types of feedback, including model confidence, feature attribution, and natural language. Our results show that *iFlip* achieves an average 57.8% higher validity than the five state-of-the-art baselines, as measured by the label flipping rate. The user study further corroborates that *iFlip* outperforms baselines in completeness, overall satisfaction, and feasibility. In addition, ablation studies demonstrate that three components are paramount for *iFlip* to generate valid counterfactuals: leveraging an appropriate number of iterations, pointing to highly attributed words, and early stopping. Finally, counterfactuals generated by *iFlip* enable effective counterfactual data augmentation, substantially improving model performance and robustness.

1 Introduction

Counterfactual examples are minimally modified inputs that cause a model to alter its prediction (Madsen et al., 2022; Wang et al., 2024; Zhao et al., 2024). Applications include elucidating opaque LLMs through contrastive causal analysis (Ross et al., 2021; Treviso et al., 2023; Nguyen et al., 2024b) and enhancing model performance and robustness (Kaushik et al., 2020; Dixit et al., 2022; Qiu et al., 2024). However, most recent approaches (Bhan et al., 2023; Bhattacharjee et al., 2024a;

Nguyen et al., 2025) rely on single-pass generation, often yielding invalid counterfactuals that are insufficient to shift the model’s original prediction. This neglects LLMs’ inherent self-correction capabilities, despite their proven efficacy in other domains and downstream tasks (Madaan et al., 2023; Gou et al., 2024; Rahmani et al., 2025).

To overcome these limitations, we propose *iFlip* (Figure 1), a framework that iteratively refines counterfactuals via diverse feedback signals to enhance validity. **First**, we evaluate *iFlip* across three datasets and three LLMs using confidence, feature attribution, and natural language feedback. Compared to five baselines – BAE (Garg and Ramakrishnan, 2020), Polyjuice (Wu et al., 2021), CGG (Nguyen et al., 2025), FIZLE (Bhattacharjee et al., 2024a), and Causal What-Ifs (Narendra and Chatterjee, 2025) – *iFlip* improves validity by 57.8% at the cost of 8.3% lower similarity, with natural language feedback proving most effective.

Second, a user study confirms *iFlip* with natural language feedback outperforms FIZLE and CGG in *completeness*, *overall satisfaction*, and *feasibility*, achieving the most substantial improvement in *overall satisfaction* (83.21%). Error analysis reveals that the iterative refinement process effectively addresses both incomplete and contextually inappropriate edits in counterfactuals (§6.2).

Third, we perform systematic ablation studies to assess the contribution of each component in *iFlip*: (1) the number of refinement iterations, (2) the choice of feedback signal, and (3) of early stopping criteria. We find that counterfactual validity can be noticeably improved across iterations, even within a limited number of rounds (e.g., $\mathcal{K} = 5$). Feedback-guided generation considerably boosts performance over the without-feedback baseline. Moreover, we establish that early stopping upon achieving validity is imperative to prevent valid counterfactuals from being erroneously overturned in subsequent iterations.

¹The code is available anonymously at <https://anonymous.4open.science/r/iFlip>.

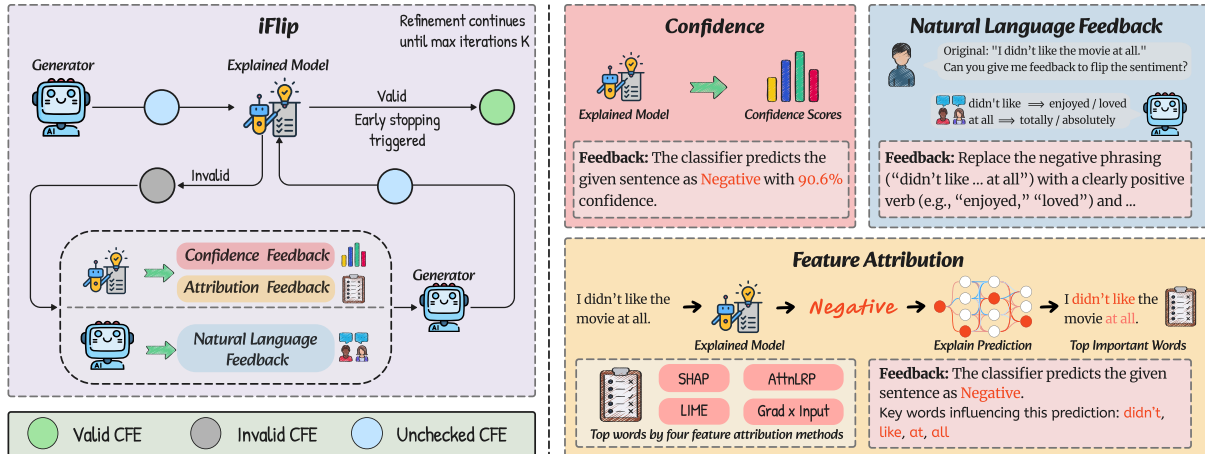


Figure 1: *iFlip* framework overview. **Left**: The core iterative loop of our method, which includes a generator \mathcal{G} and an explained model \mathcal{M} . \mathcal{G} generates and refines counterfactuals. \mathcal{M} evaluates counterfactuals under our validity criterion: a counterfactual is considered *valid* if \mathcal{M} 's predicted label is equal to the target label \tilde{y} . Otherwise, *invalid* counterfactuals are iteratively refined until the validity criterion is met to avoid unnecessary iterations or the maximal number of refinement steps is reached. **Right**: Examples of the three types of feedback we employed for *iFlip*: *Confidence*, *Feature Attribution*, and *Natural Language Feedback*.

082 **Lastly**, we show that counterfactuals generated
 083 by *iFlip* enable effective counterfactual data aug-
 084 mentation (CDA), improving model performance
 085 and robustness, measured by accuracy on both the
 086 original and the human-annotated counterfactual
 087 test sets. Additionally, our analysis confirms that
 088 the quality of the generated counterfactuals posi-
 089 tively correlates with the CDA performance gains.

090 **2 Related Work**

091 **LLM-based Counterfactual Generation.** FI-
 092 ZLE employs LLMs for zero-shot counterfactual
 093 generation to explain and evaluate black-box clas-
 094 sifiers (Bhattacharjee et al., 2024a). Bhattacharjee
 095 et al. (2024b) propose a three-step pipeline that
 096 leverages instruction-tuned LLMs to extract latent
 097 features and their associated input words. Several
 098 recent methods incorporate feature attribution sig-
 099 nals to guide counterfactual generation. ZeroCF
 100 improves zero-shot counterfactual generation by
 101 leveraging feature attribution methods to guide text
 102 edits (Wang et al., 2025b). Similarly, CGG inserts
 103 token attributions into few-shot prompts to guide
 104 LLMs in generating high-validity CFEs (Nguyen
 105 et al., 2025). Narendra and Chatterjee (2025) pro-
 106 pose an agentic framework that iteratively refines
 107 counterfactuals through self-reflection but does not
 108 incorporate feedback or early stopping, which we
 109 find crucial for enhancing counterfactual validity
 110 (§6.3.2, §6.3.3). Unlike these approaches, *iFlip*
 111 explicitly incorporates three types of feedback, in-

112 cluding feature attribution signals, and iteratively
 113 refines counterfactuals based on this feedback.

114 **Iterative Refinement with Feedback.** Xi et al.
 115 (2023) and Liu et al. (2024) empirically observe
 116 that model performance tends to improve over suc-
 117 cessive rounds of self-correction, wherein LLMs
 118 refine their answers using either intrinsic (Madaan
 119 et al., 2023; Xu et al., 2024) or external (Welleck
 120 et al., 2023) feedback. In the field of explainability,
 121 SR-NLE improves the faithfulness of post-hoc ex-
 122 planations through an iterative critique and refine-
 123 ment process (Wang and Atanasova, 2025). CROSS-
 124 REFINE enhances the quality of natural language
 125 explanations via tandem learning through feedback
 126 and critiques in an iterative manner (Wang et al.,
 127 2025a). In this work, we employ three types of
 128 feedback signals to guide iterative refinement of
 129 generated counterfactuals across multiple rounds.

130 **3 Methodology**

131 **3.1 iFlip**

132 As illustrated in Figure 1, *iFlip* employs iterative
 133 refinement driven by the interaction of two com-
 134 ponents: the counterfactual generator \mathcal{G} and the
 135 explained model \mathcal{M} . The explained model vali-
 136 dates the counterfactual candidates produced by
 137 the generator. When a candidate is unsuccessful in
 138 changing the model’s prediction, it is sent back to
 139 the generator, accompanied by specific feedback
 140 signals (§3.2), to guide the next generation step.

*i*Flip is structured into three primary stages:

Step 1: Generation. Given the original input x and the explained model \mathcal{M} , we first obtain the original model prediction $y = \mathcal{M}(x)$, a label in a classification task, then define a target label $\tilde{y} \neq y$. Generator \mathcal{G} produces an initial counterfactual candidate:

$$\tilde{x}_0 \leftarrow \mathcal{G}(x, y, \tilde{y}) \quad (1)$$

Step 2: Verification. Explained model \mathcal{M} validates the candidate \tilde{x}_0 . If $\mathcal{M}(\tilde{x}_0) = \tilde{y}$, i.e., the desired target label is achieved, we return \tilde{x}_0 (early stopping); otherwise, we proceed to **refinement**.

Step 3: Refinement. If the initial counterfactual candidate \tilde{x}_0 fails to induce the model prediction to \tilde{y} , we perform up to \mathcal{K} iterative refinement steps, indexed by $k \in \{1, 2, \dots, \mathcal{K}\}$, each guided by feedback signals f_k :

$$\tilde{x}_k \leftarrow \mathcal{G}(x, \tilde{x}_{k-1}, y, \tilde{y}, f_k) \quad (2)$$

Upon generating a new counterfactual candidate \tilde{x}_k , we return to the validation phrase (**Step 2**). This iterative process continues until either the validation succeeds ($\mathcal{M}(\tilde{x}_k) = \tilde{y}$) or the maximum iteration count \mathcal{K} is attained.

3.2 Feedback Signals

In our experiments, we cover three feedback signals $F = \{f_{\text{Conf}}, f_{\text{Attr}}, f_{\text{NL}}\}$ that are prevalently employed in the literature: *confidence*, *feature attribution*, and *natural language feedback* (Figure 1).

Confidence. The self-correction capability of language models comprises two components: confidence, defined as the ability to retain correct answers, and critique, defined as the ability to revise incorrect answers (Yang et al., 2025b). Consequently, following Hernandez et al. (2025) and Mavi et al. (2025), we incorporate the confidence score as one of feedback signals.

Feature Attribution. Following prior work that established guiding LLMs for counterfactual generation using important words (Bhan et al., 2023; Wang et al., 2025b; Nguyen et al., 2025), we apply established four feature attribution methods: SHAP (Lundberg and Lee, 2017), AttnLRP (Achtibat et al., 2024), LIME (Ribeiro et al., 2016), and Gradient \times Input (Shrikumar et al., 2017), which determine token importance in an input text.

Natural Language Feedback. LLM-generated feedback in free-text form has been shown to be effective for improving both downstream task performance and explanation generation (Madaan et al.,

2023; Wang et al., 2025a). Accordingly, we instruct the LLMs to provide natural language feedback on their own counterfactuals.

4 Experimental Setup

4.1 Datasets & Models

Datasets. We test *i*Flip on three NLP datasets that are well-studied in the counterfactual generation literature.² IMDb comprises diverse movie reviews labeled as *positive* or *negative* sentiment (Maas et al., 2011). AG News contains news articles categorized into four topics: *World*, *Sports*, *Business*, and *Sci/Tech* (Zhang et al., 2015). Each article includes a title and a description. SNLI is a dataset for natural language inference (NLI) tasks (Bowman et al., 2015). It consists of premise-hypothesis pairs labeled as *entailment*, *contradiction*, or *neutral*.

Models. We employ three state-of-the-art, open-source LLMs from different model families and with increasing parameter sizes: OLMo2-7B (OLMo et al., 2025), Qwen3-32B (Yang et al., 2025a), LLaMA3.3-70B (Grattafiori et al., 2024).³

4.2 Baselines

We compare *i*Flip against two widely adopted baselines and three state-of-the-art LLM-based counterfactual generation methods. ① BAE is an adversarial approach and perturbs inputs using a BERT masked language model to replace masked tokens based on semantic similarity (Garg and Ramakrishnan, 2020). ② Polyjuice leverages a fine-tuned GPT-2 to generate counterfactuals by framing the task as a conditional text generation problem, using control codes to produce diverse and fluent counterfactuals (Wu et al., 2021). ③ CGG uses feature attributions to select the top 25% most important words and incorporates them into a predefined prompt with factual-counterfactual examples, explicitly directing the LLM which words to modify for the target label flip (Nguyen et al., 2025). ④ FIZLE_{naive} directly prompts an LLM to minimally edit the input to achieve a label flip, without prior feature identification or guidance (Bhattacharjee et al., 2024a). ⑤ Causal What-Ifs is an agentic approach that iteratively improves counterfactual generation through self-reflection, enabling the identifi-

²Dataset examples, label distributions, and dataset sources are provided in Appendix A.

³Information about inference time and generation parameters is provided in Appendix B.

cation of causally consistent edits *without external feedback* (Narendra and Chatterjee, 2025).

5 Evaluation

5.1 Automatic Evaluation

To assess the quality of generated counterfactuals, we adopt three commonly used automatic evaluation metrics following prior work (Ross et al., 2021; Wang et al., 2024; Nguyen et al., 2024a; Bhattacharjee et al., 2024a): *validity*, *similarity*, and *fluency*.

Label Flipping Rate (LFR) evaluates the *validity* of counterfactuals by measuring the proportion of instances whose predicted label changes after modification. Given the explained model \mathcal{M}^4 , the original inputs x , and counterfactuals \tilde{x} , LFR is calculated by:

$$\text{LFR} = \frac{1}{N} \sum_{i=1}^N \mathbb{I}[\mathcal{M}(x_i) \neq \mathcal{M}(\tilde{x}_i)]$$

where $\mathbb{I}[\cdot]$ denotes the indicator function.

Semantic Similarity (SS) We compute semantic similarity between the original input x and its counterfactual \tilde{x} using cosine similarity between their sentence embeddings $\mathbf{e}(\cdot)$, where each embedding is produced by a pretrained encoder⁵:

$$\text{SS}(x_i, \tilde{x}_i) = \frac{1}{N} \sum_{i=1}^N \frac{\mathbf{e}(x_i)^\top \mathbf{e}(\tilde{x}_i)}{\|\mathbf{e}(x_i)\|_2 \|\mathbf{e}(\tilde{x}_i)\|_2}$$

Perplexity (PPL) To assess *fluency*, we compute the perplexity of generated counterfactuals using GPT-2. Given a counterfactual $\tilde{x} = (t_1, \dots, t_n)$ consisting of n tokens and a model parameterized by θ , the perplexity of \tilde{x} is defined as:

$$\text{PPL}(\tilde{x}) = \exp\left(-\frac{1}{n} \sum_{i=1}^n \log p_\theta(t_i | t_{<i})\right)$$

5.2 User Study & LLM-as-a-Judge

We further assess the quality of generated counterfactuals by conducting a *user study* and a complementary *LLM-as-a-Judge evaluation*. Participants and judge models, respectively, evaluate the counterfactuals along three dimensions (§5.2.1) on a 6-point Likert scale.

5.2.1 Subjective Ratings

Following Nguyen et al. (2024a); Domnich et al. (2025), we ask human annotators to evaluate counterfactuals across three subjective dimensions:

- **Completeness:** The counterfactual sufficiently explains the model’s decision.
- **Overall Satisfaction:** The counterfactual effectively shows how to reach a different outcome.
- **Feasibility:** The counterfactual provides actions that are practical, realistic, and actionable.

5.2.2 User Study Setup

We conduct a user study on AG News, from which we randomly sample 10 examples, with ($N = 3$) participants, all proficient in English.⁶ We evaluate two LLM-based baselines (FIZLE and CGG) alongside iFlip configured with natural language feedback, which demonstrates the best performance among all feedback types (§6.1). In Table 2, We report inter-annotator and inter-judge-model agreements with Krippendorff’s α for each dimension.

5.2.3 LLM-as-a-Judge Setup

LLM-as-a-Judge (LaaJ) has become a widely adopted approach for conducting evaluations by assigning quality scores that align with human judgment (Huang et al., 2024; Li et al., 2025). Following Gu et al. (2025), we employ three commonly used open-source LLMs of varying sizes: Gemma3-27B (Team et al., 2025), GPT-OSS-120B (OpenAI et al., 2025), and DeepSeek-R1 (DeepSeek-AI et al., 2025). Judge models are instructed to assess the quality of generated counterfactuals based on three subjective dimensions, as in the user study (§5.2.2).⁷

5.3 Ablation Study

As outlined in §3.1, our framework incorporates three essential components: (1) the number of refinement iteration steps, (2) feedback signals, and (3) early stopping. We conduct ablation studies to assess the contribution of each component.

The Number of Refinement Iterations. We aim to assess the contribution of iterative refinement to counterfactual generation effectiveness and quantify its advantages over single-pass methods. Our analysis adopts the pass@k metric (Brown et al., 2024), which measures the fraction of counterfactuals achieving successful label flips within k refinement attempts. This metric tests whether multiple refinement steps considerably enhance the LFR.

Feedback Signal. We analyze the role of different feedback signals in counterfactual generation by

⁴Model \mathcal{M} is BERT in Table 1 and RoBERTa in App. C.1.

⁵sentence-transformers/all-MiniLM-L6-v2

⁶The annotation guideline is detailed in Appendix L.

⁷The full judge prompt is provided in Appendix M.1.

Method	IMDb			AG News			SNLI (Premise)			SNLI (Hypothesis)			
	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓	
Polyjuice	0.275	0.736	60.81	0.148	0.744	93.22	0.281	0.772	96.95	0.350	0.733	114.59	
BAE	0.553	0.976	63.15	0.227	0.764	295.96	0.135	0.966	82.98	0.115	0.979	81.00	
CGG	0.885	0.837	44.67	0.510	0.380	208.56	0.169	0.882	57.03	0.253	0.948	53.92	
FIZLE	0.585	0.584	38.71	0.308	0.584	77.38	0.305	0.730	173.94	0.404	0.882	74.15	
Causal What-Ifs	0.890	0.801	37.97	0.400	0.607	37.54	0.413	0.854	47.27	0.487	0.911	35.56	
OLMo2-7B	iFlip-Conf	0.964	0.809	41.19	0.784	0.503	41.41	0.660	0.854	53.72	0.826	0.870	40.65
	iFlip-SHAP	0.968	0.805	41.87	0.802	0.488	42.95	0.587	0.847	56.81	0.760	0.867	42.39
	iFlip-AttnLRP	0.978	0.803	42.61	0.768	0.500	46.61	0.596	0.851	55.30	0.810	0.869	40.31
	iFlip-Grad×Input	0.976	0.801	43.30	0.773	0.498	50.32	0.624	0.854	56.02	0.782	0.871	41.81
	iFlip-LIME	0.968	0.805	52.82	0.730	0.504	44.32	0.558	0.866	58.18	0.736	0.875	41.02
	iFlip-NL	0.984	0.822	36.47	0.735	0.515	44.73	0.638	0.879	148.41	0.770	0.901	43.81
	CGG	0.863	0.877	62.47	0.364	0.697	97.10	0.200	0.881	50.31	0.283	0.938	47.94
FIZLE	0.684	0.900	36.00	0.164	0.864	61.46	0.454	0.901	38.66	0.524	0.918	35.97	
Causal What-Ifs	0.848	0.821	42.03	0.436	0.570	53.50	0.482	0.842	36.14	0.518	0.920	34.14	
Qwen3-32B	iFlip-Conf	0.996	0.855	33.30	0.726	0.521	41.59	0.466	0.895	62.69	0.562	0.871	47.03
	iFlip-SHAP	0.994	0.857	33.70	0.736	0.519	44.02	0.452	0.878	58.60	0.586	0.866	45.04
	iFlip-AttnLRP	1.000	0.858	33.19	0.746	0.513	44.15	0.448	0.882	58.41	0.610	0.867	44.77
	iFlip-Grad×Input	0.996	0.865	33.65	0.730	0.522	44.33	0.440	0.881	58.66	0.542	0.865	45.60
	iFlip-LIME	0.998	0.863	32.57	0.742	0.527	44.52	0.458	0.891	62.98	0.570	0.870	44.22
	iFlip-NL	0.980	0.878	32.99	0.732	0.536	49.68	0.596	0.895	68.16	0.754	0.906	47.20
	CGG	0.887	0.869	52.81	0.526	0.694	122.40	0.307	0.846	51.62	0.271	0.937	46.58
FIZLE	0.924	0.868	34.88	0.416	0.707	56.59	0.402	0.903	41.54	0.534	0.929	42.39	
Causal What-Ifs	0.922	0.788	31.93	0.636	0.461	43.56	0.372	0.816	38.97	0.420	0.904	41.29	
LLaMA.3-70B	iFlip-Conf	0.996	0.877	34.74	0.890	0.468	44.38	0.580	0.763	58.65	0.642	0.843	43.88
	iFlip-SHAP	0.996	0.878	34.32	0.860	0.481	46.07	0.522	0.743	57.62	0.606	0.828	41.09
	iFlip-AttnLRP	0.992	0.879	34.58	0.858	0.477	45.78	0.528	0.743	56.42	0.602	0.822	39.92
	iFlip-Grad×Input	0.996	0.878	34.80	0.852	0.479	46.12	0.580	0.751	55.38	0.603	0.825	39.59
	iFlip-LIME	0.996	0.877	34.54	0.852	0.475	44.20	0.558	0.759	57.87	0.608	0.825	42.91
	iFlip-NL	0.996	0.895	36.90	0.900	0.527	63.86	0.566	0.821	69.45	0.680	0.861	69.45

Table 1: Automatic evaluation results of counterfactuals generated by baselines (Polyjuice, BAE, CGG, and FIZLE) and our *iFlip* methods on the BERT models with different feedback: **1** confidence (Conf), **2** feature attribution (SHAP, AttnLRP, Grad×Input, LIME), **3** natural language (NL). Results are reported on IMDb, AG News, and SNLI using Label Flipping Rate (LFR), Semantic Similarity (SS), and Perplexity (PPL). **Boldface** indicates the best feedback type within *iFlip*. Wavy underline indicates the best result across methods.

considering three feedback settings: (i) the baseline *no feedback*, where the model refines without any external signal; (ii) a *random feedback*, where the important features are randomly selected; (iii) *least-attributed feedback*, where feedback is derived from the least important words, identified by the corresponding attribution methods.

Without Early Stopping. We investigate the impact of early stopping on the counterfactual refinement process. Early stopping halts generation upon a successful label flip; without it, the model continues to edit valid counterfactuals until \mathcal{K} iterations. The core objective is to determine if eliminating early stopping can maintain the achieved label flip while simultaneously improving the overall quality of the generated counterfactuals.

5.4 Counterfactual Data Augmentation

We examine to what extent counterfactuals generated by *iFlip* enhance both model performance and robustness through counterfactual data aug-

mentation (Kaushik et al., 2020; Dixit et al., 2022; Wang et al., 2025c). Our baseline is a model $\mathcal{M}_{\text{base}}$ which is trained only on the original dataset $\mathcal{D}_{\text{base}} = \{(x_i, y_i)\}_{i=1}^N$, while the CDA-enhanced model \mathcal{M}_c is trained on both the original data and the corresponding counterfactuals (either generated by *iFlip* or human-annotated) $\mathcal{D}_c = \{(x_i, y_i), (\tilde{x}_i, \hat{y}_i)\}_{i=1}^N$. The CDA evaluation involves assessment using both the test set data and human-annotated counterfactuals.

6 Results

6.1 Automatic Evaluation

Comparison among the baselines. Table 1 shows that perturbation-based baselines (Polyjuice, BAE) tend to make fewer edits but often struggle with the model prediction flipping, whereas LLM-based baselines (CGG, FIZLE and Causal What-Ifs) can more reliably generate counterfactuals achieving the target labels while being more natural. Among the LLM-based baselines, CGG, which leverages

feature importance methods to identify the most important words, demonstrates higher LFR on IMDb and AG News than FIZLE, where such word-level guidance facilitates more effective label flips. In contrast, FIZLE, which generates counterfactuals through direct prompting, performs better on SNLI, likely because for NLI tasks, modifying important words identified by feature importance methods often fails to fully capture the underlying logical relations between the premise and the hypothesis. Notably, Causal What-Ifs attains the highest validity among baselines on NLI tasks, though it struggles to outperform attribution-guided methods (CGG) on news topic classification (AG News). However, Causal What-Ifs requires noticeably more edits compared to FIZLE and CGG, suggesting a trade-off between validity gains and input modifications.

iFlip outperforms all baselines in terms of LFR across datasets and models. Table 1 illustrates that *iFlip* consistently achieves the highest LFR across all datasets and models while maintaining competitive fluency.⁸ Averaged across all experimental settings, *iFlip* improves LFR by 71.4% and fluency by 13.8% relative to single-pass LLM-based baselines. These gains are particularly pronounced on AG News, where *iFlip* achieves a 107% higher LFR than those baselines. Compared with self-reflection-based Causal What-Ifs, *iFlip* further improves validity by 35.7% on average. This additional gain further validates the effectiveness of the feedback mechanism (§6.3.2) and the early stopping strategy (§6.3.3).

iFlip gains involve a trade-off between validity and similarity. While *iFlip* improves the validity of generated counterfactuals, this comes at the cost of more extensive edits (Table 1)⁹, indicating a trade-off between validity and the extent of input modifications. Specifically, OLMo2-7B, despite being the smallest model employed, attains comparable or even higher LFR than larger models by incorporating more edits (Table 1). Particularly, on AG News, topic transitions typically require more intensive multi-entity and event-level modifications. Counterintuitively, we find that counterfactuals generated by larger LLMs do not necessarily achieve higher LFR, consistent with prior observa-

tions (Nguyen et al., 2024b; Wang et al., 2025b).

Comparison of different feedback signals. As shown in Figure 6, natural language feedback generally achieves the most (consistent) enhancement across all experimental setups in terms of LFR. However, the improvement comes at the cost of substantially higher inference time due to the LLM-generated natural language feedback (Madaan et al., 2023) (Table 7). Confidence-based feedback ranks second, achieving a balance between effectiveness and computational efficiency. In contrast, attribution-based feedback generally performs poorly, likely because LLMs neither strictly adhere to the identified important words nor limit themselves to targeted modifications, instead often rephrasing entire sentences.¹⁰ Among attribution approaches, propagation- and gradient-based methods (AttnLRP and Grad×Input) consistently outperform perturbation-based ones (SHAP and LIME), as further detailed in Appendix E.2.

Case Study. We examine SNLI more closely, where generating valid counterfactuals is particularly challenging due to the inherent logical relationships between premises and hypotheses, making it an outlier relative to IMDb and AG News. Following prior work on counterfactual generation for NLI (Nguyen et al., 2024b, 2025), we generate counterfactuals by modifying either the premise or hypothesis. For SNLI, editing hypotheses is substantially more effective, as their shorter length allows *iFlip* to induce label flips more easily. Empirically, however, we observe that modifying important words is less effective in improving LFR compared to other ways of generating counterfactuals. Among *iFlip* variants, attribution-based feedback yields lower LFR than confidence-based or natural language feedback (Figure 7, Appendix D), suggesting that targeting only salient words is insufficient to reverse entailment relations in NLI tasks. Moreover, SNLI exhibits both substantially lower feature attribution faithfulness than IMDb and AG News, and weaker alignment between faithfulness and counterfactual quality.¹¹

6.2 User Study & LLM-as-a-Judge

User Study. Table 2a quantitatively confirms that *iFlip*-NL consistently outperforms CGG and FIZLE across all three subjective evaluation di-

⁸App. C.2 reports the transferability of generated counterfactuals across architectures and the transferability of feedback extracted from BERT.

⁹See App. E.1.3 for a visualization of SS-LFR trade-off. App. E.1.1 and E.1.2 report the average number of refinements and the average length of counterfactuals at each iteration.

¹⁰Representative examples are presented in Appendix J.

¹¹App. G reports the faithfulness of the employed attribution methods, while App. H.2 details the correlation between the feature attribution faithfulness and counterfactual quality.

Method	Completeness	Overall Sat.	Feasibility
CGG	2.83 ± 1.69	2.67 ± 1.49	2.80 ± 1.60
FIZLE _{naive}	3.27 ± 2.00	2.93 ± 1.71	3.40 ± 1.80
iFlip-NL	5.10 ± 1.19	5.13 ± 1.12	4.83 ± 1.27
Krippendorff's α	0.6467	0.8690	0.8694

(a) Human evaluation.

Method	Completeness	Overall Sat.	Feasibility
CGG	3.20 ± 1.94	3.10 ± 2.06	3.93 ± 2.03
FIZLE _{naive}	3.10 ± 2.12	3.07 ± 2.13	3.80 ± 2.17
iFlip-NL	4.53 ± 1.78	4.47 ± 1.86	4.40 ± 1.80
Krippendorff's α	0.7615	0.8215	0.4005

(b) LLM-as-a-judge evaluation.

Table 2: Evaluation results (**mean ± std**) on three subjective dimensions: *Completeness*, *Overall Satisfaction* and *Feasibility*. Best results are **bolded**.

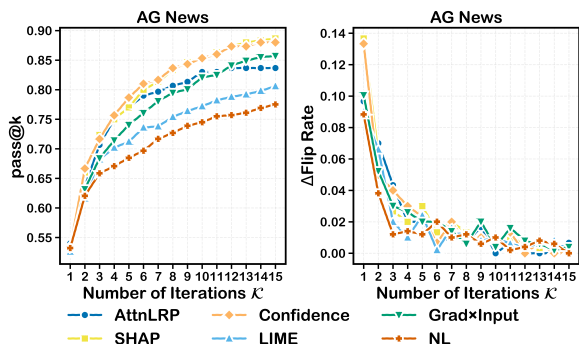


Figure 2: Iterative refinement effectiveness on OLMo2-7B (AG News) across feedback signals. Left: pass@k curves up to $\mathcal{K} = 15$. Right: per-iteration improvement in flip rate (Δ Flip Rate).

mensions (§5.2.1), achieving an average relative gain of 68.27%. Notably, the most substantial improvement occurs in *Overall Satisfaction*, with an 83.21% relative gain. To understand the source of these improvements, we **qualitatively** analyze representative failure cases in Appendix N. We observe two recurring issues in baseline methods: (i) they frequently edit only partial entity mentions, resulting in *incomplete* changes that fail to flip the model prediction; and (ii) they sometimes produce contextually inappropriate edits, yielding *unnatural* counterfactuals. In contrast, *iFlip-NL* mitigates these issues through iterative refinement, improving both *Completeness* and *Feasibility* of generated counterfactuals.¹²

LLM-as-a-Judge. Table 2b reveals that LaaJ results exhibit a trend consistent with human eval-

¹²See Appendix N.3 and N.4 for per-annotator human/LLM ratings and examples showing how iterative refinement fixes *incomplete* and *unnatural* edits

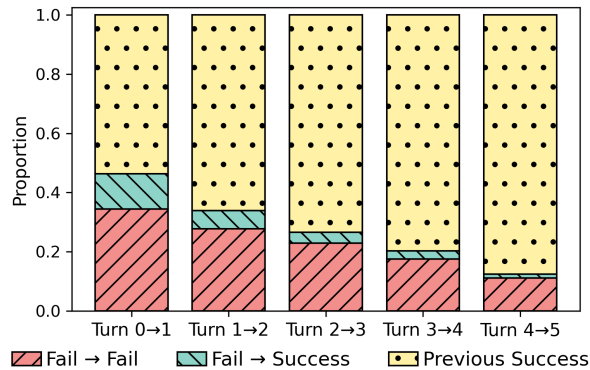


Figure 3: Iterative refinement with OLMo2-7B under early stopping, averaged across all datasets and feedback signals. *Fail* → *Fail* indicates no label change, *Fail* → *Success* denotes a successful label flip in the current turn, and *Previous Success* marks instances flipped in earlier turns.

uation: *iFlip-NL* invariably outperforms selected baselines across all three dimensions.¹³ Notably, the LLM judgments demonstrate larger standard deviations than human ratings, indicating that LLMs tend to assign more extreme scores. Moreover, the human-LLM alignment, as measured by Krippendorff's α 0.72, indicates relatively strong agreement between human and LaaJ evaluation.

6.3 Ablation Study

6.3.1 Iterative Refinement

Figure 2 illustrates that pass@k increases steadily with the number of refinement iterations, though the improvement per round gradually decreases as refinement progresses.¹⁴ This trend demonstrates LLMs' feedback-driven self-correction capacity while revealing single-pass generation's substantial performance gap relative to iterative refinement, especially when initial counterfactuals exhibit low validity (e.g., SNLI premise editing achieves less than 30% LFR in the first iteration). Even with a small number of iterations ($\mathcal{K} = 5$), iterative refinement yields markedly higher-validity counterfactuals than single-pass generation. Figure 3 further provides these dynamics under early stopping, where *Fail* → *Fail* transitions diminish and *Previous Success* cases dominate over time.¹⁵

6.3.2 Feedback Signal

We examine whether incorporating feedback is intrinsically beneficial for iterative counterfactual re-

¹³Evaluation across judge models are reported in App. M.2.

¹⁴Full pass@k curves and flip-rate improvements with OLMo2-7B across all datasets are provided in Appendix E.1.4.

¹⁵*Success* → *Fail* are not observed due to early stopping.

Feedback of iFlip	IMDb	AG News	SNLI (Premise)	SNLI (Hypothesis)
Without Feedback	0.964	0.742	0.508	0.778
Random Feedback	0.970(↑0.006)	0.794(↑0.052)	0.672(↑0.164)	0.764(↓0.014)
Least SHAP	0.970(↑0.006)	0.770(↑0.028)	0.612(↑0.104)	0.780(↑0.002)
Least AttnLRP	0.980(↑0.016)	0.776(↑0.034)	0.562(↑0.054)	0.764(↓0.014)
Least Grad×Input	0.968(↑0.004)	0.758(↑0.016)	0.593(↑0.085)	0.760(↓0.018)
Least LIME	0.968(↑0.004)	0.725(↓0.017)	0.556(↑0.048)	0.754(↓0.024)
Conf	0.964(=)	0.784(↑0.042)	0.660(↑0.152)	0.826(↑0.048)
SHAP	0.968(↑0.004)	0.802(↑0.060)	0.587(↑0.079)	0.760(↓0.018)
AttnLRP	0.978(↑0.014)	0.768(↑0.026)	0.596(↑0.088)	0.810(↑0.032)
Grad×Input	0.976(↑0.012)	0.773(↑0.031)	0.624(↑0.116)	0.782(↑0.004)
LIME	0.968(↑0.004)	0.730(↓0.012)	0.558(↑0.050)	0.736(↓0.042)
NL	0.984(↑0.020)	0.735(↓0.007)	0.638(↑0.130)	0.770(↓0.008)

Table 3: Automatic evaluation results in terms of LFR of OLMo2-7B. The tables present an ablation study of different feedback settings, including *Without Feedback*, *Random Feedback*, *Least-Attributed Feedback*, and the full variants of *iFlip*. Colored values indicate relative changes compared to the *Without Feedback* baseline (↑ = increase, ↓ = decrease).

finement. Table 3 illustrates that incorporating feedback generally improves LFR compared to the *without feedback* baseline (Appendix E.2). However, the contribution of feedback signals is not uniform; certain signals may exhibit differential utility, potentially introducing misguidance into the editing process (§6.1). We further assess the effectiveness of *iFlip* with *random feedback*, which offers only modest improvements relative to *without feedback* in terms of LFR. Among attribution-based signals, directing edits towards the most important words consistently outperforms targeting the least important words, yielding a mean LFR gain of 1.09% alongside an 11.02% reduction in edits, indicating more effective yet less disruptive edits.

6.3.3 Early Stopping

Tables 17 and 18 show that the removal of early stopping induces a decline in LFR, which is attributed to valid counterfactuals being overturned in successive iterations, as illustrated by the proportion of (*Success* → *Fail*) cases (Figure 13).¹⁶ This demonstrates the crucial role of early stopping in maintaining reliable counterfactual generation. Conversely, although additional iterations enable LLMs to enhance text fluency, they typically involve more extensive modifications. Our extended analysis in Appendix C.2 further reveals that early stopping is the primary driver of cross-architecture transferability, as it prevents the generator from overfitting to the specific decision boundary of the explained model.

¹⁶Detailed examples appear in Appendix J.3 and J.4.

Method	IMDb	CFs	AG News	SNLI (P)	CFs	SNLI (H)	CFs
Baseline	77.93	50.09	66.87	40.87	33.43	40.87	33.85
Human	92.73	91.26	–	42.27	50.90	58.40	56.95
Conf	87.93	71.09	78.60	38.47	32.98	44.13	36.88
SHAP	91.33	90.30	80.27	37.40	27.82	40.33	35.83
AttnLRP	89.27	90.28	77.87	38.13	27.97	40.13	35.53
Grad×Input	93.07	90.07	79.07	39.00	26.98	39.40	35.98
LIME	91.40	90.91	78.80	38.33	28.93	38.93	35.74
NL	90.73	71.97	81.80	40.40	30.91	37.47	33.79

Table 4: Accuracy (%) on test sets and human-annotated counterfactuals (CFs). Counterfactuals used for CDA are generated by OLMo2-7B. Best results are **bolded**.

6.4 Counterfactual Data Augmentation

Although human-annotated counterfactuals provide marginally stronger performance gains than *iFlip*-generated counterfactuals (Table 4), their prohibitive cost and time requirements motivate automated approaches. Noticeably, models trained with *iFlip*-based counterfactuals achieve substantial performance and robustness improvements over the baseline, except on SNLI (Premise). This exception may be attributed to imperfect counterfactuals, as indicated by the relatively lower LFR compared to other datasets (Table 1), which introduce ambiguous and noisy labels that adversely affect model robustness (Zhu et al., 2022; Wang et al., 2025c).¹⁷ We further observe a moderate correlation between CDA performance and counterfactual quality (Appendix H.1).

7 Conclusion

In this work, we propose *iFlip*, a feedback-driven framework that iteratively refines counterfactuals by incorporating multiple feedback signals to enhance their validity. Empirical results demonstrate that *iFlip* consistently surpasses state-of-the-art baselines, with natural language feedback yielding the strongest and most consistent improvements. In addition, a user study shows that *iFlip*-NL exceeds baseline ratings across all subjective dimensions and that its iterative refinement mechanism substantially improves the completeness and realism of generated counterfactuals. Moreover, our ablation studies reveal three key components of *iFlip*: iterative refinement, feedback signals, and early stopping, with early stopping emerging as the simplest and most cost-effective. Finally, we extend the study to counterfactual data augmentation and show that counterfactuals generated by *iFlip* effectively enhance model performance and robustness.

¹⁷Additional OOD augmentation results are provided in Appendix F. For the News Classification task, human-annotated counterfactuals are not available.

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Limitations

In this work, we propose a feedback-driven framework *iFlip* for iterative counterfactual refinement. While *iFlip* noticeably improves the validity of generated counterfactuals compared to five selected baselines, we acknowledge several limitations.

Usage of limited Feature Attribution Methods. We do not exhaustively explore all feature attribution-based feedback signals; investigating additional feature attribution methods remains future work.

Computational Costs. Despite the effectiveness of *iFlip* in producing high-quality counterfactuals, it incurs relatively high computational costs, particularly when using natural language feedback, as the iterative refinement process requires multiple rounds of generation and validation compared to single-pass methods.

English-Centric Evaluation. In addition, all experiments in this work were carried out exclusively on English datasets, and it remains unclear how well the approach would generalize to other languages. We plan to extend our evaluation to a multilingual setting in future work to assess the generalizability of our findings across languages.

Limited Scale of the User Study. Following prior work (Nguyen et al., 2024a; McAleese and Keane, 2024), we predominantly assess the quality of generated counterfactuals by three widely used automatic metrics regarding *validity*, *fluency*, and *minimality*, given that user studies for counterfactuals are uncommon in the literature. Nevertheless, to further assess textual quality beyond automatic metrics, we conduct a small-scale user study with ($N = 3$) participants evaluating *completeness*, *understandability*, and *cohesiveness*, following Domnich et al. (2025). As future work, we consider to include a comprehensive and large-scale user study to assess textual quality, e.g., coherence, feasibility, or complexity (Domnich et al., 2025; Wang et al., 2025d), and the effectiveness of counterfactuals for model predictions.

Ethics Statement

The participants in our user studies were compensated at or above the minimum wage in accordance with the standards of our host institutions' regions. The annotation took each annotator 30 minutes on average.

References

Reduan Achtibat, Sayed Mohammad Vakilzadeh Hatefi, Maximilian Dreyer, Aakriti Jain, Thomas Wiegand, Sebastian Lapuschkin, and Wojciech Samek. 2024. [AttnLRP: Attention-aware layer-wise relevance propagation for transformers](#). In *Forty-first International Conference on Machine Learning*. 617-622

Giuseppe Attanasio, Eliana Pastor, Chiara Di Bonaventura, and Debora Nozza. 2023. [ferret: a framework for benchmarking explainers on transformers](#). In *Proceedings of the 17th Conference of the European Chapter of the Association for Computational Linguistics: System Demonstrations*, page 256–266. Association for Computational Linguistics. 623-629

Milan Bhan, Jean-Noël Vittaut, Nicolas Chesneau, and Marie-Jeanne Lesot. 2023. [Tigtec: Token importance guided text counterfactuals](#). In *Machine Learning and Knowledge Discovery in Databases: Research Track*, pages 496–512, Cham. Springer Nature Switzerland. 630-635

Amrita Bhattacharjee, Raha Moraffah, Joshua Garland, and Huan Liu. 2024a. [Zero-shot LLM-guided Counterfactual Generation: A Case Study on NLP Model Evaluation](#). In *2024 IEEE International Conference on Big Data (BigData)*, pages 1243–1248, Los Alamitos, CA, USA. IEEE Computer Society. 636-641

Amrita Bhattacharjee, Raha Moraffah, Joshua Garland, and Huan Liu. 2024b. [Towards llm-guided causal explainability for black-box text classifiers](#). In *AAAI 2024 Workshop on Responsible Language Models, Vancouver, BC, Canada*. 642-646

Samuel R. Bowman, Gabor Angeli, Christopher Potts, and Christopher D. Manning. 2015. [A large annotated corpus for learning natural language inference](#). In *Proceedings of the 2015 Conference on Empirical Methods in Natural Language Processing*, pages 632–642, Lisbon, Portugal. Association for Computational Linguistics. 647-653

Bradley Brown, Jordan Juravsky, Ryan Ehrlich, Ronald Clark, Quoc V. Le, Christopher Ré, and Azalia Mirhoseini. 2024. [Large language monkeys: Scaling inference compute with repeated sampling](#). *Preprint*, arXiv:2407.21787. 654-658

DeepSeek-AI, Daya Guo, Dejian Yang, Haowei Zhang, Junxiao Song, Ruoyu Zhang, Runxin Xu, Qihao Zhu, Shirong Ma, Peiyi Wang, Xiao Bi, Xiaokang Zhang, Xingkai Yu, Yu Wu, Z. F. Wu, Zhibin Gou, Zhihong Shao, Zhuoshu Li, Ziyi Gao, and 181 others. 2025. [Deepseek-r1: Incentivizing reasoning capability in llms via reinforcement learning](#). *Preprint*, arXiv:2501.12948. 659-666

Jay DeYoung, Sarthak Jain, Nazneen Fatema Rajani, Eric Lehman, Caiming Xiong, Richard Socher, and Byron C. Wallace. 2020. [ERASER: A benchmark to evaluate rationalized NLP models](#). In *Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics*, pages 4443–4458, Online. Association for Computational Linguistics. 667-673

786	Yash Narendra and Niladri Chatterjee. 2025. Causal what-ifs: Rethinking counterfactuals with llm agents . In <i>Neural Information Processing</i> , pages 184–198, Singapore. Springer Nature Singapore.	
787		
788		
789		
790	Van Bach Nguyen, Christin Seifert, and Jörg Schlötterer. 2024a. CEval: A benchmark for evaluating counterfactual text generation . In <i>Proceedings of the 17th International Natural Language Generation Conference</i> , pages 55–69, Tokyo, Japan. Association for Computational Linguistics.	
791		
792		
793		
794		
795		
796	Van Bach Nguyen, Christin Seifert, and Jörg Schlötterer. 2025. Guiding llms to generate high-fidelity and high-quality counterfactual explanations for text classification . In <i>Explainable Artificial Intelligence</i> , pages 158–176, Cham. Springer Nature Switzerland.	
797		
798		
799		
800		
801	Van Bach Nguyen, Paul Youssef, Christin Seifert, and Jörg Schlötterer. 2024b. LLMs for generating and evaluating counterfactuals: A comprehensive study . In <i>Findings of the Association for Computational Linguistics: EMNLP 2024</i> , pages 14809–14824, Miami, Florida, USA. Association for Computational Linguistics.	
802		
803		
804		
805		
806		
807		
808	Team OLMo, Pete Walsh, Luca Soldaini, Dirk Groeneveld, Kyle Lo, Shane Arora, Akshita Bhagia, Yuling Gu, Shengyi Huang, Matt Jordan, Nathan Lambert, Dustin Schwenk, Oyvind Taffjord, Taira Anderson, David Atkinson, Faeze Brahman, Christopher Clark, Pradeep Dasigi, Nouha Dziri, and 21 others. 2025. 2 olmo 2 furious . <i>Preprint</i> , arXiv:2501.00656.	
809		
810		
811		
812		
813		
814		
815	OpenAI, :, Sandhini Agarwal, Lama Ahmad, Jason Ai, Sam Altman, Andy Applebaum, Edwin Arbus, Rahul K. Arora, Yu Bai, Bowen Baker, Haiming Bao, Boaz Barak, Ally Bennett, Tyler Bertao, Nivedita Brett, Eugene Brevdo, Greg Brockman, Sebastian Bubeck, and 108 others. 2025. gpt-oss-120b & gpt-oss-20b model card . <i>Preprint</i> , arXiv:2508.10925.	
816		
817		
818		
819		
820		
821		
822	Xiaoqi Qiu, Yongjie Wang, Xu Guo, Zhiwei Zeng, Yu Yue, Yuhong Feng, and Chunyan Miao. 2024. PairCFR: Enhancing model training on paired counterfactually augmented data through contrastive learning . In <i>Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)</i> , pages 11955–11971, Bangkok, Thailand. Association for Computational Linguistics.	
823		
824		
825		
826		
827		
828		
829		
830	Hossein A. Rahmani, Satyapriya Krishna, Xi Wang, Mohammadmehdi Naghiaei, and Emine Yilmaz. 2025. Self-correcting large language models: Generation vs. multiple choice . <i>Preprint</i> , arXiv:2511.09381.	
831		
832		
833		
834	Marco Tulio Ribeiro, Sameer Singh, and Carlos Guestrin. 2016. "why should i trust you?": Explaining the predictions of any classifier . In <i>Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, KDD '16</i> , page 1135–1144, New York, NY, USA. Association for Computing Machinery.	
835		
836		
837		
838		
839		
840		
	Alexis Ross, Ana Marasović, and Matthew Peters. 2021. Explaining NLP models via minimal contrastive editing (MiCE) . In <i>Findings of the Association for Computational Linguistics: ACL-IJCNLP 2021</i> , pages 3840–3852, Online. Association for Computational Linguistics.	841
		842
		843
		844
		845
		846
	Avanti Shrikumar, Peyton Greenside, Anna Shcherbina, and Anshul Kundaje. 2017. Not just a black box: Learning important features through propagating activation differences . <i>Preprint</i> , arXiv:1605.01713.	847
		848
		849
		850
	Gemma Team, Aishwarya Kamath, Johan Ferret, Shreya Pathak, Nino Vieillard, Ramona Merhej, Sarah Perrin, Tatiana Matejovicova, Alexandre Ramé, Morgane Rivière, Louis Rouillard, Thomas Mesnard, Geoffrey Cideron, Jean bastien Grill, Sabela Ramos, Edouard Yvinec, Michelle Casbon, Etienne Pot, Ivo Penchev, and 197 others. 2025. Gemma 3 technical report . <i>Preprint</i> , arXiv:2503.19786.	851
		852
		853
		854
		855
		856
		857
		858
	Marcos Treviso, Alexis Ross, Nuno M. Guerreiro, and André Martins. 2023. CREST: A joint framework for rationalization and counterfactual text generation . In <i>Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)</i> , pages 15109–15126, Toronto, Canada. Association for Computational Linguistics.	859
		860
		861
		862
		863
		864
		865
	Qianli Wang, Tatiana Anikina, Nils Feldhus, Simon Ostermann, Sebastian Möller, and Vera Schmitt. 2025a. Cross-refine: Improving natural language explanation generation by learning in tandem . In <i>Proceedings of the 31st International Conference on Computational Linguistics</i> , pages 1150–1167, Abu Dhabi, UAE. Association for Computational Linguistics.	866
		867
		868
		869
		870
		871
		872
	Qianli Wang, Nils Feldhus, Simon Ostermann, Luis Felipe Villa-Arenas, Sebastian Möller, and Vera Schmitt. 2025b. FitCF: A framework for automatic feature importance-guided counterfactual example generation . In <i>Findings of the Association for Computational Linguistics: ACL 2025</i> , pages 1176–1191, Vienna, Austria. Association for Computational Linguistics.	873
		874
		875
		876
		877
		878
		879
		880
	Qianli Wang, Van Bach Nguyen, Nils Feldhus, Luis Felipe Villa-Arenas, Christin Seifert, Sebastian Möller, and Vera Schmitt. 2025c. Truth or twist? optimal model selection for reliable label flipping evaluation in llm-based counterfactuals . In <i>Proceedings of the 18th International Natural Language Generation Conference</i> , pages 80–97, Hanoi, Vietnam. Association for Computational Linguistics.	881
		882
		883
		884
		885
		886
		887
		888
	Qianli Wang, Mingyang Wang, Nils Feldhus, Simon Ostermann, Yuan Cao, Hinrich Schütze, Sebastian Möller, and Vera Schmitt. 2025d. Through a compressed lens: Investigating the impact of quantization on llm explainability and interpretability . <i>Preprint</i> , arXiv:2505.13963.	889
		890
		891
		892
		893
		894
	Yingming Wang and Pepa Atanasova. 2025. Self-critique and refinement for faithful natural language explanations . In <i>Proceedings of the 2025 Conference</i>	895
		896
		897

898 *on Empirical Methods in Natural Language Process-*
899 *ing*, pages 8492–8518, Suzhou, China. Association
900 for Computational Linguistics.

901 Yongjie Wang, Xiaoqi Qiu, Yu Yue, Xu Guo, Zhiwei
902 Zeng, Yuhong Feng, and Zhiqi Shen. 2024. *A sur-*
903 *vey on natural language counterfactual generation*.
904 In *Findings of the Association for Computational*
905 *Linguistics: EMNLP 2024*, pages 4798–4818, Mi-
906 *ami, Florida, USA. Association for Computational*
907 *Linguistics*.

908 Sean Welleck, Ximing Lu, Peter West, Faeze Brah-
909 man, Tianxiao Shen, Daniel Khashabi, and Yejin
910 Choi. 2023. *Generating sequences by learning to*
911 *self-correct*. In *The Eleventh International Confer-*
912 *ence on Learning Representations*.

913 Tongshuang Wu, Marco Tulio Ribeiro, Jeffrey Heer, and
914 Daniel Weld. 2021. *Polyjuice: Generating counter-*
915 *factuals for explaining, evaluating, and improving*
916 *models*. In *Proceedings of the 59th Annual Meet-*
917 *ing of the Association for Computational Linguistics*
918 *and the 11th International Joint Conference on Natu-*
919 *ral Language Processing (Volume 1: Long Papers)*,
920 pages 6707–6723, Online. Association for Computa-
921 tional Linguistics.

922 Zhiheng Xi, Senjie Jin, Yuhao Zhou, Rui Zheng,
923 Songyang Gao, Jia Liu, Tao Gui, Qi Zhang, and
924 Xuanjing Huang. 2023. *Self-Polish: Enhance reason-*
925 *ing in large language models via problem refinement*.
926 In *Findings of the Association for Computational*
927 *Linguistics: EMNLP 2023*, pages 11383–11406, Sin-
928 *gapore. Association for Computational Linguistics*.

929 Tianyang Xu, Shujin Wu, Shizhe Diao, Xiaoze Liu,
930 Xingyao Wang, Yangyi Chen, and Jing Gao. 2024.
931 *SaySelf: Teaching LLMs to express confidence with*
932 *self-reflective rationales*. In *Proceedings of the 2024*
933 *Conference on Empirical Methods in Natural Lan-*
934 *guage Processing*, pages 5985–5998, Miami, Florida,
935 *USA. Association for Computational Linguistics*.

936 An Yang, Anfeng Li, Baosong Yang, Beichen Zhang,
937 Binyuan Hui, Bo Zheng, Bowen Yu, Chang Gao,
938 Chengen Huang, Chenxu Lv, Chujie Zheng, Day-
939 iheng Liu, Fan Zhou, Fei Huang, Feng Hu, Hao
940 Ge, Haoran Wei, Huan Lin, Jialong Tang, and 41
941 others. 2025a. *Qwen3 technical report. Preprint,*
942 *arXiv:2505.09388*.

943 Zhe Yang, Yichang Zhang, Yudong Wang, Ziyao Xu,
944 Junyang Lin, and Zhifang Sui. 2025b. *Confidence v.s.*
945 *critique: A decomposition of self-correction capabil-*
946 *ity for LLMs*. In *Proceedings of the 63rd Annual*
947 *Meeting of the Association for Computational Lin-*
948 *guistics (Volume 1: Long Papers)*, pages 3998–4014,
949 *Vienna, Austria. Association for Computational Lin-*
950 *guistics*.

951 Xiang Zhang, Junbo Zhao, and Yann LeCun. 2015.
952 *Character-level convolutional networks for text clas-*
953 *sification*. In *Advances in Neural Information Pro-*
954 *cessing Systems*, volume 28. Curran Associates, Inc.

Haiyan Zhao, Hanjie Chen, Fan Yang, Ninghao Liu,
Huiqi Deng, Hengyi Cai, Shuaiqiang Wang, Dawei
Yin, and Mengnan Du. 2024. *Explainability for large*
language models: A survey. ACM Trans. Intell. Syst.
Technol., 15(2). 955
956
957
958
959

Dawei Zhu, Michael A. Hedderich, Fangzhou Zhai,
David Ifeoluwa Adelani, and Dietrich Klakow. 2022.
Is BERT robust to label noise? a study on learning
with noisy labels in text classification. In *Proceed-*
ings of the Third Workshop on Insights from Negative
Results in NLP, pages 62–67, Dublin, Ireland. Asso-
ciation for Computational Linguistics. 960
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962
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A Dataset 967

A.1 Dataset Example 968

Figure 4 presents a representative example and its
corresponding gold label for each dataset. 969
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Figure 4: Examples from IMDb, AG News, and SNLI datasets.

A.2 Label Distributions 971

Figure 5 summarizes the label distributions across
three datasets. 972
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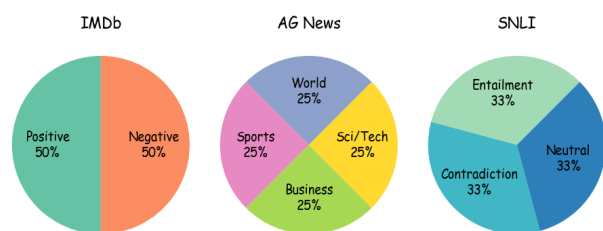


Figure 5: Label distributions across datasets.

974	A.3 Dataset Sources		1015
975	Table 5 illustrates the sources of the datasets used		
976	in our experiments.		1016
977	B Experimental Settings		
978	B.1 Experimental Parameters		
979	Table 6 summarizes the key parameters used in our		
980	experiments. These values were kept consistent		
981	across datasets unless stated otherwise.		
982	B.2 Inference Time		
983	Table 7 reports the inference time required for the		
984	OLMo2-7B generator model across all tasks.		
985	B.3 Generator Models		
986	We employ three LLMs as generator models to pro-		
987	duce counterfactuals, representing diverse scales,		
988	parameter sizes, and model families. Table 8 sum-		
989	marizes their details.		
990	B.4 Explained Models		
991	Table 9 summarizes the BERT and RoBERTa models		
992	fine-tuned on the selected datasets. These models		
993	serve as the classifier that determines whether the		
994	counterfactuals truly change the previous model		
995	prediction.		
996	C Extended Evaluation Results		
997	C.1 Evaluation Results on RoBERTa-base		
998	Table 10 presents the automatic evaluation re-		
999	sults for counterfactuals generated by <i>iFlip</i> on		
1000	the RoBERTa-base model, using LLaMA3.3-70B as		
1001	the generator. While agentic baselines like Causal		
1002	What-Ifs remain competitive on NLI tasks, <i>iFlip</i>		
1003	demonstrates superior consistency, particularly on		
1004	sentiment analysis and news topic classification		
1005	where it frequently outperforms baselines.		
1006	C.2 Transferability		
1007	C.2.1 Transferability of the counterfactuals		
1008	across architectures		
1009	Table 11 reports the <i>transferability</i> of the gener-		
1010	ated counterfactuals across classifier architectures.		
1011	Specifically, all counterfactuals are generated for		
1012	BERT classifiers, while the automatic evaluation is		
1013	conducted by replacing the original BERT classifier		
1014	with a RoBERTa classifier.		
	C.2.2 Transferability of the feedback		
	extracted from BERT		
	Table 12 evaluates the <i>transferability</i> of feedback		1017
	signals extracted from BERT. We use these signals		1018
	to guide <i>iFlip</i> in generating counterfactuals, and		1019
	then evaluate the resulting counterfactuals with		1020
	RoBERTa.		1021
	C.2.3 Discussion		1022
	Early stopping is the key factor for transfer-		1023
	ability. Regarding transferability, early stopping		1024
	emerges as the primary driver of robustness across		1025
	architectures. In Table 11, when counterfactu-		1026
	als generated for BERT are evaluated on RoBERTa,		1027
	methods employing early stopping (e.g., <i>iFlip</i> and		1028
	Causal What-Ifs) exhibit substantial validity re-		1029
	ductions compared to counterfactuals generated		1030
	directly for RoBERTa (Table 10). This pattern indi-		1031
	cates that early stopping enhances transferability		1032
	by providing the LLM with direct validity feedback		1033
	on whether candidate counterfactuals successfully		1034
	flip classifier predictions.		1035
	The source of the feedback has limited impact		1036
	on transferability. Table 12 suggests that the		1037
	<i>source</i> of the feedback (extracted from BERT or		1038
	RoBERTa) is comparatively less influential on trans-		1039
	ferability: using feedback from different models		1040
	yields only small performance differences, and the		1041
	resulting counterfactuals achieve similar quality		1042
	to those guided by RoBERTa feedback (Table 10).		1043
	Nevertheless, feedback is still beneficial for coun-		1044
	terfactual generation, where our ablation results		1045
	showing that removing feedback leads to worse		1046
	performance than using feedback (see §6.3.2).		1047
	C.2.4 Summary of experimental settings		1048
	Table 13 summarizes the experimental settings		1049
	used in Tables 10, 11, and 12, including (i) the <i>feed-</i>		1050
	<i>back source</i> model, (ii) the model used for <i>early</i>		1051
	<i>stopping</i> (validity check during generation), and		1052
	(iii) the <i>evaluation</i> classifier.		1053
	D Feedback Signal Comparison		1054
	We compare different feedback signals in terms of		1055
	their label flipping rate (LFR) across models and		1056
	tasks. Figure 6 shows the results across models,		1057
	and Figure 7 shows the results across tasks.		1058

Dataset	Citation	Source
IMDb	Maas et al. (2011)	https://huggingface.co/datasets/stanfordnlp/imdb
AG News	Zhang et al. (2015)	https://huggingface.co/datasets/sentence-transformers/agnews
SNLI	Bowman et al. (2015)	https://huggingface.co/datasets/stanfordnlp/snli

Table 5: Datasets employed in our experiments with their citations and sources.

Parameter	Value
<i>Generator Parameters</i>	
Temperature	0.9
Top-p	0.95
Top-k	50
Max new tokens	4096
Number of iterations	5
Top-k important words	$\max(10, \lfloor 0.10 \times \text{orig_words} \rfloor)$
<i>Explained Model Settings</i>	
Voting Strategy	Majority voting
Window Size	512
Stride	256
<i>Hardware</i>	
OLMo2-7B	1× V100 (32 GB)
Qwen3-32B	1× H100 (80 GB)
LLaMA3.3-70B	2× H100 (80 GB)

Table 6: Experimental settings.

Task	Method	Duration (hours)
IMDb	Conf	3.40
	AttnLRP	3.22
	SHAP	3.75
	Grad×Input	3.45
	LIME	3.72
	NL	4.55
	AG News	Conf
AttnLRP		7.22
SHAP		9.73
Grad×Input		7.37
LIME		9.86
NL		17.90
SNLI-Premise		Conf
	AttnLRP	1.64
	SHAP	2.10
	Grad×Input	1.55
	LIME	4.80
	NL	7.57
	SNLI-Hypothesis	Conf
AttnLRP		1.13
SHAP		1.37
Grad×Input		1.14
LIME		3.45
NL		5.26

Table 7: Inference time (in hours) for OLMo2-7B across SNLI, IMDb, and AG News.

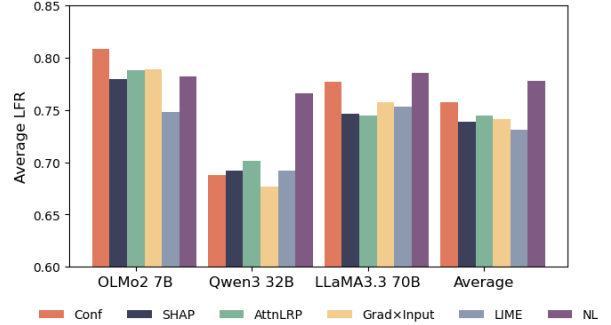


Figure 6: Averaged label flipping rate (LFR) across feedback signals and models on the IMDb, AG News, and SNLI datasets.

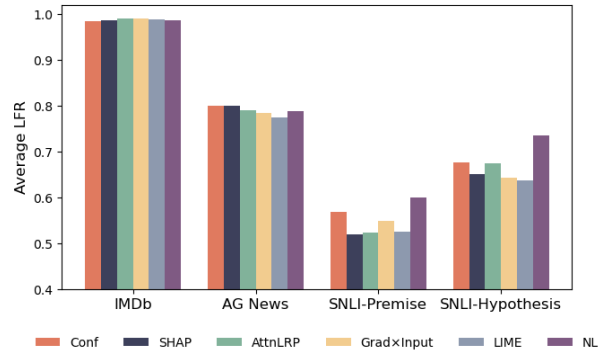


Figure 7: Average label flipping rate (LFR) across feedback signals and tasks on the IMDb, AG News, and SNLI datasets.

E Extended Ablation Results 1059

E.1 Iterative Refinement 1060

E.1.1 Average Early Stop Rounds 1061

Table 14 reports the average number of refinement rounds before early stopping across datasets and models. 1062 1063 1064

E.1.2 Counterfactual Length across Iteration Rounds 1065 1066

Figure 8 illustrates how the average length of generated counterfactuals evolves over refinement iterations. 1067 1068 1069

Name	Citation	Size	Source
OLMo2-7B	OLMo et al. (2025)	7B	https://huggingface.co/allenai/OLMo-2-1124-7B-Instruct
Qwen3-30B	Yang et al. (2025a)	32B	https://huggingface.co/Qwen/Qwen3-32B
Llama3.3-70B	Grattafiori et al. (2024)	70B	https://huggingface.co/meta-llama/Llama-3.3-70B-Instruct

Table 8: Generator models employed in our experiments.

Task	Model	Source
IMDb	textattack/bert-base-uncased-imdb	https://huggingface.co/textattack/bert-base-uncased-imdb
	textattack/roberta-base-imdb	https://huggingface.co/textattack/roberta-base-imdb
AG News	textattack/bert-base-uncased-ag-news	https://huggingface.co/textattack/bert-base-uncased-ag-news
	textattack/roberta-base-ag-news	https://huggingface.co/textattack/roberta-base-ag-news
SNLI	textattack/bert-base-uncased-snli	https://huggingface.co/textattack/bert-base-uncased-snli
	utahnlp/snli_roberta-base_seed-2	https://huggingface.co/utahnlp/snli_roberta-base_seed-2

Table 9: Explained models (BERT and RoBERTa) used for different datasets.

Method	IMDb			AG News			SNLI (Premise)			SNLI (Hypothesis)			
	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓	
RoBERTa-base													
Polyjuice	0.274	0.736	60.81	0.165	0.744	93.22	0.212	0.772	96.95	0.260	0.733	114.59	
BAE	0.637	0.977	62.26	0.443	0.813	246.61	0.518	0.894	103.32	0.665	0.914	92.10	
LLaMA 3.3-70B	CGG	0.930	0.892	54.57	0.748	0.542	130.31	0.635	0.893	59.23	0.680	<u>0.944</u>	54.23
	FIZLE	0.956	0.868	34.88	0.345	<u>0.707</u>	56.59	<u>0.759</u>	<u>0.908</u>	41.54	0.821	0.929	<u>42.39</u>
	Causal What-Ifs	0.908	0.788	<u>32.78</u>	0.656	0.442	<u>46.18</u>	0.750	0.864	<u>41.07</u>	0.740	0.892	43.63
	iFlip-Conf	1.000	0.895	37.48	0.880	0.575	55.55	0.665	0.688	62.94	0.830	0.799	47.43
	iFlip-SHAP	1.000	0.895	36.19	0.885	0.542	57.69	0.680	0.700	57.99	0.800	0.795	44.69
iFlip-NL	1.000	0.893	36.48	<u>0.915</u>	0.583	57.66	0.730	0.789	77.00	0.815	0.815	52.91	

Table 10: Automatic evaluation results of counterfactuals on the RoBERTa-base model using iFlip methods with different feedback types: ① confidence (Conf), ② feature attribution (SHAP), and ③ natural language (NL). **Boldface** indicates the best feedback type within iFlip. Wavy underline indicates the best result across methods.

E.1.3 Trade-off between Validity and Similarity

Figure 9 plots the trade-off between semantic similarity (SS) and label flipping rate (LFR). Figure 10 further breaks down this trade-off by showing how the SS-LFR trajectory evolves across iFlip-NL iteration steps k on each task. After $\mathcal{K} = 4$, the degradation in semantic similarity accelerates, so for practical applications requiring high fidelity, $\mathcal{K} = 3$ or $\mathcal{K} = 4$ may offer a better balance.

E.1.4 Iterative Refinement Effectiveness

Figures 11 and 12 show that iterative refinement with OLMo2-7B yields steady pass@k gains across IMDb, AG News, and SNLI up to $k = 15$, while the largest marginal improvements in flip rate occur in the early rounds and taper off thereafter depending on the feedback signal.

E.2 Feedback Signals

Table 15 reports the evaluation results of our feedback signal ablations on IMDb and AG News, while Table 16 presents the corresponding results on SNLI.

E.3 Without Early Stopping

Table 17 reports the evaluation results of our without early stopping ablations on IMDb and AG News, while Table 18 presents the corresponding results on SNLI. Figure 13 presents the distribution of state transitions during iterative refinement when the early-stopping mechanism is disabled.

F Counterfactual Data Augmentation

Tables 19 and 20 report the results of data augmentation on in-domain (ID), out-of-domain (OOD), and human-annotated counterfactual (Human CFs)

Method	IMDb			AG News			SNLI (Premise)			SNLI (Hypothesis)			
	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓	
Polyjuice	0.274	0.736	60.81	0.165	0.744	93.22	0.212	0.772	96.95	0.260	0.733	114.59	
BAE	0.090	0.976	63.15	0.157	0.764	295.96	0.068	0.966	82.98	0.095	0.979	81.00	
OLMo2-7B	CGG	0.891	0.837	44.67	0.560	0.380	208.56	0.257	0.882	57.03	0.323	0.948	53.92
	FIZLE	0.585	0.584	38.71	0.236	0.584	77.38	0.586	0.730	173.94	0.634	0.882	74.15
	Causal What-Ifs	0.850	0.801	37.97	0.273	0.607	37.54	0.443	0.854	47.27	0.627	0.911	35.56
	iFlip-Conf	0.895	0.809	41.19	0.552	0.504	41.41	0.440	0.854	53.52	0.620	0.870	40.65
	iFlip-SHAP	0.906	0.805	41.87	0.552	0.489	42.95	0.441	0.847	52.76	0.594	0.867	42.38
	iFlip-AttnLRP	0.923	0.803	42.61	0.536	0.501	46.61	0.458	0.851	51.89	0.624	0.869	40.31
	iFlip-Grad×Input	0.912	0.801	43.30	0.516	0.499	50.32	0.432	0.854	52.93	0.634	0.871	41.81
	iFlip-LIME	0.911	0.805	52.82	0.522	0.506	44.32	0.420	0.866	52.33	0.606	0.875	41.02
	iFlip-NL	0.931	0.822	36.47	0.532	0.516	44.73	0.444	0.879	148.41	0.636	0.901	43.81
	Qwen3-32B	CGG	0.890	0.877	62.47	0.364	0.697	97.10	0.273	0.881	50.31	0.343	0.938
FIZLE		0.686	0.900	36.00	0.140	0.864	61.46	0.689	0.901	38.66	0.810	0.918	35.97
Causal What-Ifs		0.798	0.821	42.03	0.436	0.570	53.50	0.580	0.842	36.14	0.680	0.920	34.18
iFlip-Conf		0.940	0.855	33.30	0.622	0.521	41.59	0.490	0.895	50.44	0.640	0.871	47.03
iFlip-SHAP		0.936	0.857	33.70	0.604	0.520	44.02	0.542	0.878	47.16	0.634	0.866	45.04
iFlip-AttnLRP		0.934	0.858	33.19	0.626	0.513	44.15	0.532	0.882	46.93	0.648	0.867	44.77
iFlip-Grad×Input		0.934	0.865	33.65	0.592	0.522	44.33	0.528	0.881	47.40	0.658	0.865	45.60
iFlip-LIME		0.938	0.863	32.57	0.624	0.527	44.52	0.498	0.891	50.60	0.654	0.870	44.22
iFlip-NL		0.922	0.878	32.99	0.618	0.537	49.68	0.546	0.895	68.16	0.668	0.906	47.20
LLaMA3.3-70B		CGG	0.851	0.869	52.81	0.516	0.694	122.40	0.357	0.846	51.62	0.412	0.937
	FIZLE	0.956	0.868	34.88	0.345	0.707	56.59	0.759	0.903	41.54	0.821	0.929	42.39
	Causal What-Ifs	0.852	0.788	31.93	0.628	0.461	43.56	0.528	0.816	38.97	0.560	0.904	41.29
	iFlip-Conf	0.944	0.877	34.74	0.804	0.468	44.38	0.654	0.763	45.99	0.678	0.843	43.88
	iFlip-SHAP	0.944	0.878	34.32	0.794	0.481	46.07	0.652	0.743	45.15	0.678	0.828	41.09
	iFlip-AttnLRP	0.946	0.879	34.58	0.816	0.477	45.78	0.642	0.743	44.66	0.684	0.822	39.92
	iFlip-Grad×Input	0.942	0.878	34.80	0.814	0.479	46.12	0.666	0.751	44.14	0.696	0.825	39.55
	iFlip-LIME	0.944	0.877	34.54	0.796	0.476	44.20	0.654	0.759	45.51	0.680	0.825	42.91
	iFlip-NL	0.942	0.895	36.90	0.782	0.527	63.86	0.624	0.821	69.45	0.726	0.861	49.74

Table 11: Automatic evaluation results of counterfactual generated for BERT models, and evaluated on RoBERTa classifiers. Baselines (Polyjuice, BAE, CGG, and FIZLE) are compared with our iFlip variants under different feedback types: ❶ confidence (Conf), ❷ feature attribution (SHAP, AttnLRP, Grad×Input, LIME), and ❸ natural language (NL). Results are reported on IMDb, AG News, and SNLI using Label Flipping Rate (LFR), Semantic Similarity (SS), and Perplexity (PPL). **Boldface** indicates the best feedback type within iFlip. Wavy underline indicates the best result across methods.

Method	IMDb			AG News			SNLI (Premise)			SNLI (Hypothesis)			
	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓	
LLaMA 3.3-70B	iFlip-Conf	0.995	0.897	37.17	0.896	0.539	58.65	0.672	0.702	62.81	0.816	0.792	46.84
	iFlip-SHAP	1.000	0.897	37.12	0.905	0.516	57.88	0.677	0.697	62.30	0.831	0.790	44.08
	iFlip-AttnLRP	1.000	0.895	36.66	0.876	0.524	59.95	0.677	0.706	56.80	0.841	0.796	45.66
	iFlip-Grad×Input	1.000	0.897	36.78	0.910	0.518	59.34	0.672	0.699	55.40	0.811	0.792	44.98
	iFlip-LIME	1.000	0.898	36.92	0.905	0.509	57.58	0.662	0.704	55.88	0.846	0.788	45.36

Table 12: Automatic evaluation results of counterfactual generated by iFlip using feedback extracted from BERT models, and evaluated on RoBERTa models. We report results on IMDb, AG News, and SNLI using Label Flipping Rate (LFR), Semantic Similarity (SS), and Perplexity (PPL). Feedback types include ❶ confidence (Conf), ❷ feature attribution (SHAP, AttnLRP, Grad×Input and LIME). **Boldface** indicates the best feedback type within iFlip.

test data across four tasks: Sentiment Analysis, News Classification, NLI Premise, and NLI Hypothesis. The CFEs for Table 19 are produced with iFlip using the OLMo2-7B model, while those for Table 20 are generated using the LLaMA3-70B model.

G Faithfulness Evaluation

Given that feature attribution-based feedback serve as a central component of our framework, it is essential to assess the faithfulness of different attri-

bution methods. Faithfulness measures how accurately explanations reflect the true reasoning of the model (Lyu et al., 2024). We evaluate attribution methods using FERRET (Attanasio et al., 2023) with three metrics: comprehensiveness, sufficiency (DeYoung et al., 2020), and Kendall’s τ correlation with Leave-One-Out (Jain and Wallace, 2019). These metrics jointly assess whether highlighted words faithfully capture the model’s decision process.

The results in Table 21 show clear differences in

Table	Feedback source	Early stop under	Evaluation model
Table 10	RoBERTa-base	RoBERTa-base	RoBERTa-base
Table 11	BERT	BERT	RoBERTa-base
Table 12	BERT	RoBERTa-base	RoBERTa-base

Table 13: Overview of experimental settings of *iFlip* across tables: feedback source, early-stopping model, and evaluation classifier.

Dataset	OLMo2-7B	Qwen3-32B	LLaMA3.3-70B
IMDb	0.13	0.05	0.01
AG News	1.48	1.53	0.80
SNLI (Premise)	2.20	3.20	2.75
SNLI (Hypothesis)	1.83	2.62	2.41

Table 14: Average early stop rounds per dataset and model.

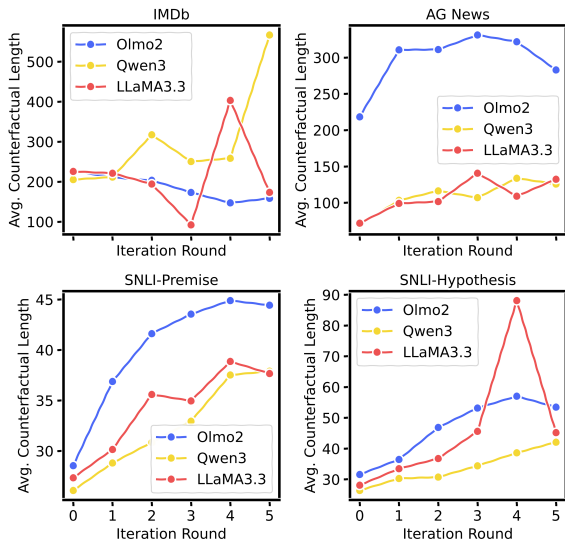


Figure 8: Average counterfactual length vs. iteration round across tasks and models.

1124 how attribution methods capture the model’s reasoning process. Among the evaluated approaches, AttnLRP provides the most faithful explanations, showing strong performance across comprehensiveness, sufficiency, and Kendall’s τ . Propagation-based methods exhibit solid alignment with the model’s decision-making process, which aligns with our earlier observations in Section 6.1. SHAP follows as the next most faithful method across datasets and models, with competitive scores on comprehensiveness and sufficiency, though less consistent on τ .

1136 We further observe that the results on the SNLI dataset show weaker faithfulness compared to sentiment and news classification. In particular, attribution methods on SNLI exhibit lower comprehensiveness, together with less favorable sufficiency values, indicating that the most important

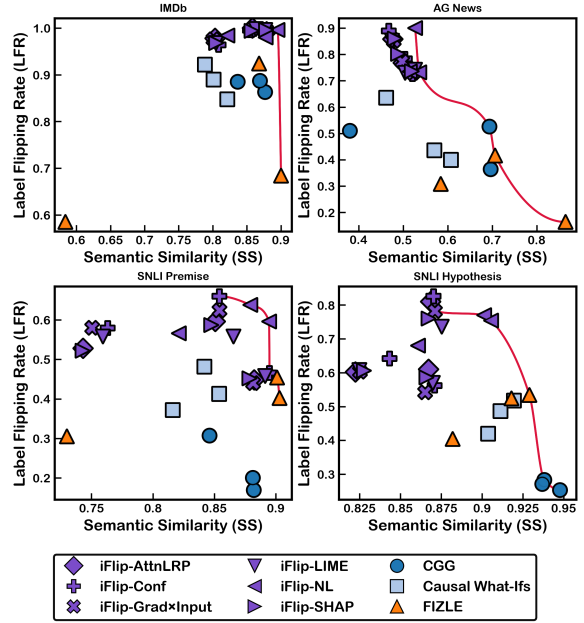


Figure 9: Trade-off between semantic similarity and label flipping rate. The upper-right region indicates the most favorable trade-off. The red curve denotes the Pareto frontier.

1142 words identified by attribution methods capture the
1143 model’s reasoning less effectively in NLI tasks.
1144 This suggests that attribution methods are more
1145 challenging when explanations must account for
1146 subtle entailment relations rather than more direct
1147 sentiment or news topic.

1148 H Correlation Analysis

1149 We further analyze the relationship between counterfactual quality and two key aspects: their performance in Counterfactual Data Augmentation (CDA) and their alignment with attribution-based faithfulness. To assess counterfactual quality, we employ the *label flipping rate* and derive feedback-specific rankings. CDA performance is measured by the ranking of average OOD accuracy on test sets obtained from models trained with different counterfactual sets. Faithfulness is captured through attribution-based metrics – *comprehensiveness* (DeYoung et al., 2020), *sufficiency* (DeYoung et al., 2020), and Kendall’s τ correlation with

Feedback of iFlip	IMDb			AG News		
	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓
Without Feedback	0.964	0.803	39.12	0.742	0.494	44.71
Random Feedback	0.970(↑0.006)	0.803(—)	44.58(↑5.46)	0.794(↑0.052)	0.498(↑0.004)	43.59(↓1.12)
Least SHAP	0.970(↑0.006)	0.802(↓0.001)	41.10(↑1.98)	0.770(↑0.028)	0.490(↓0.004)	41.78(↓2.93)
Least AttnLRP	0.980(↑0.016)	0.805(↑0.002)	41.34(↑2.22)	0.776(↑0.034)	0.495(↑0.001)	40.74(↓3.97)
Least Grad×Input	0.968(↑0.004)	0.803(—)	43.02(↑3.90)	0.758(↑0.016)	0.495(↑0.001)	49.09(↑4.38)
Least LIME	0.968(↑0.004)	0.800(↓0.003)	44.99(↑5.87)	0.725(↓0.017)	0.508(↑0.014)	43.53(↓1.18)
Conf	0.964(—)	0.809(↑0.006)	41.19(↑2.07)	0.784(↑0.042)	0.503(↑0.009)	41.41(↓3.30)
SHAP	0.968(↑0.004)	0.805(↑0.002)	41.87(↑2.75)	0.802(↑0.060)	0.488(↓0.006)	42.95(↓1.76)
AttnLRP	0.978(↑0.014)	0.803(—)	42.61(↑3.49)	0.768(↑0.026)	0.500(↑0.006)	46.61(↑1.90)
Grad×Input	0.976(↑0.012)	0.801(↓0.002)	43.30(↑4.18)	0.773(↑0.031)	0.498(↑0.004)	50.32(↑5.61)
LIME	0.968(↑0.004)	0.805(↑0.002)	52.82(↑13.70)	0.730(↓0.012)	0.504(↑0.010)	44.32(↓0.39)
NL	0.984(↑0.020)	0.822(↑0.019)	36.47(↓2.65)	0.735(↓0.007)	0.515(↑0.021)	44.73(↑0.02)

Table 15: Automatic evaluation results of OLMo2-7B on IMDb and AG News. The tables present an ablation study of different feedback settings, including *Without Feedback*, *Random Feedback*, *Least-Attributed Feedback*, and the full variants of iFlip. Colored values indicate relative changes compared to the *Without Feedback* baseline (↑ = increase, ↓ = decrease).

Feedback of iFlip	SNLI (Premise)			SNLI (Hypothesis)		
	LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓
Without Feedback	0.508	0.872	66.42	0.778	0.879	41.61
Random Feedback	0.672(↑0.164)	0.865(↓0.007)	53.64(↓12.78)	0.764(↓0.014)	0.870(↓0.009)	40.25(↓1.36)
Least SHAP	0.612(↑0.104)	0.854(↓0.018)	54.51(↓11.91)	0.780(↑0.002)	0.874(↓0.005)	41.30(↓0.31)
Least AttnLRP	0.562(↑0.054)	0.860(↓0.012)	55.31(↓11.11)	0.764(↓0.014)	0.869(↓0.010)	40.58(↓1.03)
Least Grad×Input	0.593(↑0.085)	0.868(↓0.004)	56.99(↓9.43)	0.760(↓0.018)	0.870(↓0.009)	41.25(↓0.36)
Least LIME	0.556(↑0.048)	0.868(↓0.004)	57.02(↓9.40)	0.754(↓0.024)	0.870(↓0.009)	41.27(↓0.34)
Conf	0.660(↑0.152)	0.854(↓0.018)	53.72(↓12.70)	0.826(↑0.048)	0.870(↓0.009)	40.65(↓0.96)
SHAP	0.587(↑0.079)	0.847(↓0.025)	56.81(↓9.61)	0.760(↓0.018)	0.867(↓0.012)	42.39(↑0.78)
AttnLRP	0.596(↑0.088)	0.851(↓0.021)	55.30(↓11.12)	0.810(↑0.032)	0.869(↓0.010)	40.31(↓1.30)
Grad×Input	0.624(↑0.116)	0.854(↓0.018)	56.02(↓10.40)	0.782(↑0.004)	0.871(↓0.008)	41.81(↑0.20)
LIME	0.558(↑0.050)	0.866(↓0.006)	58.18(↓8.24)	0.736(↓0.042)	0.875(↓0.004)	41.02(↓0.59)
NL	0.638(↑0.130)	0.879(↑0.007)	148.41(↑81.99)	0.770(↓0.008)	0.901(↑0.022)	43.81(↑2.20)

Table 16: Automatic evaluation results of OLMo2-7B on SNLI. The tables present an ablation study of different feedback settings, including *Without Feedback*, *Random Feedback*, *Least-Attributed Feedback*, and the full variants of iFlip. Colored values indicate relative changes compared to the *Without Feedback* baseline (↑ = increase, ↓ = decrease).

1162 Leave-One-Out token removal (Jain and Wallace,
1163 2019).

1174 factu-als, which in turn lead to enhanced model
1175 performance and robustness.

1164 H.1 Correlation between CDA performance 1165 and counterfactual quality

1166 Figure 14 shows the Pearson correlation between
1167 CDA performance and counterfactual quality
1168 across datasets. Among the datasets examined,
1169 AG News exhibits a strong correlation between
1170 the counterfactuals quality and CDA effectiveness,
1171 whereas IMDb and SNLI demonstrate only moder-
1172 ate correlation. Nonetheless, feedback-based
1173 refinement generally yields effective counter-

1174 H.2 Correlation between Faithfulness 1175 measures and counterfactual quality.

1176 Figure 15 reports the Spearman correlation be-
1177 tween faithfulness measures and counterfactual
1178 quality. The results reveal heterogeneous patterns
1179 across tasks: while datasets such as IMDb and
1180 AG News show positive correlations between flip-
1181 rate quality and faithfulness metrics, SNLI yields
1182 weaker or even negative correlations, especially
1183
1184
1185

Feedback of <i>iFlip</i>		IMDb			AG News		
		LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓
OLMo2-7B	Conf	0.677 (↓0.287)	0.774 (↓0.035)	41.32 (↑0.13)	0.507 (↓0.277)	0.539 (↑0.036)	40.15 (↓1.26)
	SHAP	0.859 (↓0.109)	0.762 (↓0.043)	41.34 (↓0.53)	0.600 (↓0.202)	0.485 (↓0.003)	40.03 (↓2.92)
	AttnLRP	0.922 (↓0.056)	0.782 (↓0.021)	40.75 (↓1.86)	0.610 (↓0.158)	0.502 (↑0.002)	38.75 (↓7.86)
	Grad×Input	0.916 (↓0.060)	0.778 (↓0.023)	40.11 (↓3.19)	0.559 (↓0.214)	0.499 (↑0.001)	38.61 (↓11.71)
	LIME	0.890 (↓0.078)	0.784 (↓0.021)	38.47 (↓14.35)	0.600 (↓0.130)	0.503 (↓0.001)	37.56 (↓6.76)
	NL	0.980 (↓0.004)	0.747 (↓0.075)	39.87 (↑3.40)	0.548 (↓0.187)	0.499 (↓0.016)	38.52 (↓6.21)

Table 17: Evaluation of OLMo2-7B *Without Early Stopping* on IMDb and AG News. Colored values indicate relative changes compared to *Early Stopping* (↑ = increase, ↓ = decrease).

Feedback of <i>iFlip</i>		SNLI (Premise)			SNLI (Hypothesis)		
		LFR↑	SS↑	PPL↓	LFR↑	SS↑	PPL↓
OLMo2-7B	Conf	0.340 (↓0.320)	0.860 (↑0.006)	52.47 (↓1.25)	0.560 (↓0.266)	0.873 (↑0.003)	39.46 (↓1.19)
	SHAP	0.340 (↓0.247)	0.848 (↑0.001)	57.20 (↑0.39)	0.543 (↓0.217)	0.871 (↑0.004)	41.47 (↓0.92)
	AttnLRP	0.343 (↓0.253)	0.858 (↑0.007)	58.07 (↑2.77)	0.563 (↓0.247)	0.871 (↑0.002)	40.60 (↑0.29)
	Grad×Input	0.347 (↓0.277)	0.854 (—)	55.76 (↓0.26)	0.520 (↓0.262)	0.871 (—)	40.76 (↓1.05)
	LIME	0.323 (↓0.235)	0.875 (↑0.009)	57.04 (↓1.14)	0.497 (↓0.239)	0.872 (↓0.003)	40.38 (↓0.64)
	NL	0.387 (↓0.251)	0.844 (↓0.035)	54.87 (↓93.54)	0.546 (↓0.224)	0.903 (↑0.002)	43.81 (—)

Table 18: Evaluation of OLMo2-7B *Without Early Stopping* on SNLI (Premise) and SNLI (Hypothesis). Colored values indicate relative changes compared to *Early Stopping* (↑ = increase, ↓ = decrease).

Methods	Sentiment Analysis				News Classification				NLI - Premise				NLI - Hypothesis			
	<i>Test Data</i>				<i>Test Data</i>				<i>Test Data</i>				<i>Test Data</i>			
	ID	OOD			ID	OOD			ID	OOD			ID	OOD		
	IMDb	Amazon	SST-2	CFs	AG News	BBC	20NG	CFs	SNLI	MNLI	ANLI	CFs	SNLI	MNLI	ANLI	CFs
Baseline	77.93	75.00	67.43	50.09	66.87	62.80	41.07	—	40.87	34.87	35.00	33.43	40.87	34.87	35.00	33.85
Human	92.73	89.53	85.55	91.26	—	—	—	—	42.27	37.47	33.93	50.90	58.40	52.07	30.13	56.95
Conf	87.93	88.33	83.83	71.09	78.60	45.30	55.80	—	38.47	36.33	32.80	32.98	44.13	33.13	32.87	36.88
SHAP	91.33	89.33	83.94	90.30	80.27	48.60	56.33	—	37.40	34.93	32.93	27.82	40.33	36.87	33.13	35.83
AttnLRP	89.27	88.00	84.75	90.28	77.87	42.50	53.60	—	38.13	35.67	32.87	27.97	40.13	36.33	33.13	35.53
Grad×Input	93.07	88.00	82.45	90.07	79.07	43.70	55.80	—	39.00	31.93	32.93	26.98	39.40	34.13	33.20	35.98
LIME	91.40	88.73	83.37	90.91	78.80	42.50	54.53	—	38.33	32.60	32.93	28.93	38.93	35.80	32.93	35.74
NL	90.73	88.27	84.40	71.97	81.80	46.10	58.47	—	40.40	33.60	32.73	30.91	37.47	33.27	33.20	33.79

Table 19: Accuracy (%) on in-domain (ID), out-of-domain (OOD), and human-annotated counterfactual (Human CFs) test data across four tasks: Sentiment Analysis, News Classification, NLI Premise, and NLI Hypothesis. Best results are bolded. The CFEs used for data augmentation, produced with *iFlip*, are generated by an OLMo2-7B model.

Methods	Sentiment Analysis				News Classification				NLI - Premise				NLI - Hypothesis			
	<i>Test Data</i>				<i>Test Data</i>				<i>Test Data</i>				<i>Test Data</i>			
	ID	OOD			ID	OOD			ID	OOD			ID	OOD		
	IMDb	Amazon	SST-2	CFs	AG News	BBC	20NG	CFs	SNLI	MNLI	ANLI	CFs	SNLI	MNLI	ANLI	CFs
Baseline	77.93	75.00	67.43	50.09	66.87	62.80	41.07	—	40.87	34.87	35.00	33.43	40.87	34.87	35.00	33.85
Human	92.73	89.53	85.55	91.26	—	—	—	—	42.27	37.47	33.93	50.90	58.40	52.07	30.13	56.95
Conf	91.67	88.60	84.29	90.92	83.07	66.80	58.33	—	34.53	33.00	32.80	33.49	48.40	37.40	32.00	41.09
SHAP	91.53	88.27	82.80	90.71	79.73	59.30	62.40	—	36.20	32.47	32.73	33.16	40.60	34.20	31.40	38.03
AttnLRP	88.80	88.80	84.40	91.21	80.33	58.50	61.33	—	33.27	31.87	32.80	32.32	39.80	33.40	32.73	36.58
Grad×Input	92.27	88.87	83.72	90.89	81.60	59.00	62.73	—	34.47	32.27	32.73	31.84	45.47	36.00	32.07	38.71
LIME	91.00	88.80	84.06	90.83	79.80	57.30	62.47	—	36.13	32.87	32.60	33.28	41.47	35.47	33.40	35.86
NL	91.67	88.73	83.83	90.89	81.73	69.50	66.27	—	37.13	31.00	32.87	33.94	39.73	36.33	32.27	36.94

Table 20: Accuracy (%) on in-domain (ID), out-of-domain (OOD), and human-annotated counterfactual (Human CFs) test data across four tasks: Sentiment Analysis, News Classification, NLI Premise, and NLI Hypothesis. Best results are bolded. The CFEs used for data augmentation, produced with *iFlip*, are generated by an LLaMA3.3-70B model.

for SNLI Hypothesis. These findings suggest that higher-quality counterfactuals tend to align better

Model	Feedback	IMDb			AG News			SNLI-Premise			SNLI-Hypothesis		
		comp.	suff.	$\tau(\text{loo})$	comp.	suff.	$\tau(\text{loo})$	comp.	suff.	$\tau(\text{loo})$	comp.	suff.	$\tau(\text{loo})$
OLMo2-7B	SHAP	0.28	-0.01	0.02	0.56	0.04	0.03	0.09	-0.19	0.21	0.07	-0.22	0.20
	AttnLRP	0.76	-0.00	0.09	0.53	0.20	0.18	0.12	-0.23	0.18	0.12	-0.25	0.17
	Grad×Input	0.05	0.07	-0.00	0.31	0.27	0.01	0.00	-0.07	0.05	-0.02	-0.11	0.03
	LIME	0.12	0.03	0.01	0.39	0.21	0.04	0.10	-0.16	0.23	0.08	-0.20	0.23
Qwen-32B	SHAP	0.34	-0.01	0.04	0.66	-0.03	0.08	0.08	-0.22	0.23	0.06	-0.26	0.22
	AttnLRP	0.78	-0.01	0.11	0.38	0.19	0.22	0.10	-0.26	0.22	0.10	-0.27	0.24
	Grad×Input	0.06	0.08	-0.00	0.24	0.20	0.05	-0.01	-0.10	0.06	-0.03	-0.11	0.07
	LIME	0.15	0.05	0.02	0.43	0.06	0.08	0.08	-0.19	0.26	0.07	-0.24	0.26
Llama-70B	SHAP	0.34	-0.00	0.03	0.59	-0.00	0.07	0.06	-0.21	0.19	0.06	-0.25	0.19
	AttnLRP	0.79	-0.00	0.11	0.32	0.19	0.22	0.07	-0.24	0.20	0.08	-0.28	0.21
	Grad×Input	0.05	0.06	-0.00	0.22	0.16	0.06	-0.02	-0.09	0.05	-0.04	-0.12	0.04
	LIME	0.12	0.04	0.02	0.36	0.08	0.06	0.07	-0.19	0.25	0.06	-0.24	0.23

Table 21: Faithfulness evaluation results: **AOPC Comprehensiveness** (comp., \uparrow), **AOPC Sufficiency** (suff., 0 best), and **Kendall’s τ correlation with Leave-One-Out** ($\tau(\text{loo})$, \uparrow). Higher \uparrow and lower \downarrow are better. Best results per column are **bold**.

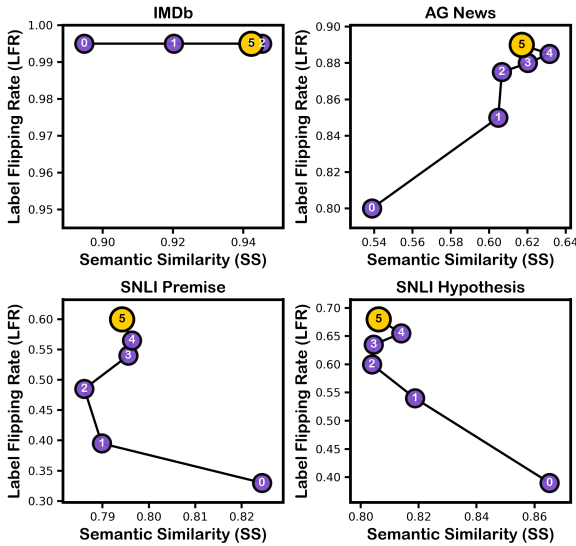


Figure 10: Trade-off between semantic similarity and label flipping rate. Markers show iteration \mathcal{K} . Results are from *iFlip-NL* using LLaMA3.3-70B.

with attribution signals in sentiment and topic classification, whereas this alignment is less stable in NLI due to the complexity of entailment reasoning.

I Highlighted Words from Attribution Methods

Table 22 illustrate how different attribution methods identify most important words within the same IMDb review.

J Additional Examples

This section presents illustrative case studies of counterfactual generation, showcasing both successful refinements and common failure patterns of

the proposed framework.

J.1 Example 1: Undesired Flip

Observation: Table 23 shows that the framework can produce label flips, but not always toward the desired direction. The label was flipped from **NEUTRAL** to **ENTAILMENT** instead of the expected **CONTRADICTION**.

J.2 Example 2: Failed Flip

Observation: Table 24 shows a common failure case: the generator tends to produce longer and more elaborate counterfactuals, but the label remains unchanged despite multiple refinement rounds.

J.3 Example 3: No Early Stopping (Flip-Flop)

Observation: Table 25 shows another failure pattern: even though the generator kept producing essentially the same counterfactual, the classifier’s prediction oscillated between **NEUTRAL** and **CONTRADICTION**, suggesting instability near the decision boundary.

J.4 Example 4: No Early Stopping (Flip-Flop)

Observation: Table 26 illustrates a flip-flop failure pattern: the classifier initially flipped correctly to **CONTRADICTION**, but subsequent refinements pushed the prediction back to **NEUTRAL**, showing instability in the refinement loop.

K Prompts

This section presents the full set of prompts employed in our counterfactual generation pipeline.

Method	IMDb Review
AttenLRP	This movie is on the level with Welcome Home Roxy Carmichael for biggest pieces of garbage that have ever hit the silver screen. If these guys weren't Adam Sandler's gay friends, this script would have ended up where it should have: as some big time movie exec's toilet paper. I hate this movie, it makes me want to injure people. I will admit that I have high standards, but honestly I'd rather watch Step Up 2. The ultra sad part was when I logged onto IMDb and read that you pieces of trash actually gave this movie a 6.9 rating. This is a testament to all of the retards in our society that will go watch terrible movies that are just hour and a half long dick, fart, and weed jokes with little to no originality. After seeing this rating, I would like to suggest Tyler Perry's House of Pain to all of you guys who enjoyed this film; you'll see some high quality humor there on about the same level of this abhorrent abomination.
SHAP	This movie is on the level with Welcome Home Roxy Carmichael for biggest pieces of garbage that have ever hit the silver screen. If these guys weren't Adam Sandler's gay friends, this script would have ended up where it should have: as some big time movie exec's toilet paper. I hate this movie, it makes me want to injure people. I will admit that I have high standards, but honestly I'd rather watch Step Up 2. The ultra sad part was when I logged onto IMDb and read that you pieces of trash actually gave this movie a 6.9 rating. This is a testament to all of the retards in our society that will go watch terrible movies that are just hour and a half long dick, fart, and weed jokes with little to no originality. After seeing this rating, I would like to suggest Tyler Perry's House of Pain to all of you guys who enjoyed this film; you'll see some high quality humor there on about the same level of this abomination.
LIME	This movie is on the level with Welcome Home Roxy Carmichael for biggest pieces of garbage that have ever hit the silver screen. If these guys weren't Adam Sandler's gay friends, this script would have ended up where it should have: as some big time movie exec's toilet paper. I hate this movie, it makes me want to injure people. I will admit that I have high standards, but honestly I'd rather watch Step Up 2. The ultra sad part was when I logged onto IMDb and read that you pieces of trash actually gave this movie a 6.9 rating. This is a testament to all of the retards in our society that will go watch terrible movies that are just hour and a half long dick, fart, and weed jokes with little to no originality. After seeing this rating, I would like to suggest Tyler Perry's House of Pain to all of you guys who enjoyed this film; you'll see some high quality humor there on about the same level of this abhorrent abomination.
Grad×Input	This movie is on the level with Welcome Home Roxy Carmichael for biggest pieces of garbage that have ever hit the silver screen. If these guys weren't Adam Sandler's gay friends, this script would have ended up where it should have: as some big time movie exec's toilet paper. I hate this movie, it makes me want to injure people. I will admit that I have high standards, but honestly I'd rather watch Step Up 2. The ultra sad part was when I logged onto IMDb and read that you pieces of trash actually gave this movie a 6.9 rating. This is a testament to all of the retards in our society that will go watch terrible movies that are just hour and a half long dick, fart, and weed jokes with little to no originality. After seeing this rating, I would like to suggest Tyler Perry's House of Pain to all of you guys who enjoyed this film; you'll see some high quality humor there on about the same level of this abhorrent abomination.

Table 22: IMDb review with Top-k important words highlighted under different attribution methods.

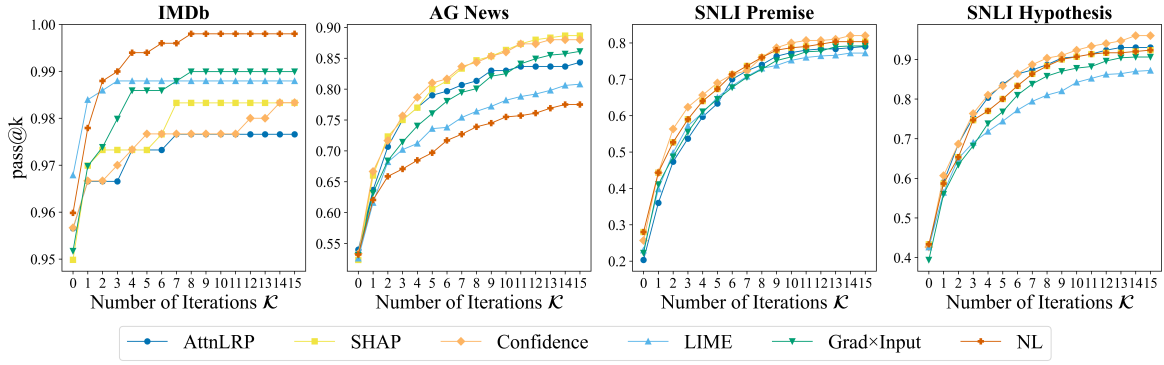


Figure 11: Iterative refinement effectiveness on OLMo2-7B. pass@k curves for each dataset (IMDb, AG News, SNLI), evaluated up to $\mathcal{K} = 15$ refinement steps.

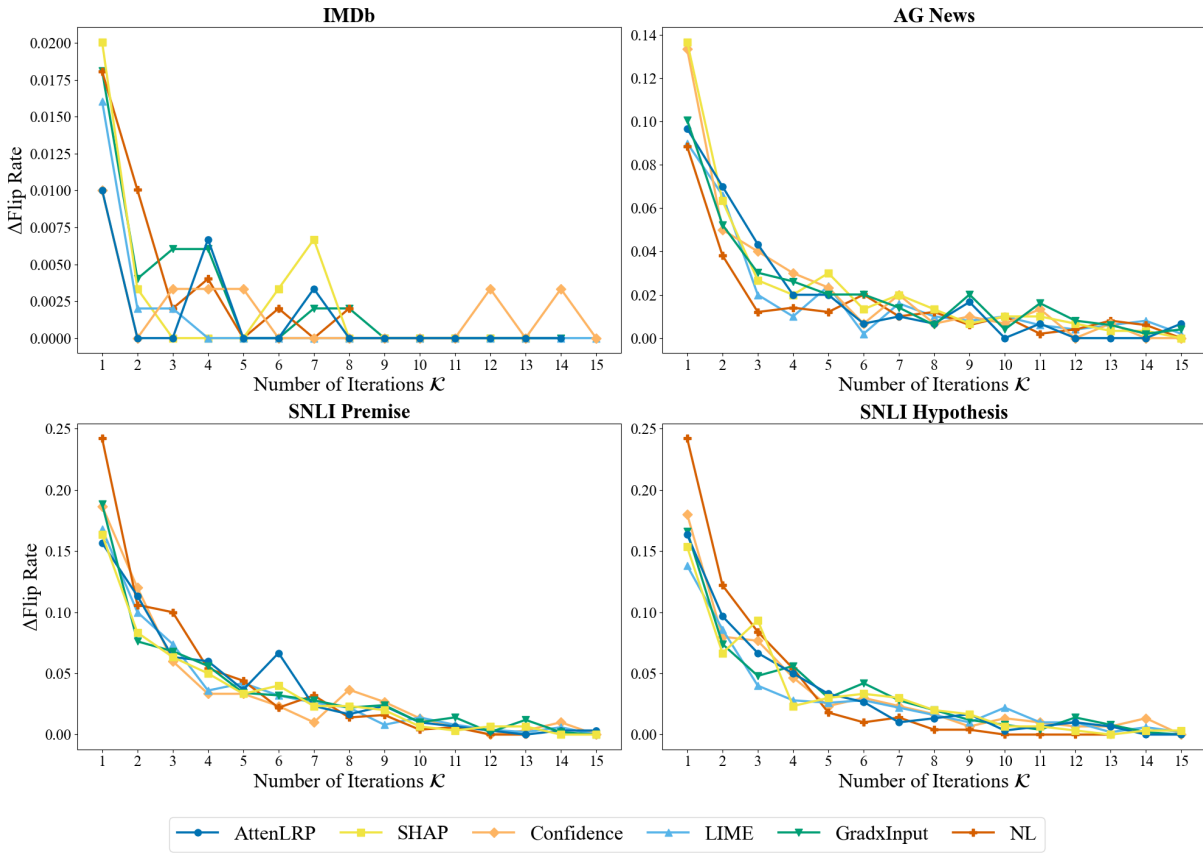


Figure 12: Change in flip rate (Δ Flip Rate) across iterative refinement rounds with OLMo2-7B for different feedback signals. The results show how much additional gain each refinement step contributes beyond the previous round.

1229 The Base Counterfactual Prompt in Section K.1
 1230 is used to initially generate a counterfactual example.
 1231 The subsequent refinement stage then improves
 1232 this initial counterfactual using one of our three
 1233 feedback mechanisms: the Confidence-Based Re-
 1234 finement Prompt in Section K.2, the Attribution-
 1235 Based Refinement Prompt in Section K.3, and the
 1236 Natural-Language Feedback Refinement Prompt in
 1237 Section K.4.

K.1 Base Counterfactual Prompt

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A classifier has determined that the label
 of the following text is [ORIGINAL_LABEL].
 Please flip it to [TARGET_LABEL] with
 minimal changes. Wrap your answer in
 <cf>...</cf>.
 Original input:
 [INPUT_TEXT]
 Hint: [TASK-SPECIFIC HINT]

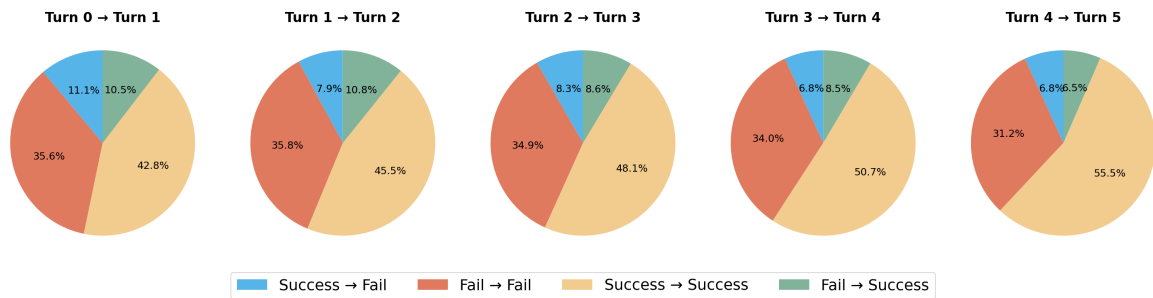


Figure 13: Iterative refinement with OLMo2-7B **without early stopping**, averaged across all datasets and all feedback signals. A substantial share of *Success* → *Fail* transitions indicates reduced stability compared to early-stopping.

Round	Counterfactual Example	Classifier Prediction
Original	Premise: A small girl with short brown hair is pushing a pink scooter over grass with brown leaves with trees in the background. Hypothesis: The girl is outside.	NEUTRAL (Expected: Contradiction)
Round 1	Premise: A small girl with short brown hair is inside playing with a pink scooter . Hypothesis: The girl is outside.	NEUTRAL (Expected: Contradiction)
Round 2	Counterfactual: <i>invalid output</i>	NEUTRAL
Round 3	Premise: A small girl with short brown hair is playing inside with a pink scooter . Hypothesis: The girl is outside.	NEUTRAL (Expected: Contradiction)
Round 4	Premise: A small girl with short brown hair is indoors riding a pink scooter . Hypothesis: The girl is outside.	ENTAILMENT (Expected: Contradiction)

Table 23: Iterative counterfactual refinement on an SNLI Premise. Top-*k* important words identified by AttnLRP are highlighted. *i*Flip flips the label, but not always to the desired class.

K.2 Confidence-based Refinement Prompt

The classifier now predicts your text as [PRED_LABEL] ([CONF]% confidence), which is the desired label.
Your task is to minimize the edits compared to the original while preserving the current label: [PRED_LABEL].
Make the revision as close as possible to the original, but do not revert to the original label: [ORIGINAL_LABEL].
Wrap ONLY the final text in <cf>...</cf>.
Original input (classifier label [ORIGINAL_LABEL]):
[INPUT_TEXT]
Current counterfactual:
[CF_TEXT]
Hint: [TASK-SPECIFIC HINT]

Make the revision as close as possible to the original, but do not revert to the original label: [ORIGINAL_LABEL].
Wrap ONLY the final text in <cf>...</cf>.
Original input (classifier label [ORIGINAL_LABEL]):
[INPUT_TEXT]
Current counterfactual:
[CF_TEXT]
Hint: [TASK-SPECIFIC HINT]

K.4 Natural-Language Feedback Refinement Prompt

Natural-language refinement first asks the model to generate NL feedback analyzing how to minimally achieve the target label. This feedback is then used to guide a second prompt that produces the counterfactual.

K.3 Attribution-based Refinement Prompt

The classifier now predicts your text as [PRED_LABEL], which is the desired label.
Key words influencing this prediction: [TOP_WORDS].
Your task is to minimize the edits compared to the original while preserving the current label: [PRED_LABEL].

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Round	Counterfactual Example	Classifier Prediction
Original	Premise: A ballerina standing on the toes of one foot with one arm up in the air and one leg lifted behind her. Hypothesis: The ballerina hates this.	CONTRADICTION (Expected: Neutral)
Round 1	Premise: A ballerina stands gracefully on the toes of one foot, her arm reaching towards the sky, while the other leg is lifted behind her, a look of intense concentration on her face as she perfectly captures the beauty and intricacy of the moment in dance, amidst a bustling cityscape outside the studio window, completely unaware of the chaos beyond her focus. Hypothesis: The ballerina hates this.	CONTRADICTION (Expected: Neutral)
Round 2	Premise: A ballerina stands gracefully on the toes of one foot, her arm reaching towards the sky, while the other leg is lifted behind her, a look of intense concentration on her face as she perfectly captures the beauty and intricacy of the moment in dance, happening during her first solo performance in front of a packed theater, completely unaware of the standing ovation from the enthralled audience outside the proscenium arch. Hypothesis: The ballerina hates this.	CONTRADICTION (Expected: Neutral)
Round 3	Premise: A ballerina stands gracefully on the toes of one foot, her arm reaching towards the sky, while the other leg is lifted behind her, capturing the serene beauty of a peaceful morning scene in the park, completely unaware of the beautiful sunrise illuminating the clouds overhead. Hypothesis: The ballerina hates this.	CONTRADICTION (Expected: Neutral)
Round 4	Premise: A ballerina stands gracefully , her arm elegantly raised, foot poised on the tip, as she prepares for a grand performance on a bustling city stage, her eyes filled with determination and focus. The bright lights above illuminate her, casting long shadows on the polished wooden floor. The audience's anticipation is palpable in the silent, charged air of the theatre. Hypothesis: The ballerina hates this.	CONTRADICTION (Expected: Neutral)
Round 5	Premise: A ballerina stands gracefully on a beach, one arm stretched upward towards the sky as if greeting the sun, the other hand resting lightly on her hip, amidst a sea of beachgoers. The air is salty and warm, and the sand is soft beneath her feet. Around her, people are lounging, laughing, and enjoying the freedom of the day. The city's skyline is visible in the distance, with skyscrapers gleaming against the azure sky. Hypothesis: The ballerina hates this.	CONTRADICTION (Expected: Neutral)

Table 24: Iterative counterfactual refinement on an SNLI Premise. Top- k important words identified by AttnLRP are highlighted. Despite multiple refinements, the prediction remains CONTRADICTION instead of flipping to the expected NEUTRAL.

K.4.1 Feedback Generation Prompt (NL Feedback)

Analyze the current counterfactual and suggest improvements to achieve the target label [TARGET_LABEL].
You should make the smallest possible edits to the text while still achieving the target.
Wrap your reasoning inside
<think>...</think>.

Original (classifier label
[ORIGINAL_LABEL]):
[INPUT_TEXT]

Current counterfactual:
[CF_TEXT]

K.4.2 Counterfactual Editing Prompt (Using NL Feedback)

Based on the feedback below, revise the text so that it flips to [TARGET_LABEL].

Feedback:
[FEEDBACK_TEXT]

Wrap ONLY the final counterfactual in
<cf>...</cf>.

Original text (classifier label:
[ORIGINAL_LABEL]):
[INPUT_TEXT]

Current counterfactual:
[CF_TEXT]

1250
1251

Round	Counterfactual Example	Classifier Prediction
Original	Premise: A man in a business suit silently meditating in front of the camera. Hypothesis: A business man is giving a heated interview for the local news.	NEUTRAL (Expected: Contradiction)
Round 1	Premise: A man in a business suit silently meditating in front of the camera. Hypothesis: A business man is giving a heated interview for the local news.	NEUTRAL (Expected: Contradiction)
Round 2	Premise: A man in a business suit silently meditating in front of the camera. Hypothesis: A business man is giving a heated interview for the local news.	CONTRADICTION (Expected: Contradiction)
Round 3	Premise: A man in a business suit silently meditating in front of the camera. Hypothesis: A business man is giving a heated interview for the local news.	NEUTRAL (Expected: Contradiction)
Round 4	Premise: A man in a business suit silently meditating in front of the camera. Hypothesis: A business man is giving a heated interview for the local news.	CONTRADICTION (Expected: Contradiction)
Round 5	Premise: A man in a business suit silently meditating in front of the camera. Hypothesis: A business man is giving a heated interview for the local news.	NEUTRAL (Expected: Contradiction)

Table 25: Iterative counterfactual refinement on an SNLI premise. Top- k important words identified by AttnLRP are highlighted. Despite producing nearly identical counterfactuals, the classifier oscillates between CONTRADICTION and NEUTRAL, illustrating instability near the decision boundary.

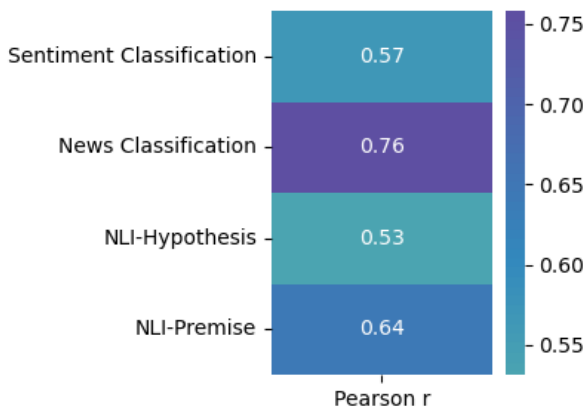


Figure 14: Pearson correlation between augmentation performance and counterfactual quality across datasets.

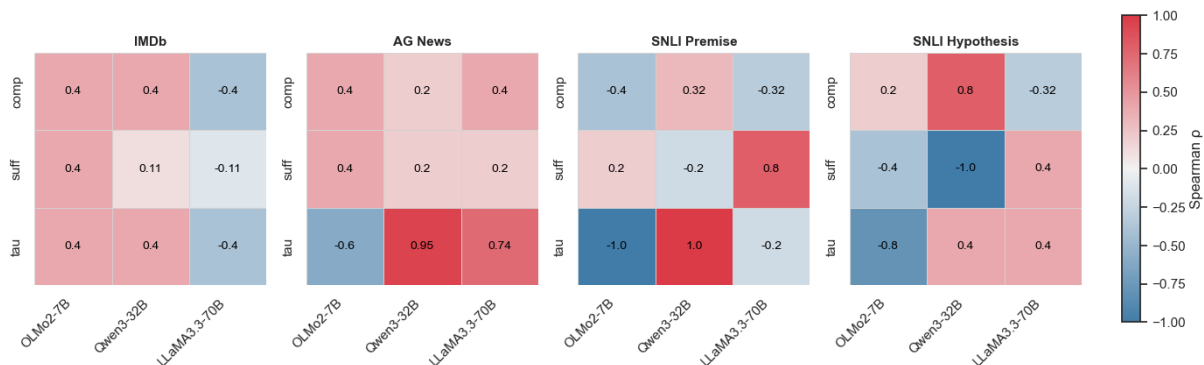


Figure 15: Spearman correlation between faithfulness and counterfactual quality across datasets.

Round	Counterfactual Example	Prediction (Expected)
Original	Premise: Man in robe making designs on dirt ground. Hypothesis: A man making designs in the dirt outside.	NEUTRAL
Round 1	Hypothesis: A man making designs in the dirt outdoors.	NEUTRAL (Expected: Contradiction)
Round 2	Hypothesis: A man is carefully cleaning a spotless carpet indoors.	CONTRADICTION (Expected: Contradiction)
Round 3	Hypothesis: A man is carefully cleaning a spotless carpet indoors while there's a man in a robe making designs on a dirt ground outside.	NEUTRAL (Expected: Contradiction)
Round 4	Hypothesis: A man is meticulously cleaning a spotless carpet indoors while simultaneously, there's a man in a robe making designs on a dirt ground outside, in total contradiction to the original scene where there's no mention of indoor cleaning and only a man making designs on dirt.	NEUTRAL (Expected: Contradiction)
Round 5	Hypothesis: A man indoors is vacuuming a spotless carpet while another man outside is making intricate designs on a dirt ground, representing a total contradiction as it juxtaposes cleaning indoors with design-making outdoors, and a spotless carpet with a dirt ground.	NEUTRAL (Expected: Contradiction)

Table 26: Iterative counterfactual refinement on an SNLI Hypothesis. Top- k important words identified by AttnLRP are highlighted. The classifier briefly flipped to CONTRADICTION in Round 2 but reverted back to NEUTRAL.

L User Study Guidelines

User Study Guidelines

Dear participants,

Thank you for participating in our user study. This study focuses on evaluating model-generated explanations, specifically counterfactual explanations (definitions and examples follow). We generate counterfactuals using three approaches in total, and you will evaluate 10 counterfactuals generated by each approach. You will subjectively rate each explanation based on the following three dimensions: **completeness**, **understandability**, and **cohesiveness**.

Counterfactual Example (CFE): the smallest change to an input that would cause a model to output a different prediction. It is important to note that “change in prediction” refers to the model’s predicted label, not the ground truth label.

Simple Example (Sentiment Classification):

- Original: “The movie was boring.” → Model predicts **negative**.
- CFE: “The movie was great.” → Model predicts **positive**.

In our questionnaire, the task is more complex: the model modifies news sentences from AG News, which has four categories: Business, Sports, World, Sci/Tech. You will manually rate CFEs using the following metrics. Higher scores indicate higher quality.

1. Completeness (1–6): The explanation is sufficient in explaining the outcome. In other words, does the CFE provide enough information to clearly support the new predicted label?

- **1** – The CFE is not enough to justify the new label; explanation is insufficient
- **3** – Partially justifies the new label; some key information is missing
- **6** – Fully justifies the new label; enough information to clearly support the prediction shift

We give two special cases to help you rate:

• **Case I:**

Original: “The company reported lower profits this quarter.” → Model predicts Business.

CFE: “The company reported lower profits this sports quarter.” → Model predicts Sports.

We may rate this CFE a low completeness score (e.g., 1–2). Because the topic of CFE is still Business, though it did mention sports quarter.

• **Case II:**

Original: “The president met with foreign leaders to discuss regional security.” → Model predicts World.

CFE: “The president met with foreign leaders to discuss new technology.” → Model predicts Sci/Tech.

We may rate this CFE a low completeness score (e.g., 1–2). The sentence still mainly describes political or diplomatic meetings; the small mention of “technology” is not enough to justify Sci/Tech.

2. Overall satisfaction (1–6): This scenario effectively explains how to reach a different outcome.

- **1** – Does not explain how to reach a different outcome
- **3** – Explains it partially but lacks clarity
- **6** – Clearly and fully explains how to reach a different outcome

We give one special case to help you rate:

• **Case I:**

Original: “Leaders met to discuss international security and trade sanctions.” → Model predicts World.

CFE: “Leaders met to discuss international sports security and trade sanctions.” → Model predicts World.

We may rate this CFE a low Overall Satisfaction score (e.g., 1–2), because the change from “security” to “sports security” is too minor to meaningfully alter the sentence’s topic.

3. Feasibility (1–6): The actions suggested by the explanation are practical, realistic to implement and actionable.

- **1** – unrealistic or impossible
- **3** – partly feasible but unclear or difficult
- **6** – fully realistic and actionable

We give one special case to help you rate:

• **Case I:**

Original: “Apple Inc. won an international innovation award.” → Model predicts Business.

CFE: “Apple Inc. won the World Cup” → Model predicts Sports.

We may rate this CFE a low score (e.g., 1–2), because the change is unrealistic. A company cannot win the World Cup.

M LLM-as-a-Judge Evaluation

We adopt an LLM-as-a-judge protocol to assess the explanatory quality of counterfactual from three subjective perspectives: *Completeness*, *Overall Satisfaction*, and *Feasibility*.

M.1 Prompt

The following prompt instructs the judge model to rate each CFE using integer scores from 1 to 6.

You are an evaluation model (LLM-as-a-judge). You will be given:

- Original text
- Counterfactual example (CFE): A minimally edited version of the input text that results in a change in the model’s prediction.
- Original prediction and counterfactual prediction
- Whether the prediction flips (isFlip)

Your task is to score the CFE scenario’s explanatory quality on three metrics. Use integer scores from 1 to 6 (1 = lowest, 6 = highest).

Metrics:

- 1) Completeness (1-6): The explanation is sufficient in explaining the outcome.
- 2) Overall satisfaction (1-6): This scenario effectively explains how to reach a different outcome.
- 3) Feasibility (1-6): The actions suggested by the explanation are practical, realistic to implement and actionable.

Output MUST be exactly in the following format (three tags, integers only):
 <completeness>score</completeness><satisfaction>score</satisfaction><feasibility>score</feasibility>

Do not output anything else.

M.2 Evaluation Across Judge Models

Table 27 reports the mean ratings for all counterfactuals across three judge models.

Model	Method	Compleat.	Overall Sat.	Feasib.	Kripp. α
Gemini3 -27B	CGG	3.4	3.4	4.5	0.649
	FIZLE	3.2	3.2	3.3	
	#Flip-NL	5.2	5.3	5.1	
GPT-OSS -120B	CGG	2.7	2.6	2.9	0.666
	FIZLE	2.7	2.7	3.3	
	#Flip-NL	3.4	3.4	3.5	
DeepSeek -KI	CGG	3.5	3.3	4.4	0.571
	FIZLE	3.4	3.3	4.8	
	#Flip-NL	5.0	4.7	4.6	

Table 27: Evaluation results on *Completeness*, *Overall Satisfaction*, and *Feasibility* across three judge models. Best results are bolded. Krippendorff’s α denotes Krippendorff’s alpha measuring agreement between the judge model ratings and human ratings.

N Error Analysis

Subsection N.1 and N.2 discusses Incomplete and Unrealistic CFE Candidates, and Subsection N.4 shows how iterative refinement can enhance the completeness and feasibility of CFE candidates.

N.1 Incomplete CFE Candidates

As illustrated in Table 28, a common failure case occurs when only partial entity mentions are edited, resulting in incomplete modifications that fail to sufficiently alter the model’s predictions.

Dataset	AG News
Method	CGG
Original	Senate approves tax relief bill for manufacturers The Senate today passed a far-reaching, \$136 billion corporate tax package that cuts taxes for businesses ranging from film companies to bow-and-arrow makers while closing tax loopholes and bringing US exporters in line with Prediction: business
CFE	Senate approves research funding bill for innovators The Senate today passed a far-reaching, \$136 billion scientific research package that cuts funding for projects ranging from space companies to robotics makers while closing research gaps and bringing US scientists in line with Prediction: business
Issue	Although many business-related entities are replaced with scientific terms, enough business cues remain and the overall prediction does not change.

Table 28: Error analysis for incomplete CFE candidates

N.2 Unnatural CFE Candidates

As shown in Table 29, another common failure case is when modifications produce counterfactuals that are unnatural. The generated CFE candidates contain contexts that are inconsistent with real-world facts and scenarios.

Dataset	AG News
Method	FIZLE
Original	IBM Claims Computing Crown (The Motley Fool) The Motley Fool - IBM (NYSE: IBM - News) has new bragging rights. Press reports indicate that the technology giant has created the world’s fastest supercomputer two years after a Japanese computer claimed that title. Prediction: sci/tech
CFE	IBM Claims Tennis Crown (The Sports Fool) The Sports Fool - IBM (NYSE: IBM - News) has new bragging rights. Press reports indicate that the tennis giant has created the world’s fastest serve two years after a Japanese player claimed that title. Prediction: sci/tech
Issue	The CFE unrealistically portrays IBM, a technology company, as a tennis giant, creating a scenario that conflicts with real world.

Table 29: Error analysis for unnatural CFE candidates.

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N.3 Per-annotator Human and LLM Ratings

Table 31 presents two concrete examples that report detailed per-annotator ratings from a human user study (H1–H3) and an LLM-as-a-judge evaluation (L1–L3; Gemma3–27B, GPT–OSS–120B, and DeepSeek–R1) on three dimensions: *Completeness*, *Overall Satisfaction*, and *Feasibility*.

N.4 Enhancing Completeness and Feasibility with Iterative Refinement

As shown in Table 30, iterative refinement helps address both incompleteness and unnatural counterfactual scenarios in CFE candidates.

Dataset	AG News
Method	iFlip
Original	<p>Gold Fields wins appeal to fight takeover Gold Fields Ltd. won an appeal on Friday in its battle to stave off a hostile \$7.1 billion takeover by Harmony Gold Mining Co. that would create the world #39;s largest gold mining company.</p> <p style="text-align: right;">Prediction: business</p>
CFE (a) (Iter: $\mathcal{K} = 1$)	<p>Gold Fields wins global appeal to address international concerns Gold Fields Ltd. won a global appeal on Friday in its effort to address international concerns by Harmony Gold Mining Co. that would impact global stability, sparking concerns at the United Nations and among nations worldwide.</p> <p style="text-align: right;">Prediction: business</p>
CFE (b) (Iter: $\mathcal{K} = 2$)	<p>Gold Fields wins global appeal to address international concerns, sparking widespread discussion on the world stage about the global implications of mining operations and their potential impact on international stability, prompting concerns at the United Nations and among nations worldwide.</p> <p style="text-align: right;">Prediction: world</p>
Observation	<p>Although CFE (a) adds world-related context, it is still mainly about the legal appeal, so the model keeps the <i>business</i> label and the claim about affecting global stability is not very realistic.</p> <p>After one round of iterative refinement, CFE (b) becomes more complete and realistic by highlighting the global debate around mining operations, and consequently the model prediction changes to <i>world</i>.</p>

Table 30: Error analysis for Iterative Refinement.

Dataset	AG News			
Original	<i>"Senate approves tax relief bill for manufacturers The Senate today passed a far-reaching, \$136 billion corporate tax package that cuts taxes for businesses ranging from film companies to bow-and-arrow makers while closing tax loopholes and bringing US exporters in line with "</i>			
CFE by CGG	<i>"Senate approves research funding bill for innovators The Senate today passed a far-reaching, \$136 billion scientific research package that cuts funding for projects ranging from space companies to robotics makers while closing research gaps and bringing US scientists in line with"</i>			
	Orig. Pred	business	Completeness	H1–H3: 3/2/4 L1–L3: 3/1/2
	CFE Pred	business	Overall Satisfaction	H1–H3: 2/2/3 L1–L3: 3/1/2
	isFlip	Yes	Feasibility	H1–H3: 3/2/2 L1–L3: 4/1/4
CFE by FIZLE	<i>"Sports fans are approval of tax relief bill for sports manufacturers The Senate today passed a far-reaching, \$136 billion corporate tax package that cuts taxes for businesses ranging from sports equipment companies to athletic wear makers while closing tax loopholes and bringing US sports exporters in line with international standards, which is expected to boost the sports industry and create new jobs for athletes and sports enthusiasts."</i>			
	Orig. Pred	business	Completeness	H1–H3: 6/3/1 L1–L3: 6/5/5
	CFE Pred	sport	Overall Satisfaction	H1–H3: 3/3/5 L1–L3: 6/5/5
	isFlip	No	Feasibility	H1–H3: 3/2/3 L1–L3: 6/5/5
CFE by iFlip	<i>"Senate approves research funding bill for sci/tech innovators. The Senate today passed a far-reaching, \$136 billion research package that funds cutting-edge projects in areas like quantum computing, biotechnology, and advanced materials for companies ranging from artificial intelligence startups to renewable energy labs, while supporting collaborations with institutions like NASA, Google, and MIT, and enhancing the global competitiveness of US tech exporters."</i>			
	Orig. Pred	business	Completeness	H1–H3: 5/5/6 L1–L3: 6/5/6
	CFE Pred	sci/tech	Overall Satisfaction	H1–H3: 6/6/6 L1–L3: 6/5/6
	isFlip	Yes	Feasibility	H1–H3: 6/5/6 L1–L3: 6/4/6

Table 31: Detailed ratings from three human annotators (H1–H3) and three LLM judges (L1–L3), where L1=Gemma3-27B, L2=GPT-OSS-120B, and L3=DeepSeek-R1.