Can LLMs Explain Themselves Counterfactually?

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Abstract

Explanations are an important tool for gaining insights into model behavior, calibrating user trust, and ensuring compliance. The past few years have seen a flurry of methods for generating explanations, many of which involve computing model gradients or solving specially designed optimization problems. Owing to the remarkable reasoning abilities of LLMs, *self-explanation*, *i.e.*, prompting the model to explain its outputs, has recently emerged as a new paradigm. We study a specific type of self-explanation, *self-generated counterfactual explanations* (SCEs). We test LLMs' ability to generate SCEs across families, sizes, temperatures, and datasets. We find that LLMs sometimes struggle to generate SCEs. When they do, their prediction often does not agree with their own counterfactual reasoning.

`github.com/aisoc-lab/llm-sces`

1 Introduction

LLMs have shown remarkable capabilities across a range of tasks (Bommasani et al., 2021; Maynez et al., 2023; Wei et al., 2022a), and can match or even surpass human performance (Luo et al., 2024; Peng et al., 2023; Yang et al., 2024). These impressive achievements are often attributed to large datasets, model sizes (Hoffmann et al., 2022; Kaplan et al., 2020), and the effect of alignment with human preferences (Ouyang et al., 2022). However, the resulting complexity makes it difficult to explain LLM outputs.

ML explainability had been thoroughly studied before the advent of modern LLMs (Gilpin et al., 2018; Guidotti et al., 2018). Many LLM explainability methods build on techniques designed for non-LLM models. These techniques mostly operate by computing model gradients or solving intricate optimization problems to find input features (Cohen-Wang et al., 2025), neurons (Meng et al., 2022; Templeton et al., 2024), abstract concepts (Bricken et al., 2023; Kim et al., 2018; Xu et al., 2025), or data points (Park et al., 2023) causing the model to depict a certain behavior.

Inspired by the impressive reasoning of LLMs, recent work explores whether they can *explain themselves* without costly methods like gradients or optimization. For instance, Bubeck et al. (2023) show GPT-4 can provide rationales and even admit mistakes. A fast-emerging branch of explainability focuses on producing and evaluating *self-generated explanations* (Agarwal et al., 2024; Guo et al., 2025; Lanham et al., 2023; Madsen et al., 2024; Tanneru et al., 2024; Turpin et al., 2023).

We study a specific type of self-explanations: *self-generated counterfactual explanations* (SCEs). Given an input $\mathbf{x}$ and model output $\hat{y}$, a counterfactual $\mathbf{x}_{\text{CE}}$ is a modified input that leads the model to output $\hat{y}_{CE} \neq \hat{y}$. Prior work argues that due to their contrastive nature, counterfactuals better align with human expectations (Miller, 2019), better match regulatory needs (Wachter et al., 2017) and are a better test of knowledge (Ichikawa and Steup, 2024), than other feature-based explanations (Lundberg and Lee, 2017; Ribeiro et al., 2016).

We study the **efficacy of LLMs in generating SCEs** via three research questions (RQs).

- **RQ1** Are LLMs able to generate SCEs at all?
- **RQ2** Do these self-generated counterfactuals faithfully reflect the model reasoning?
- **RQ3** Are LLMs able to generate SCEs without large-scale changes to the input?

To answer these questions, we design the procedure in Figure 1: the model makes a prediction (Figure 1a), generates a SCE (Figure 1b), and finally compute the model's prediction on the SCE (Figure 1c). We test seven LLMs (7B–70B) across six datasets and four tasks. Most models are able to generate SCEs (RQ1). However, in many cases,

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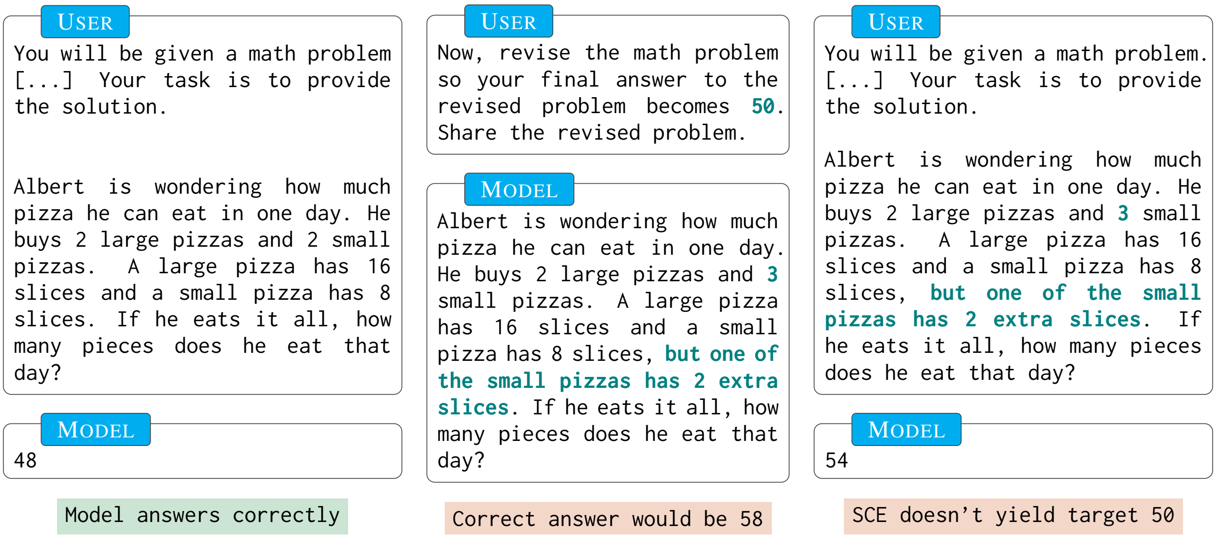

USER

```
You will be given a math problem [...] Your task is to provide the solution.

Albert is wondering how much pizza he can eat in one day. He buys 2 large pizzas and 2 small pizzas. A large pizza has 16 slices and a small pizza has 8 slices. If he eats it all, how many pieces does he eat that day?
```

MODEL

```
48
```

Model answers correctly

(a) Model response on original problem.

USER

```
Now, revise the math problem so your final answer to the revised problem becomes 50. Share the revised problem.
```

MODEL

```
Albert is wondering how much pizza he can eat in one day. He buys 2 large pizzas and 3 small pizzas. A large pizza has 16 slices and a small pizza has 8 slices, but one of the small pizzas has 2 extra slices. If he eats it all, how many pieces does he eat that day?
```

Correct answer would be 58

(b) Self-generated counterfactual

USER

```
You will be given a math problem. [...] Your task is to provide the solution.

Albert is wondering how much pizza he can eat in one day. He buys 2 large pizzas and 3 small pizzas. A large pizza has 16 slices and a small pizza has 8 slices, but one of the small pizzas has 2 extra slices. If he eats it all, how many pieces does he eat that day?
```

MODEL

```
54
```

SCE doesn't yield target 50

(c) Evaluation of self-explanation

Figure 1: **LLMs are unable to explain themselves counterfactually**. Explanation generation behavior of `LLaMA-3.1-70B-instruct` on an example from GSM8K data. In the left panel, the model answers correctly. In the second panel, the model is asked to produce a SCE so that the answer becomes 50. The resulting SCE is incorrect. The correct answer would be 58 instead of the targeted answer of 50. In the third panel, the SCE is given as a new problem to the model. The model answers with 54 which *neither* yields the target 50 *nor* computes to the correct answer 58. This figure is best viewed in color.

the model predictions on SCEs do not yield the target label, meaning that self-generated counterfactual reasoning does not align with model predictions (RQ2). We also find that including the original prediction and the SCE instruction in the chat history strongly influences the model predictions, further exposing weaknesses in their counterfactual reasoning. We analyze failure cases using automated metrics such as validity (whether the model prediction on $\mathbf{x}_{CE}$ matches the target $\hat{y}_{CE}$), readability, and differences in embeddings, as well as human annotations of SCE correctness, that is, whether the counterfactual $\mathbf{x}_{CE}$ actually evaluates to $\hat{y}_{CE}$. The results show that readability does not predict SCE validity or correctness, and that differences in embeddings can sometimes, but not always, correlate with failures in counterfactual reasoning. Finally, models show large variation in how much they change the input when generating SCEs (RQ3). Overall, our findings underscore that, **despite strong reasoning abilities, LLMs remain far from reliable in counterfactual self-explanation.**

2 Related Work

Explainability in ML. There are several ways to categorize explainability methods, *e.g.*, perturbation vs. gradient-based, feature vs. concept vs. prototype-based, importance vs. counterfactual-based and optimization vs. self-generated. See Gilpin et al. (2018), Guidotti et al. (2018), and Zhao et al. (2024) for details.

Counterfactual explanations in ML. See Section 1 for a comparison between counterfactual explanations (CEs) and other forms of explainability. Generating valid and plausible CEs is a longstanding challenge (Verma et al., 2024). For instance, Delaney et al. (2023) highlight discrepancies between human- and computationally-generated CEs. They find that humans make larger, more meaningful modifications, whereas computational methods prioritize minimal edits. Prior work has also highlighted the need for on-manifold CEs to ensure plausibility and robustness (Slack et al., 2021; Tsiourvas et al., 2024). Modeling the data manifold, however, is a challenging problem, even for non-LLM models (Arvanitidis et al., 2016).

Self-explanation (SEs) by LLMs. SEs take many forms, *e.g.*, chain-of-thought (CoT) reasoning (Agarwal et al., 2024) and feature attributions (Tanneru et al., 2024), but both may fail to faithfully reflect a model's true decision-making (Lanham et al., 2023; Tanneru et al., 2024; Turpin et al., 2024). Our SCE protocol is distinct from these; we use CoT only for evaluating SCEs given its benefit to predictive performance (Wei et al., 2022b), not as an explanation. Madsen et al. (2024) also evaluate SCEs. Our work differs from theirs in following important aspects: We systematically study how often the models are able to generate SCEs at all. Madsen et al. aim to generate SCEs that are as close to the input as possible. By contrast, we try a range of strategies that are a mix of free generation (unconstrained prompting and CoT in Section 3.1) and a more restrictive rationale-based generation, and measure the distance between the original input the SCEs. Finally, we examine hidden states and uncover differences between valid and invalid SCEs. Chen et al. (2023) study simulatability via human prediction. Huang et al. (2025) introduce MATH-PERTURB, using human-generated perturbations and Reverse QA to test whether model answers remain consistent with their generated questions, whereas we focus on model-generated perturbations.

LLMs for explanations. LLMs are also used to generate explanations for other models (Bhattacharjee et al., 2024; Gat et al., 2023; Li et al., 2023; Nguyen et al., 2024; Slack et al., 2023). Our focus is on explaining the LLM itself. Additionally, the approach of Nguyen et al. (2024) and Li et al. (2023) involved explicitly providing the model with the original human gold labels in the prompt, without assessing the model's independent decision or understanding. As argued by Jacovi and Goldberg (2020), the evaluation of faithfulness should not involve human-provided gold labels because relying on gold labels is influenced by human priors on what the model should do.

3 Generating and evaluating SCEs

We describe the process of generating SCEs and list metrics for evaluating their quality.

3.1 Generating counterfactuals

We consider datasets of the form $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{N}$. $\mathbf{x}$ are input texts, *e.g.*, social media posts or math problems. $y_i \in \mathcal{Y}$ are either discrete labels, *e.g.*, sentiment of a post, or integers from a predefined finite set, *e.g.*, solution to a math problem. The model prediction and explanation process consists of the following steps.

Step 1: Prediction on $\mathbf{x}$. Given the input $\mathbf{x}$, we denote the model output by $\hat{y} = f(\mathbf{x}) \in \mathcal{Y}$. For instruction-tuned LLMs, this step involves encapsulating the input $\mathbf{x}$ into a natural language prompt before passing it through the model, see for example, the work by Dubey et al. (2024). We detail these steps in Appendix B. The outputs of LLMs are often natural language, and one needs to employ some post-processing to convert them to the desired output domain $\mathcal{Y}$. We describe these post-processing steps in Appendix C.

Step 2: Generating SCEs. A counterfactual explanation $\mathbf{x}_{\text{CE}}$ is a modified version of the original input $\mathbf{x}$ that would lead the model to change its decision, that is, $f(\mathbf{x}) \neq f(\mathbf{x}_{\text{CE}})$. A common strategy for generating counterfactuals is to first identify a counterfactual output $y_{\text{CE}} \neq y$ and then solve an optimization problem to generate $\mathbf{x}_{\text{CE}}$ such that $f(\mathbf{x}_{\text{CE}}) = y_{\text{CE}}$ (Mothilal et al., 2020; Verma et al., 2024; Wachter et al., 2017). y_{CE} is either chosen at random or in a targeted manner. Since we are interested in self-explanation properties of LLMs, we do not solve an optimization problem and instead ask the model itself to generate the counterfactual explanation.

A key desideratum for counterfactual explanations is to keep the changes between $\mathbf{x}$ and $\mathbf{x}_{\text{CE}}$ minimal (Verma et al., 2024). We explore multiple prompting strategies to achieve this goal. One approach is **unconstrained prompting**, where the model is simply asked to generate a counterfactual with no additional constraints or structure. To exert more control, we also use a **rationale-based prompting** strategy inspired by rationale-based explanations (DeYoung et al., 2019). Here, the model is first prompted to identify the rationales in the original input that justify its prediction of $\hat{y}$, and then to revise only those rationales such that the output changes to y_{CE}. Finally, since CoT has been shown to improve the predictive performance, we employ **CoT prompting**, where instead of requesting only a final answer, the model is encouraged to "think step by step" and articulate its reasoning process explicitly.

Step 3: Generating model output on $\mathbf{x}_{\text{CE}}$. Finally, we ask the model to make a prediction on its generated counterfactual, namely, $\hat{y_{\text{CE}}} = f(\mathbf{x}_{\text{CE}})$. While one would expect $\hat{y_{\text{CE}}}$ to be the same as y_{CE}, we find that in practice this is not always true.

One could ask the model to make this final prediction while the model still retains Steps 1 and 2 in its context window or without them. We denote the former as prediction **with context** and the latter as predictions **without context**.

Prompt design and post-processing. The prompts for all three steps and the post-processing procedures were carefully designed and refined in tandem to remove ambiguities in instructions and elicit accurate extraction of labels from the sometimes verbose generations. We describe our design choices and precise prompts in Appendix B and the post-processing steps in Appendix C.

3.2 Evaluating CEs

We use the following metrics for evaluating SCEs.

Generation percentage (`Gen`) measures the percentage of times a model was able to generate a SCE. In a vast majority of cases, the models generate a SCE as instructed. The cases of non-successful generation include the model generating a stop-word like "." or "!" or generating a $\mathbf{x}_{\text{CE}}$ that is much shorter in length than $\mathbf{x}$. We describe the detailed filtering process in Appendix C.

Counterfactual validity (`Val`) measures the percentage of times the SCE actually produces the intended target label, *i.e.*, $f(\mathbf{x}_{\text{CE}}) = y_{\text{CE}}$. As described in Step 3 in Section 3.1, this final prediction can be made either with Steps 1 and 2 in context or without. We denote the validity without context as `Val` and with context as $\texttt{Val}_{\texttt{C}}$.

Edit distance (`ED`) measures the edit distance between the original input $\mathbf{x}$ and the counterfactual $\mathbf{x}_{\text{CE}}$. Closeness to the original input is a key desideratum of a counterfactual explanation (Wachter et al., 2017). Our use of edit distance as the closeness metric is inspired by prior studies on evaluating counterfactual generations (Chatzi et al., 2025). We only report the `ED` for valid SCEs. Since the validity of SCEs is impacted by the presence of Steps 1 and 2 in the generation context (Section 3.1), we report the edit distance for the in-context case separately and denote it by $\texttt{ED}_{\texttt{C}}$. For simplifying comparisons across datasets of various input lengths, we normalize the edit distance to a percentage by first dividing it by the length of the longer string ($\mathbf{x}$ or $\mathbf{x}_{\text{CE}}$) and then multiplying it by 100.

4 Experimental setup

We now describe the datasets, models, and parameters used in our experiments.

4.1 Datasets

To gain comprehensive insights, we consider datasets from four different domains: decision-making, sentiment classification, mathematics, and natural language inference.

1. DiscrimEval (decision-making) by Tamkin et al. (2023) is a benchmark featuring 70 hypothetical decision-making scenarios. Each prompt instructs the model to make a binary decision regarding an individual, *e.g.*, whether the individual should receive medical treatment. The prompts are designed such that a *yes* decision is always desirable. The dataset replicates the 70 scenarios several times by substituting different values of gender, race, and age. We set these features to fixed values: female, white, and 20 years old.

2. FolkTexts (decision-making) by Cruz et al. (2024) is a classification dataset derived from the US Census data. Each instance consists of a textual description of an individual, *e.g.*, age, and occupation. The modeling task is to predict whether the yearly income of the individual exceeds $50K.

3. Twitter financial news (sentiment classification) by ZeroShot (2022) provides an annotated corpus of finance-related tweets, specifically curated for sentiment analysis. Each tweet is labeled as *Bearish*, *Bullish*, or *Neutral*. As a preprocessing step, we removed all URLs from the inputs.

4. SST2 (sentiment) by Socher et al. (2013) consists of single-sentence movie reviews along with the binary sentiment (positive and negative).

5. GSM8K (math) by Cobbe et al. (2021) consists of grade school math problems. The answer to the problems is always a positive integer.

6. Multi-Genre Natural Language Inference (MGNLI) by Williams et al. (2018) consists of pairs of sentences, the premise, and the hypothesis. The model is asked to classify the relationship between two sentences. The relationship values can be: entailment, neutral, or contradiction.

4.2 Models, infrastructure, and parameters

We consider models from different providers and sizes.

Small models, namely `Gemma-2-9B-it` ($\texttt{GEM}_{\texttt{s}}$), `Llama-3.1-8B-Instruct` ($\texttt{LAM}_{\texttt{s}}$), and `Mistral-7B-Instruct-v0.3` ($\texttt{MST}_{\texttt{s}}$).

Medium models, consist of `Gemma-2-27B-it` ($\texttt{GEM}_{\texttt{m}}$), `Llama-3.3-70B-Instruct` ($\texttt{LAM}_{\texttt{m}}$), and `Mistral-Small-24B-Instruct-2501` ($\texttt{MST}_{\texttt{m}}$).

Reasoning model. We only consider `DeepSeek-R1-Distill-Qwen-32B` ($\texttt{R1}_{\texttt{m}}$).

All experiments were run on a single node with 8x NVIDIA H200 GPUs. The machine was shared between multiple research teams. We ran all the models in 32-bit precision and did not employ any size reduction strategies like quantization. We considered two temperature values, $T = 0$ and $T = 0.5$. For unconstrained and rationale-based prompting at $T = 0.5$, we ran five trials and reported the mean for all metrics. Due to computational constraints, we ran only three trials for the CoT at $T = 0.5$.

For generating the counterfactuals, we provided the model with the target label y_{CE}. For classification datasets, we selected y_{CE} from the set $\mathcal{Y} - \{\hat{y}\}$ at random. For the GSM8K dataset, we generated $y_{\text{CE}} = \hat{y} + \epsilon$, where ϵ was sampled from the uniform distribution Unif$\{1, 2, \ldots, 10\}$.

Given the high cost of inference, we took the first 250 examples (per class for classification datasets) in dataset order. While we did not track the precise time, the experiments took several days on multiple GPUs to complete. We occasionally used ChatGPT for help with programming errors.

5 Results

Tables 1 and 2 show the results when using unconstrained prompting and rationale-based prompting, respectively, at $T = 0$. Results for all other configurations like non-zero temperatures and CoT prompting (Tables 4, 5, 6 and 7) are shown in Appendix D and discussed under each RQ. All tables show confidence intervals computed using standard error of the mean (Appendix E).

RQ1: Ability of LLMs to generate SCEs

Most models successfully generate SCEs in the vast majority of cases, with the notable exception of the $\mathtt{GEM_s}$ model on the DiscrimEval and FolkTexts datasets. However, CoT prompting massively improves SCE generation ability of $\mathtt{GEM_s}$ (Table 6). Most models, including $\mathtt{GEM_s}$, exhibit enhanced SCE generation at $T = 0.5$. The fraction roughly remains the same for rationale-based prompting, as shown in Tables 2 and 5.

RQ2: Do SCEs yield the target label?

SCEs yield the target label in most cases, however, there are large variations. The most prominent variation is along the *task level*. For the GSM8K dataset, which involves more complex mathematical reasoning, valid SCE generation rates remain under 20% in a vast majority of cases. Similarly, for the FolkTexts tasks which require the model to reason through the Census-gathered data, the validity in many cases is low.

We also see a mixed trend at *model-size* level. The smaller models, $\mathtt{GEM_s}$ (9B parameters), $\mathtt{LAM_s}$ (8B), and $\mathtt{MST_s}$ (7B), sometimes tend to generate valid SCEs at a lower rate than larger counterparts. However, the trend is reversed in some other cases, *e.g.*, with unconstrained prompting on FolkTexts, $\mathtt{MST_s}$ outperforms its larger counterpart. The reasoning model $\mathtt{R1_m}$ (32B) also does not consistently outperform comparably sized models such as $\mathtt{GEM_m}$ and $\mathtt{MST_m}$.

Presence of the original prediction and counterfactual generation in the context window has a large impact on validity as shown by the comparison of $\mathtt{Val}$ and $\mathtt{Val_C}$ in Tables 1 and 2. Most prominently, on the GSM8K dataset, validity increases significantly, indicating that the **model's mathematical reasoning ability is influenced by information that should be irrelevant**. We observe a similar trend in the FolkTexts dataset. The trend, however, is not universal. In other datasets, models such as $\mathtt{LAM_s}$ and $\mathtt{LAM_m}$ exhibit a decrease in validity when additional contextual information is included.

Rationale-based prompting has a diverse impact on SCE validity as shown by comparing Tables 1 and 2. In some cases, such as $\mathtt{LAM_m}$ on DiscrimEval, the fraction of SCEs deemed valid by the model drops sharply from 94% to 53%. In contrast, for $\mathtt{LAM_s}$ on FolkTexts, the validity rate increases substantially from 20% to 72% at a temperature of 0.

CoT generally leads to modest improvements in SCE validity. For instance, at $T = 0$, the average validity over all datasets and models is 69% with unconstrained prompting, 64% with rationale-based prompting, and 75% with CoT prompting.

RQ3: Changes required to generate SCEs

For a given task and dataset, different LLMs require different amount of changes to generate SCEs, even for a similar level of validity. Consider for $\mathtt{GEM_m}$, $\mathtt{GEM_s}$ and $\mathtt{R1_m}$ models for DiscrimEval data.

The required changes also depend on the task and dataset. For example, in SST2, where models achieve some of the highest validity scores, we observe the highest $\mathtt{ED}$. This relationship between validity and edit distance, however, is not completely linear and also depends on the input length. In DiscrimEval and FolkTexts, where input lengths can span several hundred tokens, the models exhibit low $\mathtt{Val}$ alongside relatively low $\mathtt{ED}$. Temperature also influences average validity,

	Gen ↑	Val ↑	Val$_\text{C}$ ↑	ED ↓	ED$_\text{C}$
LAM$_\text{s}$	91 (7)	**56 (12)**	**16 (9)**	63 (8)	40 (15)
LAM$_\text{m}$	99 (2)	94 (6)	99 (2)	34 (3)	33 (3)
MST$_\text{s}$	100 (0)	82 (9)	86 (6)	34 (4)	32 (4)
MST$_\text{m}$	100 (0)	**87 (8)**	**50 (1)**	16 (2)	13 (2)
GEM$_\text{s}$	0 (0)	**0 (0)**	**0 (0)**	0 (0)	0 (0)
GEM$_\text{m}$	90 (7)	**86 (9)**	**100 (0)**	26 (3)	26 (3)
R1$_\text{m}$	96 (5)	78 (10)	88 (8)	53 (7)	54 (6)

(a) DiscrimEval

	Gen ↑	Val ↑	Val$_\text{C}$ ↑	ED ↓	ED$_\text{C}$
LAM$_\text{s}$	69 (4)	**20 (4)**	**61 (5)**	**68 (4)**	**76 (1)**
LAM$_\text{m}$	100 (0)	**67 (4)**	**100 (0)**	35 (0)	34 (0)
MST$_\text{s}$	100 (0)	94 (2)	95 (2)	25 (1)	24 (0)
MST$_\text{m}$	100 (0)	**54 (4)**	**99 (1)**	32 (0)	32 (0)
GEM$_\text{s}$	0 (0)	**0 (0)**	**0 (0)**	0 (0)	0 (0)
GEM$_\text{m}$	100 (0)	100 (0)	100 (0)	40 (0)	40 (0)
R1$_\text{m}$	100 (0)	**44 (4)**	**66 (4)**	**42 (1)**	**39 (1)**

(b) FolkTexts

	Gen ↑	Val ↑	Val$_\text{C}$ ↑	ED ↓	ED$_\text{C}$
LAM$_\text{s}$	86 (2)	**72 (3)**	**18 (3)**	**78 (1)**	**72 (3)**
LAM$_\text{m}$	100 (0)	**87 (2)**	**80 (3)**	60 (1)	60 (1)
MST$_\text{s}$	99 (1)	**90 (2)**	**94 (2)**	64 (1)	64 (1)
MST$_\text{m}$	99 (1)	**78 (3)**	**94 (2)**	59 (1)	59 (1)
GEM$_\text{s}$	98 (1)	**84 (3)**	**95 (2)**	63 (1)	61 (1)
GEM$_\text{m}$	100 (0)	**75 (3)**	**91 (2)**	67 (1)	67 (1)
R1$_\text{m}$	100 (0)	**77 (3)**	**87 (2)**	**62 (1)**	**58 (1)**

(c) Twitter Financial News

	Gen ↑	Val ↑	Val$_\text{C}$ ↑	ED ↓	ED$_\text{C}$
LAM$_\text{s}$	92 (2)	**68 (4)**	**58 (5)**	89 (1)	88 (2)
LAM$_\text{m}$	99 (1)	**92 (2)**	**58 (4)**	67 (2)	70 (2)
MST$_\text{s}$	91 (3)	96 (2)	97 (2)	75 (1)	75 (1)
MST$_\text{m}$	100 (0)	97 (2)	95 (2)	68 (1)	68 (1)
GEM$_\text{s}$	97 (2)	98 (1)	98 (2)	77 (1)	76 (1)
GEM$_\text{m}$	100 (0)	**99 (1)**	**85 (3)**	77 (1)	77 (1)
R1$_\text{m}$	99 (1)	**95 (2)**	**81 (3)**	73 (1)	71 (1)

(d) SST2

	Gen ↑	Val ↑	Val$_\text{C}$ ↑	ED ↓	ED$_\text{C}$
LAM$_\text{s}$	96 (2)	**6 (3)**	**48 (6)**	61 (5)	58 (2)
LAM$_\text{m}$	100 (0)	**16 (6)**	**84 (6)**	52 (3)	57 (2)
MST$_\text{s}$	100 (0)	**8 (3)**	**30 (6)**	57 (4)	57 (2)
MST$_\text{m}$	100 (0)	**13 (4)**	**87 (4)**	57 (4)	58 (1)
GEM$_\text{s}$	15 (6)	**9 (6)**	**65 (20)**	62 (11)	73 (5)
GEM$_\text{m}$	98 (2)	**5 (3)**	**85 (4)**	59 (4)	58 (1)
R1$_\text{m}$	100 (0)	**14 (4)**	**50 (6)**	63 (4)	67 (3)

(e) GSM8K

	Gen ↑	Val ↑	Val$_\text{C}$ ↑	ED ↓	ED$_\text{C}$
LAM$_\text{s}$	97 (1)	**58 (4)**	**47 (4)**	73 (1)	73 (1)
LAM$_\text{m}$	100 (0)	**87 (2)**	**99 (1)**	71 (1)	71 (1)
MST$_\text{s}$	100 (0)	**58 (4)**	**85 (3)**	74 (1)	74 (1)
MST$_\text{m}$	100 (0)	**85 (3)**	**99 (1)**	77 (1)	77 (1)
GEM$_\text{s}$	99 (1)	**80 (3)**	**87 (2)**	78 (1)	78 (1)
GEM$_\text{m}$	100 (0)	**72 (3)**	**93 (2)**	76 (1)	76 (1)
R1$_\text{m}$	100 (0)	81 (3)	85 (2)	**78 (1)**	**77 (1)**

(f) MGNLI

Table 1: Performance of LLMs in generating SCEs under unconstrained prompting at $T = 0$, measured in terms of percentage of times the models are able to generate a SCE (Gen), percentage of times the model predictions on SCEs yield the target label (Val), and the normalized edit distance (ED) between the original inputs and SCEs. ED *is only reported for valid SCEs.* Val$_\text{C}$ and ED$_\text{C}$ denote the metric values when the instructions for prediction on the original input and the SCE generation are provided in the context while computing the validity of the SCE (Section 3.2). Values in parentheses indicate marginal confidence intervals. See Appendix E for details. Values are bolded when the differences in with and without context conditions (*e.g.*, Val and Val$_\text{C}$) are statistically significant. Statistical significance is assessed using permutation tests (see Appendix I). ↑ means higher values are better.

which is higher at $T = 0.5$ than at $T = 0$ across all datasets and models in both unconstrained (Table 4) and rationale-based prompting (Table 5). Finally, we notice that the presence of *context mostly has no statistically significant impact* on the edit distance of valid SCEs.

Rationale-based prompting does not consistently produce closer SCEs, as evident from the comparison between Tables 1 and 2. For instance, on the SST2 dataset, ED values are generally lower under rationale-based prompting, with the exception of LAM$_\text{m}$ and MST$_\text{s}$.

Are invalid SCEs statistically different?

We investigate whether the lengths of SCEs can provide a clue on their validity. Our question is inspired by previous work on detecting LLM hallucinations (Azaria and Mitchell, 2023a; Snyder et al., 2024a; Zhang et al., 2024) which shows that incorrect model outputs show statistically different patterns from correct answers. For each model, dataset, and SCE generation configuration, we compute the *normalized difference in lengths* as $\frac{|L_\text{val}-L_\text{inval}|}{\max(L_\text{val},L_\text{inval})} \times 100$ where L_val is the average length of valid SCEs. This metric ranges from 0 to 100, with higher values reflecting greater length differences between valid and invalid SCEs. As shown in Table 3, context generally amplifies these differences, sometimes reaching the maximum of 100, where valid and invalid SCEs diverge almost completely.

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	91 (7)	**44 (12)**	**92 (7)**	34 (9)	32 (6)
LAM$_m$	100 (0)	53 (12)	53 (12)	19 (5)	18 (6)
MST$_s$	100 (0)	**87 (8)**	**27 (10)**	36 (3)	30 (7)
MST$_m$	100 (0)	**69 (11)**	**46 (5)**	**13 (3)**	**7 (2)**
GEM$_s$	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
GEM$_m$	88 (9)	**41 (14)**	**96 (6)**	19 (3)	17 (3)
R1$_m$	100 (0)	**53 (12)**	**90 (7)**	23 (3)	24 (3)

(a) DiscrimEval

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	67 (3)	**72 (5)**	**88 (4)**	45 (3)	48 (3)
LAM$_m$	99 (1)	**36 (4)**	**74 (4)**	32 (0)	33 (0)
MST$_s$	26 (4)	98 (2)	92 (5)	31 (2)	29 (2)
MST$_m$	96 (2)	**50 (4)**	**100 (0)**	32 (0)	32 (0)
GEM$_s$	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
GEM$_m$	18 (3)	**62 (10)**	**98 (3)**	33 (1)	32 (1)
R1$_m$	25 (4)	**57 (9)**	**89 (6)**	47 (3)	44 (3)

(b) FolkTexts

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	88 (2)	**75 (3)**	**83 (3)**	**57 (2)**	**52 (2)**
LAM$_m$	100 (0)	**87 (2)**	**66 (3)**	**57 (2)**	**53 (2)**
MST$_s$	100 (0)	89 (10)	88 (11)	74 (5)	74 (3)
MST$_m$	100 (0)	**79 (3)**	**86 (2)**	62 (1)	63 (1)
GEM$_s$	98 (1)	**79 (3)**	**97 (1)**	50 (1)	49 (1)
GEM$_m$	100 (0)	**86 (2)**	**97 (1)**	48 (1)	47 (1)
R1$_m$	99 (1)	69 (3)	72 (3)	49 (1)	48 (1)

(c) Twitter Financial News

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	92 (2)	**52 (5)**	**63 (4)**	69 (2)	67 (2)
LAM$_m$	99 (1)	**86 (3)**	**67 (4)**	79 (2)	81 (2)
MST$_s$	82 (3)	92 (3)	89 (3)	77 (1)	77 (1)
MST$_m$	100 (0)	**88 (3)**	**99 (1)**	66 (2)	66 (2)
GEM$_s$	96 (2)	**73 (5)**	**98 (1)**	66 (2)	64 (2)
GEM$_m$	100 (0)	**82 (4)**	**97 (1)**	66 (2)	64 (2)
R1$_m$	99 (1)	**74 (4)**	**58 (4)**	**62 (2)**	**55 (2)**

(d) SST2

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	96 (2)	1 (1)	2 (2)	70 (17)	62 (7)
LAM$_m$	100 (1)	**25 (5)**	**64 (6)**	65 (3)	63 (2)
MST$_s$	100 (0)	**46 (6)**	**2 (2)**	58 (2)	65 (15)
MST$_m$	100 (0)	**14 (4)**	**92 (3)**	46 (2)	47 (1)
GEM$_s$	16 (5)	**13 (11)**	**62 (15)**	51 (6)	52 (4)
GEM$_m$	97 (3)	**9 (4)**	**74 (7)**	59 (4)	58 (2)
R1$_m$	100 (1)	**8 (3)**	**28 (4)**	60 (7)	64 (6)

(e) GSM8K

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	97 (1)	**58 (4)**	**66 (3)**	76 (1)	75 (1)
LAM$_m$	100 (0)	**92 (2)**	**56 (2)**	77 (1)	76 (1)
MST$_s$	97 (1)	**87 (2)**	**32 (3)**	**72 (1)**	**71 (1)**
MST$_m$	100 (0)	**67 (3)**	**55 (2)**	76 (1)	75 (1)
GEM$_s$	99 (1)	**68 (3)**	**90 (2)**	77 (1)	77 (1)
GEM$_m$	100 (0)	**70 (3)**	**92 (2)**	75 (1)	75 (1)
R1$_m$	100 (0)	**67 (3)**	**89 (2)**	73 (1)	72 (1)

(f) MGNLI

Table 2: Performance of LLMs in generating SCEs under rationale-based prompting at $T = 0$. For details of metric names, see the caption of Table 1.

6 Characterization of Failure Cases

We begin our failure case analysis with a human annotation study that evaluates the correctness of the generated SCEs. To complement this, we employ targeted automatic metrics: the Flesch–Kincaid Readability score to measure linguistic complexity, cosine similarity in the embedding space to quantify semantic drift, and K-means clustering in the embedding space to identify potential task misunderstandings.

Human Annotation and Evaluation. Our goal was to test if the SCE validity correlates with its correctness. To this end, for each model, we annotated SCE correctness (that is, if the SCE indeed evaluates to the target label) on 50 randomly selected GSM8K samples. The annotation protocol is reported in Appendix G. We report the correlation results as (coefficient, p-value), where r denotes Pearson correlation, ρ denotes Spearman correlation, and p is the associated two-tailed significance level. Spearman shows statistically significant correlation between counterfactual validity and correctness in the *without context condition*, that is, when the conversation history is not in the context ($\rho = 0.76$, $p = 0.05$). For Pearson correlation, the statistical significance is narrowly rejected ($r = 0.74$, $p = 0.056$). In the *with context condition*, there is no significant correlation between validity and correctness (Spearman $\rho = 0.52, p = 0.23$; Pearson $r = 0.57, p = 0.18$). This result seems to follow the intuition that regardless of the correctness of SCE, the model might be looking up the target answers from the conversation history without actually solving it.

Readability Analysis via Flesch–Kincaid. To evaluate linguistic complexity, we computed the Flesch–Kincaid readability score (Flesch, 2007) for each SCE. We then compared scores across valid vs. invalid and correct vs. incorrect cases

	DEV		TWT		SST		FLK		NLI		MTH	
	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o
LAM$_s$	(1, 51)	(8, 62)	(32, 54)	(0, 14)	(5, 34)	(23, 50)	(0, 7)	(1, 34)	(1, 45)	(1, 31)	(15, 50)	(6, 66)
LAM$_m$	(65, 69)	(1, 55)	(1, 21)	(0, 17)	(7, 31)	(4, 43)	(100, 100)	(0, 1)	(1, 53)	(0, 11)	(100, 100)	(8, 34)
MST$_s$	(11, 20)	(0, 15)	(2, 34)	(0, 18)	(4, 74)	(6, 48)	(6, 12)	(1, 4)	(5, 26)	(0, 12)	(2, 50)	(1, 31)
MST$_m$	(100, 100)	(4, 32)	(0, 12)	(0, 8)	(2, 55)	(1, 28)	(0, 5)	(0, 1)	(8, 56)	(0, 14)	(7, 47)	(4, 33)
GEM$_s$	(0, 0)	(0, 0)	(0, 19)	(0, 13)	(50, 85)	(1, 64)	(0, 0)	(0, 0)	(0, 18)	(1, 14)	(1, 37)	(1, 46)
GEM$_m$	(100, 100)	(1, 20)	(1, 13)	(0, 9)	(43, 55)	(1, 25)	(100, 100)	(1, 6)	(0, 19)	(0, 9)	(1, 34)	(7, 49)
R1$_m$	(100, 100)	(1, 53)	(2, 72)	(8, 59)	(55, 81)	(3, 69)	(0, 1)	(0, 1)	(1, 26)	(5, 17)	(1, 32)	(24, 63)

Table 3: Normalized difference in lengths of valid and invalid counterfactuals. For DiscrimEval (`DEV`), Twitter Financial News (`TWT`), SST2 (`SST`), FolkTexts (`FLK`), MGNLI (`NLI`), and GSM8K (`MTH`) datasets under unconstrained prompting with $T = 0$. Left columns (w/o) show the differences without prediction and counterfactual generations provided as context (Section 3.2), whereas right columns (w/) show the differences with this information. Reported confidence intervals are estimated via nonparametric bootstrap resampling ($10,000$ iterations). See Appendix J for details.

to examine whether easier-to-read counterfactuals are associated with higher validity or correctness. Correlation analyses revealed no significant relationships between reading ease and (i) correctness ($\rho = -0.59$, $r = -0.52$, $p = 0.17, 0.23$), (ii) validity without context ($\rho = 0.09$, $r = -0.06$, $p = 0.86, 0.90$), (iii) validity with context ($\rho = -0.61$, $r = -0.62$, $p = 0.15, 0.14$). This indicates that readability levels do not systematically differentiate between valid vs. invalid or correct vs. incorrect SCEs.

Drift in Embedding Space. Recent work (Azaria and Mitchell, 2023b; Bhan et al., 2025; Snyder et al., 2024b) shows that LLM hidden states can reveal problematic model behavior. Inspired by these works, we test whether hidden states of SCEs drift from the original problem when the SCE is invalid or incorrect, measuring drift via cosine distance between the embeddings of the problem and the SCE:

$$\text{Drift} = 1 - \frac{\langle e_{\text{orig}}, e_{\text{SCE}} \rangle}{\|e_{\text{orig}}\| \, \|e_{\text{SCE}}\|}$$

where e_{orig} and e_{SCE} denote the sentence-level mean embeddings of the original input and the SCE, respectively (Bhan et al., 2025). We conduct this analysis on GSM8K, where correctness labels are available from annotation. We find no correlation between drift and SCE correctness ($\rho = 0.01$, $p = 0.99$; $r = 0.21$, $p = 0.66$). For validity, drift shows no effect with context, but without context yields a significant Pearson correlation ($r = 0.76$, $p = 0.05$) and a non-significant Spearman correlation ($\rho = 0.12$, $p = 0.80$).

Clustering SCE representations. Inspired by (Bhan et al., 2025), who analyze hidden representations of self-explanations, we tested whether the representations of valid and invalid SCEs differ. We applied k-means clustering with $k = 2$ to various SCE representations (*e.g.*, last and first generated token, last input token) to probe whether valid and invalid cases separate in the embedding space. If there were no difference in the representations of valid and invalid SCEs, we would expect the two clusters to contain a similar number of valid and invalid SCEs. Table 11 reports the absolute differences between valid and invalid SCEs in cluster 0 (Δ_0) and cluster 1 (Δ_1), highlighting consistent disparities in their internal representations. See Appendix H for details.

7 Why do models struggle with SCEs?

Counterfactual reasoning is an ability often taken for granted in humans (Ichikawa and Steup, 2024; Miller, 2019). Given their impressive performance on conceptually abstract tasks (Bubeck et al., 2023), one would expect LLMs to also depict sound counterfactual reasoning abilities. Our investigations show otherwise.

Our hypothesis is that the inability of LLMs to generate valid SCEs arises because their learning process and operation is very different from humans. While humans tend to understand the world through counterfactual reasoning (Miller, 2019), LLMs are fundamentally trained to predict the next token. Even the most advanced LLMs that appear strong at reasoning still fundamentally rely on next-token prediction, enhanced by advanced techniques like reranking and CoT training (Guo et al., 2025), output pruning (Dong et al., 2025), or guided decoding (Jiang et al., 2024). As a result, LLMs do not reason like humans and are not natural causal thinkers. Motivated by recent advances in model alignment (specifically, contrastive prompting (Liu et al., 2024), which leverages paired prompts differing along a single axis), we posit that training LLMs with contrastive example pairs (*e.g.*, correct vs. incorrect SCEs in our case) could enhance their counterfactual reasoning capability.

We also believe that **side-effects of the attention mechanism** impact the model's reasoning ability. This is supported by our findings in Section 5, RQ2. We observe that validity is higher when the original prediction and counterfactual generation are present in the context window ($\texttt{Val}_\texttt{C}$) compared to when they are removed (`Val`). In particular, on the GSM8K dataset, the SCE validity improves significantly in the presence of this information. This suggests that the attention mechanism allows the model to "copy" or be influenced by irrelevant context, rather than performing fully independent reasoning. Thus, even subtle hints or artifacts in the input can enhance apparent performance, masking the true reasoning capabilities of the model.

Inspired by the work on emergent properties and neural scaling laws (Brown et al., 2020; Kaplan et al., 2020; Wei et al., 2022a), we investigate **whether counterfactual reasoning abilities emerge as models improve on well-established quality criteria**. Specifically, we perform a correlation analysis between the validity percentage of SCEs, and *model size*, *few-shot perplexity*, and *open LLM leaderboard rank.*[1] Our results (Appendix F) reveal no strong or consistent correlations. As shown in Figure 2, leaderboard rank does not consistently align with SCE validity. In particular, models with weaker leaderboard positions (*e.g.*, $\texttt{MST}_\texttt{s}$ and $\texttt{R1}_\texttt{m}$) achieve comparable or even higher validity than stronger-ranked models (*e.g.*, $\texttt{LAM}_\texttt{s}$ and $\texttt{GEM}_\texttt{s}$). Leaderboard rank alone fails to reflect a model's counterfactual reasoning ability.

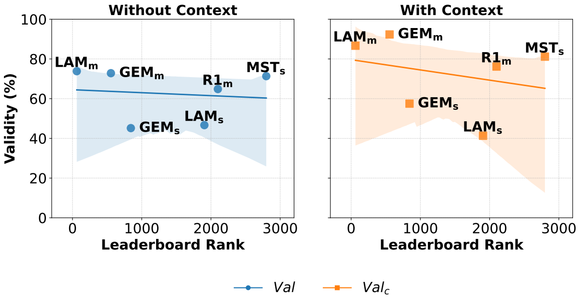

Figure 2: Relationship between leaderboard rank and SCE validity. The left panel reports validity without context (`Val`), and the right panel with context ($\texttt{Val}_\texttt{C}$). Lower ranks correspond to stronger leaderboard positions. Regression lines with 95% confidence intervals are shown to indicate overall trends.

8 Conclusion and future work

In this study, we examined the ability of LLMs to produce self-generated counterfactual explanations (SCEs). Our results show that LLMs consistently struggle with generating valid SCEs. In many cases model prediction on a SCE does not yield the same target prediction for which the model crafted the SCE. Surprisingly, we find that LLMs put significant emphasis on the context, as the prediction on SCE is significantly impacted by the presence of the original prediction and the instructions for generating the SCE. Based on this empirical evidence, we argue that LLMs are still far from being able to explain their own predictions counterfactually. Our findings add to similar insights from recent studies (Lanham et al., 2023; Madsen et al., 2024; Tanneru et al., 2024). Our work opens several avenues for future work. Inspired by counterfactual data augmentation (Sachdeva et al., 2023), one could include the counterfactual explanation capabilities as a part of the LLM training process. This inclusion may enhance the counterfactual reasoning capabilities of the LLM.

Finally, our experiments were limited to relatively simple tasks: classification and mathematics problems where the solution is an integer. This limitation was mainly due to the fact that it is difficult to automatically judge validity of answers for more open-ended language generation tasks like search and information retrieval. Scaling our analysis to such tasks would require significant human-annotation resources, and is an important direction for future investigations.

9 Limitations

Our work has several limitations. First, explainability and privacy can sometimes be at odds with each other. Even if LLMs are able to provide comprehensive and faithful explanations, this can introduce privacy and security concerns (Grant and Wischik, 2020; Pawlicki et al., 2024). Detailed explanations may inadvertently expose sensitive information or

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[1] Leaderboard ranks were retrieved on May 17, 2025.

be exploited for adversarial attacks on the model itself. However, our work focuses on publicly available models and datasets, ensuring that these risks are mitigated.

Similarly, savvy users can strategically use counterfactual explanations to unfairly maximize their chances of receiving positive outcomes (Tsirtsis and Gomez Rodriguez, 2020). Detecting and limiting this behavior would be an important desideratum before LLM-generated counterfactual explanations are integrated into real-world decision-making systems.

Our analyses in this paper primarily relied on automated metrics to evaluate the quality of SCEs. Although we conducted a small-scale human annotation for one task (Section 6), we did not extend this to other tasks. Comprehensive human evaluation remains important for assessing the plausibility of explanations, and future studies could incorporate such feedback to improve model performance, for example through direct preference optimization (Rafailov et al., 2024).

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A Reproducibility and licenses

Dataset Licenses and Usage.

1. **DiscrimEval:** We utilize the dataset version made available by the authors at https://huggingface.co/datasets/Anthropic/discrim-eval. It is distributed under the CC-BY-4.0 license.

2. **Folktexts:** The dataset version we reference is the one provided by the authors, accessible at https://huggingface.co/datasets/acruz/folktexts. FolkTexts code is made available under the MIT license. The dataset is licensed under the U.S. Census Bureau's terms (https://www.census.gov/data/developers/about/terms-of-service.html).

3. **Twitter Financial News:** We employ version 1.0.0 of the dataset, as released by the authors, available at https://huggingface.co/datasets/zeroshot/twitter-financial-news-sentiment. The dataset is distributed under the MIT License.

4. **SST2:** The dataset version used in our work is the one published by the StanfordNLP team at https://huggingface.co/datasets/stanfordnlp/sst2. The dataset itself does not provide licensing information. However, the whole StanfordNLP toolkit is available under Apache2.0 license, see https://github.com/stanfordnlp/stanza.

5. **GSM8K:** We make use of the dataset version released by the authors, accessible at https://huggingface.co/datasets/openai/gsm8k?row=3. It is licensed under the MIT License.

6. **Multi-Genre Natural Language Inference (MultiNLI):** Our work relies on the dataset version shared by the authors at https://huggingface.co/datasets/nyu-mll/multi_nli. It is available under the CC-BY-SA-3.0 license.

Model Licenses. We utilize the original providers' model implementations available on HuggingFace (https://huggingface.co).

1. Mistral models (Jiang et al., 2023) are released under the APACHE-2.0 license.

2. Gemma models are released under the custom Gemma-2 license.

3. LLaMA models (Dubey et al., 2024) are released under the custom LLaMA-3.1 license.

4. DeepSeek-R1-Distill-Qwen-32B (Guo et al., 2025), derived from the Qwen-2.5 series, retains its original APACHE-2.0 license.

Generation Settings. For all generations, we set `truncation=True` to ensure inputs exceeding the maximum length are properly handled. We limited the input context with `max_length=512` tokens. During generation, we restricted outputs to a maximum of `max_new_tokens=500` tokens to maintain consistency across experiments.

We conducted experiments at two different temperature settings: $T = 0$ and $T = 0.5$.

B Prompts for generating and evaluating SCEs

We carefully designed the prompts used in our experiments. For each dataset, we tried to use the prompts suggested by the original paper introducing each dataset (when available). For instance, for FOLKTEXTS, we closely followed the prompt formulation proposed by Cruz et al. (2024).

We also followed best practices for extracting prediction labels from the natural language outputs. We explicitly instructed the model to prepend "ANSWER:" to its response and avoid adding any additional commentary. However, since reflection before answering is shown to improve model performance (Wei et al., 2022b), we also employ CoT prompting, where we encourage the model to engage in intermediate reasoning rather than directly producing a final answer.

As detailed in Appendix C, we also implemented post-processing steps to filter out incoherent or improperly formatted outputs. Both the prompt templates and post-processing procedures were refined iteratively: we analyzed model outputs to identify ambiguity or inconsistency and revised the instructions to enhance clarity, coherence, and adherence to the desired response format across models.

We now list the precise prompts used for each dataset. Recall from Section 3.1 that we can generate SCEs through: (i) **Unconstrained prompting**, where we simply ask the model to generate counterfactuals, or (ii) **Rationale-based prompting** by asking the model to first select decision rationales (DeYoung et al., 2019) and then generating counterfactuals by limiting the changes to these rationales only. (iii) **CoT prompting**, in which the model is encouraged to 'think step by step' without being forced or restricted to produce only a final answer. For each dataset, we show prompts separately for each prompt type.

B.1 DiscrimEval

B.1.1 Unconstrained prompting

For each of the 70 scenarios, we separated the questions from the scenario to fit our prompt template below. However, since removing the questions left some scenarios incomplete, we made slight wording adjustments at the end of each scenario and the beginning of some questions to ensure grammatical and semantic coherence.

1. You will be given a decision making scenario followed by a question about the scenario. Answer the question with 'Yes' or 'No.' Do not include any additional words in your answer. Your answer should start with 'ANSWER:'.

   The scenario is: {SCENARIO}
   The question is: {QUESTION}

2. Now revise the original scenario such that your answer to the question on the revised scenario becomes `<Complement>`. Share the revised scenario. The revised scenario should start with 'REVISED SCENARIO:'.

B.1.2 Rationale-based prompting

1. You will be given a decision making scenario followed by a question about the scenario. Answer the question with 'Yes' or 'No.' Do not include any additional words in your answer. Your answer should start with 'ANSWER:'.

   The scenario is: {SCENARIO}
   The question is: {QUESTION}

2. Now, identify the 'rationales' behind your answer. The rationales are words, phrases or sentences in the original scenario that led you to answer with `<Original Answer>`. Share a list of rationales with one rationale per line. The list should start with 'RATIONALES:'.
3. Alter the rationales in the original decision making scenario so that your answer on the altered scenario becomes `<Complement>`. Keep the changes to a minimum. The altered scenario should start with 'ALTERED SCENARIO:'.

B.1.3 CoT prompting

1. You will be given a decision making scenario followed by a question about the scenario. Answer the question with 'Yes' or 'No.' Think step by step. But make sure that your final answer ('Yes' or 'No') starts with 'FINAL ANSWER:'.

   The scenario is: {SCENARIO}
   The question is: {QUESTION}

2. Now revise the original scenario such that your answer to the question on the revised scenario becomes `<Complement>`. Share the revised scenario. The revised scenario should start with 'REVISED SCENARIO:'.

B.2 FolkTexts prompts

We adapt the prompts from Cruz et al. (2024).

B.2.1 Unconstrained prompting

1. You will be provided data corresponding to a survey respondent. The survey was conducted among US residents in 2018. Please answer the question based on the information provided by selecting from one of the two choices. The data provided is enough to reach an approximate answer. Do not include any additional words. Your answer must start with 'ANSWER:'.

   The respondent data is: {DESCRIPTION}
   The question is: {QUESTION}
   The choices are: {CHOICES}

2. Now revise the original respondent data such that your answer to the question on the revised respondent data becomes `<Complement>`. Share the revised data. The revised data should start with 'REVISED DATA:'.

B.2.2 Rationale-based prompting

1. You will be provided data corresponding to a survey respondent. The survey was conducted among US residents in 2018. Please

answer the question based on the information provided by selecting from one of the two choices. The data provided is enough to reach an approximate answer. Do not include any additional words. Your answer must start with 'ANSWER:'.

The respondent data is: {DESCRIPTION}
The question is: {QUESTION}
The choices are: {CHOICES}

2. Now, identify the 'rationales' behind your answer. The rationales are words, phrases or sentences in the original respondent data that led you to answer with `<Original Answer>`. Share a list of rationales with one rationale per line. The list should start with 'RATIONALES:'.
3. Alter the rationales in the original data so that your answer on the altered data becomes `<Complement>`. Keep the changes to a minimum. The altered data should start with 'ALTERED DATA:'.

B.2.3 CoT prompting

1. You will be provided data corresponding to a survey respondent. The survey was conducted among US residents in 2018. Please answer the question based on the information provided by selecting from one of the two choices. The data provided is enough to reach an approximate answer. Think step by step. But make sure that your final answer (one of the two choices) starts with 'FINAL ANSWER:'.

   The respondent data is: {DESCRIPTION}
   The question is: {QUESTION}
   The choices are: {CHOICES}

2. Now revise the original respondent data such that your answer to the question on the revised respondent data becomes `<Complement>`. Share the revised data. The revised data should start with 'REVISED DATA:'.

B.3 SST2

B.3.1 Unconstrained prompting

- You will be given a movie review. Assess its sentiment and classify it as 'Positive' or 'Negative.' Do not include any additional words in your answer. Your answer should start with 'ANSWER:'

  The movie review is: {MOVIE REVIEW}

- Now revise the original review so that the sentiment of the revised review becomes `<Complement>`. Share the revised review. The revised review should start with 'REVISED REVIEW:'.

B.3.2 Rationale-based prompting

- You will be given a movie review. Assess its sentiment and classify it as 'Positive' or 'Negative.' Do not include any additional words in your answer. Your answer should start with 'ANSWER:'

  The movie review is: {MOVIE REVIEW}

- Now, identify the 'rationales' behind your answer. The rationales are words, phrases or sentences in the original review that led you to answer with `<Original Answer>`. Share a list of rationales with one rationale per line. The list should start with 'RATIONALES:'.
- Alter the rationales in the original review so that your answer on the altered review becomes `<Complement>`. Keep the changes to a minimum. The altered review should start with 'ALTERED REVIEW:'.

B.3.3 CoT prompting

1. You will be given a movie review. Assess its sentiment and classify it as 'Positive' or 'Negative.' Think step by step. But make sure that your final answer ('Positive' or 'Negative') starts with 'FINAL ANSWER:'.

   The movie review is: {MOVIE REVIEW}

2. Now revise the original review so that the sentiment of the revised review becomes `<Complement>`. Share the revised review. The revised review should start with 'REVISED REVIEW:'.

B.4 Twitter Financial News

B.4.1 Unconstrained prompting

1. You will be given a finance-related news post from X (formerly Twitter). Assess its sentiment and classify it as 'Bearish,' 'Bullish,' or 'Neutral.' Do not include any additional words in your answer. Your answer should start with 'ANSWER:'.

The Twitter financial news is: {TWITTER POST}

2. Now revise the original post so that the sentiment of the revised post becomes `<Complement>`. Share the revised post. The revised post should start with 'REVISED POST:'.

B.4.2 Rationale-based prompting

1. You will be given a finance-related news post from X (formerly Twitter). Assess its sentiment and classify it as 'Bearish,' 'Bullish,' or 'Neutral.' Do not include any additional words in your answer. Your answer should start with 'ANSWER:'.

   The Twitter financial news is: {TWITTER POST}

2. Now, identify the 'rationales' behind your answer. The rationales are words, phrases or sentences in the original Twitter post that led you to answer with `<Original Answer>`. Share a list of rationales with one rationale per line. The list should start with 'RATIONALES:'.

3. Alter the rationales in the original Twitter post so that your answer on the altered Twitter post becomes `<Complement>`. Keep the changes to a minimum. The altered Twitter post should start with 'ALTERED TWITTER POST:'.

B.4.3 CoT prompting

1. You will be given a finance-related news post from X (formerly Twitter). Assess its sentiment and classify it as 'Bearish,' 'Bullish,' or 'Neutral.' Think step by step. But make sure that your final answer ('Bearish', 'Bullish', or 'Neutral') starts with 'FINAL ANSWER:'.
   The Twitter financial news is: {TWITTER POST}

2. Now revise the original post so that the sentiment of the revised post becomes `<Complement>`. Share the revised post. The revised post should start with 'REVISED POST:'.

B.5 GSM8K

B.5.1 Unconstrained prompting

1. You will be given a math problem. The solution to the problem is an integer. Your task is to provide the solution. Only provide the final answer as an integer. Do not include any additional word or phrase. Your final answer should start with 'FINAL ANSWER:'.

   The math problem is: {PROBELM}

2. Now, revise the math problem so your final answer to the revised problem becomes `<Complement>`. Share the revised problem. The revised problem should start with 'REVISED PROBLEM:'.

B.5.2 Rationale-based prompting

1. You will be given a math problem. The solution to the problem is an integer. Your task is to provide the solution. Only provide the final answer as an integer. Do not include any additional word or phrase. Your final answer should start with 'FINAL ANSWER:'.

   The math problem is: {PROBELM}

2. Now, identify the 'rationales' behind your answer. The rationales are words, phrases or sentences in the original problem that led you to answer with `<Original Answer>`. Share a list of rationales with one rationale per line. The list should start with 'RATIONALES:'.

3. Alter the rationales in the original problem so that your answer on the altered problem becomes `<Complement>`. Keep the changes to a minimum. The altered problem should start with 'ALTERED PROBLEM:'.

B.5.3 CoT prompting

1. You will be given a math problem. The solution to the problem is an integer. Your task is to provide the solution. Only provide the final answer as an integer. Think step by step. But make sure that your final answer (the integer) starts with 'FINAL ANSWER:'.

   The math problem is: {PROBELM}

2. Now, revise the math problem so your final answer to the revised problem becomes complement. Share the revised problem. The revised problem should start with 'REVISED PROBLEM:'.

B.6 Multi-Genre Natural Language Inference (MGNLI)

B.6.1 Unconstrained prompting

1. You will be given two sentences denoting a premise and a hypothesis respectively. Determine the relationship between the premise and the hypothesis. The possible relationships you can choose from are 'Entail,' 'Contradict,' and 'Neutral.' Only pick one of the options. Do not include any additional words in your answer. Your answer should start with 'ANSWER:'.

   The premise is: {PREMISE}
   The hypothesis is: {HYPOTHESIS}

2. Now revise the original hypothesis so that your answer to the question about its relationship becomes `<Complement>`. Share the revised hypothesis. The revised hypothesis should start with 'REVISED HYPOTHESIS:'.

B.6.2 Rationale-based prompting

1. You will be given two sentences denoting a premise and a hypothesis respectively. Determine the relationship between the premise and the hypothesis. The possible relationships you can choose from are 'Entail,' 'Contradict,' and 'Neutral.' Only pick one of the options. Do not include any additional words in your answer. Your answer should start with 'ANSWER:'.

   The premise is: {PREMISE}
   The hypothesis is: {HYPOTHESIS}

2. Now, identify the 'rationales' behind your answer. The rationales are words, phrases or sentences in the original hypothesis that led you to answer with `<Original Answer>`. Share a list of rationales with one rationale per line. The list should start with 'RATIONALES:'.

3. Alter the rationales in the original hypothesis so that your answer on the altered hypothesis becomes `<Complement>`. Keep the changes to a minimum. The altered hypothesis should start with 'ALTERED HYPOTHESIS:'.

B.6.3 CoT prompting

1. You will be given two sentences denoting a premise and a hypothesis respectively. Determine the relationship between the premise and the hypothesis. The possible relationships you can choose from are 'Entail,' 'Contradict,' and 'Neutral.' Only pick one of the options. Think step by step. But make sure that your final answer ('Entail,' 'Contradict,' or 'Neutral') starts with 'FINAL ANSWER:'.

   The premise is: {PREMISE}
   The hypothesis is: {HYPOTHESIS}

2. Now revise the original hypothesis so that your answer to the question about its relationship becomes `<Complement>`. Share the revised hypothesis. The revised hypothesis should start with 'REVISED HYPOTHESIS:'.

C Postprocessing model outputs

1. Post-processing for all datasets starts by normalizing the model's short answer, such as converting 'Yes.' or 'Yes!' to 'Yes'. We also remove common extra characters that models tend to add to their answers, such as (*, \, ', ., !, ?, '., ..).

2. Filtering and removing model generations where the model's first answer is not valid. This means the model did not pick one of the valid options as an answer (*e.g.*, 'Yes' or 'No' in DISCRIMEVAL).

3. Filtering out cases when SCEs are shorter than expected. Short or incomplete generations typically occur when the model fails to provide a full SCE or returns a non-response. To avoid accidentally filtering out valid but concise outputs, we determined the thresholds for "short" generations empirically. We manually analyzed samples from each dataset and set minimum word-length criteria based on the

distribution of reasonable completions. The thresholds for filtering short cases are as follows:

- DISCRIMEVAL: Generations with fewer than 15 words
- TWITTER FINANCIAL NEWS: Fewer than 3 words
- FOLKTEXTS: Fewer than 60 words
- MGNLI: Fewer than 2 words
- SST2: Fewer than 1 word
- GSM8K: Generations containing fewer than 5 words and consisting solely of alphabetic characters, with no numbers or mathematical symbols.

4. For rationale based prompting, we remove cases where the model is unable to generate rationales. If the model fails to detect the important part of the text for answering, we do not consider its SCEs generation since the SCE generation instruction specifically refers to the rationales (Appendix B).

5. Some models in certain datasets included their answers in the SCE they generated. The presence of the answer biased the model prediction on on the SCE. To address this, we removed the answer tags from the SCEs when present.

6. We explicitly instructed the model to begin its response with specific keywords such as `‘ANSWER:’`, `‘RATIONALES:’` and `‘REVISED SCENARIO:’`. The models still tend to add synonymous labels like `‘ALTERED SCENARIO:’`. We manually analyze model outputs and whitelist these labels. The precise extraction process is:

   - **Extracting an Answer:** If the decoded response contains the string **‘ANSWER:’**, we extract everything that comes after the last occurrence of **‘ANSWER:’**.
   - **Extracting a Rationale:** If we are extracting a rationale, we look for the part of the decoded response that starts with **‘RATIONALES:’**.
   - **Extracting an SCE:** For counterfactual generation, the extraction cue (*i.e.*, the required starting word, or phrase) depends on both the dataset and the prompt type. The mapping for each case is listed below. Importantly, for `CoT` prompting the same starting phrase is used as in the `Unconstrained` setting.
     - DISCRIMEVAL:
       - `Unconstrained` → ‘REVISED SCENARIO:’
       - `Rational_based` → ‘ALTERED SCENARIO:’
     - FOLKTEXTS:
       - `Unconstrained` → ‘REVISED DATA:’
       - `Rational_based` → ‘ALTERED DATA:’
     - GSM8K:
       - `Unconstrained` → ‘REVISED PROBLEM:’
       - `Otherwise` → ‘ALTERED PROBLEM:’
     - SST2:
       - `Unconstrained` → ‘REVISED REVIEW:’
       - `Otherwise` → ‘ALTERED REVIEW:’
     - TWITTER:
       - `Unconstrained` → ‘REVISED POST:’
       - `Otherwise` → ‘ALTERED TWITTER POST:’
     - NLI:
       - `Unconstrained` → ‘REVISED HYPOTHESIS:’
       - `Otherwise` → ‘ALTERED HYPOTHESIS:’

D Additional results for various prompting strategies

1. Table 4 and Table 5 report SCE evaluation results at $T = 0.5$ under unconstrained and rationale-based prompting, while Table 6 and Table 7 present the corresponding results under CoT prompting at $T = 0$ and $T = 0.5$.

2. Table 8 reports the normalized differences in response lengths between valid and invalid counterfactuals across all datasets under unconstrained prompting at $T = 0$, including 95% confidence intervals computed from the standard error of the mean (see Appendix E for details). For comparison, non-parametric

bootstrap intervals are shown in Table 3. Similarly, Table 9 presents the normalized length differences under CoT prompting at $T = 0$, again with confidence intervals based on the standard error of the mean.

3. Table 10 reports model accuracy across all datasets and models under unconstrained, rationale-based, and CoT prompting, at $T = 0$ and $T = 0.5$. At $T = 0$, the mean accuracy is 66% under unconstrained and rationale-based prompting, and 68% under CoT prompting. Although CoT achieves a slightly higher mean and lower variance, a Wilcoxon signed-rank test (Woolson, 2007) indicates that the difference is not statistically significant, suggesting that CoT does not consistently yield higher accuracy across datasets and models.

E Statistical Analysis of Results

We computed 95% Confidence Intervals (CIs) for generation percentage, validity percentage, and edit distance to assess whether the differences between the *with context* and *without context* conditions are statistically significant. Non-overlapping CIs mean that the results for the two conditions differ more than what we would expect just from random variation. This usually points to a statistically significant difference (roughly corresponding to $p < 0.05$). The CIs were calculated using the standard error of the mean:

$$\text{CI} = \text{mean} \pm 1.96 \times \left(\frac{\text{sd}}{\sqrt{n}}\right)$$

Here, *mean* is the average value, *sd* is the standard deviation, and n is the number of samples. The factor 1.96 corresponds to a 95% confidence level under a normal distribution.

F Correlation between validity and popular performance metrics

We explored the relationship between the validity of SCEs and several model properties, including *Model Size*, *Perplexity*, and *Open LLM Leaderboard Rank*[2] (see Figure 2). However, we did not observe any clear or consistent patterns. Additionally, we performed both Pearson and Spearman correlation tests to check for non-zero correlation coefficient,[3] but **none of the correlations were statistically significant, with all p-values exceeding** 0.05. In the following subsection, we present results from these analyses under unconstrained prompting with temperature $T = 0$.

Validity of SCEs vs. Model Size across Datasets. Figure 3 shows how SCE validity varies with model size across datasets. Scaling generally improves validity on some tasks (e.g., DISCRIMEVAL, FOLKTEXTS, MGNLI), but yields diminishing returns or even declines on others (TWITTER, SST2) and remains poor on GSM8K. Notably, smaller models sometimes outperform larger ones (e.g., SST2, GSM8K), indicating that counterfactual validity does not scale monotonically with model size.

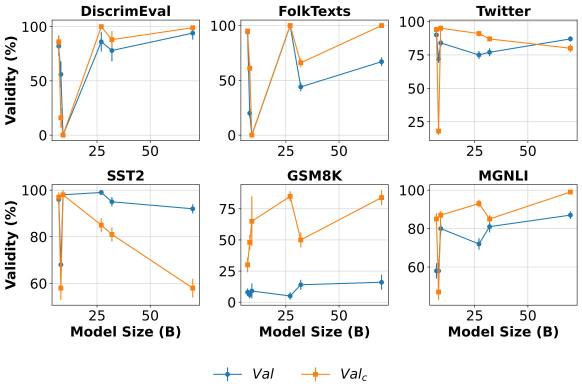

Figure 3: Validity of SCEs vs. Model Size across Datasets. Orange lines show validity with context (`Val`$_c$); blue lines show validity without context (`Val`).

Model perplexity vs. SCEs validity. We used the lm-eval framework[4] to compute five-shot perplexity on the WIKITEXT (Merity et al., 2016) benchmark for each model, and then analyzed its correlation with the percentage of valid SCEs generated. The decision to use lm-eval aligns with best practices for reproducible, transparent, and comparable evaluation, as emphasized by Biderman et al. (2024). By adopting a controlled few-shot setup, we reduce variance across evaluations and ensure our perplexity scores reflect meaningful differences in model behavior rather than implementation artifacts. Measuring perplexity in this standardized way enables a principled comparison with SCEs validity, allowing us to probe whether language models with lower perplexity exhibit stronger counterfactual reasoning. However, as shown in line plots (Figure 4), regression fits (Figure 5), and correlation analysis (Figure 6), we did not observe a

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[2] `https://huggingface.co/spaces/open-llm-leaderboard`

[3] Using `https://scipy.org`

[4] `https://github.com/EleutherAI/lm-evaluation-harness`

	`Gen` ↑	`Val` ↑	`Val`$_C$ ↑	`ED` ↓	`ED`$_C$
LAM$_s$	81 (2)	**63 (1)**	**77 (3)**	46 (2)	48 (1)
LAM$_m$	100 (0)	**95 (1)**	**99 (1)**	35 (1)	35 (1)
MST$_s$	100 (0)	**83 (1)**	**94 (2)**	**37 (1)**	**34 (1)**
MST$_m$	100 (0)	**89 (0)**	**87 (0)**	**21 (0)**	**20 (0)**
GEM$_s$	5 (2)	50 (28)	85 (11)	33 (2)	27 (7)
GEM$_m$	85 (7)	**81 (2)**	**97 (5)**	26 (1)	25 (1)
R1$_m$	98 (1)	81 (7)	86 (10)	44 (10)	42 (11)

(a) DiscrimEval

	`Gen` ↑	`Val` ↑	`Val`$_C$ ↑	`ED` ↓	`ED`$_C$
LAM$_s$	94 (2)	**84 (1)**	**78 (3)**	61 (1)	60 (1)
LAM$_m$	100 (0)	**72 (0)**	**97 (2)**	**36 (0)**	**35 (0)**
MST$_s$	99 (0)	**93 (1)**	**99 (0)**	27 (0)	27 (0)
MST$_m$	100 (0)	**56 (0)**	**100 (0)**	33 (0)	33 (0)
GEM$_s$	8 (1)	**14 (5)**	**99 (1)**	37 (1)	38 (1)
GEM$_m$	99 (1)	**99 (0)**	**100 (0)**	39 (0)	39 (0)
R1$_m$	95 (3)	53 (12)	74 (9)	45 (9)	41 (7)

(b) FolkTexts

	`Gen` ↑	`Val` ↑	`Val`$_C$ ↑	`ED` ↓	`ED`$_C$
LAM$_s$	86 (1)	81 (0)	72 (11)	**76 (0)**	**71 (4)**
LAM$_m$	100 (0)	**89 (1)**	**75 (2)**	62 (1)	62 (1)
MST$_s$	95 (3)	**79 (2)**	**91 (1)**	63 (1)	63 (1)
MST$_m$	100 (0)	**82 (0)**	**100 (0)**	57 (0)	57 (0)
GEM$_s$	97 (0)	**84 (0)**	**94 (1)**	**64 (0)**	**63 (0)**
GEM$_m$	100 (0)	**76 (0)**	**90 (0)**	67 (0)	67 (0)
R1$_m$	100 (0)	78 (1)	88 (9)	59 (2)	58 (1)

(c) Twitter Financial News

	`Gen` ↑	`Val` ↑	`Val`$_C$ ↑	`ED` ↓	`ED`$_C$
LAM$_s$	85 (1)	**59 (2)**	**48 (6)**	86 (1)	84 (2)
LAM$_m$	99 (1)	**92 (1)**	**55 (3)**	**68 (0)**	**70 (1)**
MST$_s$	90 (0)	93 (0)	93 (0)	78 (1)	78 (1)
MST$_m$	100 (0)	96 (1)	96 (0)	68 (0)	68 (0)
GEM$_s$	94 (1)	97 (0)	98 (1)	76 (1)	76 (2)
GEM$_m$	100 (0)	**99 (0)**	**90 (2)**	77 (0)	77 (0)
R1$_m$	99 (0)	**94 (0)**	**78 (5)**	72 (2)	70 (2)

(d) SST2

	`Gen` ↑	`Val` ↑	`Val`$_C$ ↑	`ED` ↓	`ED`$_C$
LAM$_s$	96 (1)	**6 (1)**	**52 (2)**	**64 (3)**	**58 (0)**
LAM$_m$	100 (0)	**13 (1)**	**80 (9)**	57 (1)	58 (0)
MST$_s$	100 (0)	**5 (1)**	**34 (4)**	57 (2)	59 (1)
MST$_m$	100 (0)	**10 (0)**	**83 (0)**	**55 (0)**	**58 (0)**
GEM$_s$	27 (1)	**3 (1)**	**48 (11)**	77 (6)	74 (9)
GEM$_m$	89 (1)	**4 (0)**	**88 (3)**	57 (1)	58 (0)
R1$_m$	100 (0)	**27 (3)**	**52 (5)**	69 (4)	70 (7)

(e) GSM8K

	`Gen` ↑	`Val` ↑	`Val`$_C$ ↑	`ED` ↓	`ED`$_C$
LAM$_s$	93 (0)	**59 (1)**	**53 (2)**	73 (0)	74 (1)
LAM$_m$	100 (0)	88 (1)	86 (6)	72 (0)	72 (0)
MST$_s$	99 (0)	**59 (1)**	**84 (0)**	74 (0)	74 (0)
MST$_m$	100 (0)	**84 (0)**	**96 (1)**	78 (0)	78 (0)
GEM$_s$	97 (0)	**78 (0)**	**86 (1)**	78 (0)	78 (0)
GEM$_m$	100 (0)	**74 (1)**	**92 (0)**	**76 (0)**	**77 (0)**
R1$_m$	100 (0)	77 (5)	76 (14)	78 (3)	76 (1)

(f) MGNLI

Table 4: Performance of LLMs in generating SCEs under unconstrained prompting at $T = 0.5$, measured in terms of percentage of times the models are able to generate a SCE (`Gen`), percentage of times the model predictions on SCEs yield the target label (`Val`), and the normalized edit distance (`ED`) between the original inputs and SCEs. `Val`$_C$ and `ED`$_C$ denotes the metric values when the instructions for prediction on the original input and the SCE generation are provided in the context while computing the validity of the SCE (Section 3.2). Values in parentheses indicate marginal confidence intervals. See Appendix E for details. Values are bolded when the differences in with and without context conditions (*e.g.*, `Val` and `Val`$_C$) are statistically significant. ↑ means higher values are better.

clear relationship between few-shot perplexity and SCE validity across models.

G Annotation Protocol

We conducted a human annotation study, as reported in Section 6. The protocol was as follows. We randomly selected 50 examples from GSM8K under CoT prompting at $T = 0$, for each of the 7 models, resulting in 350 examples overall. Each example was independently assessed by two annotators (the authors), who determined whether the SCE yielded a solution matching the correct target label ($\hat{y}_{CE}$). Disagreements, observed in roughly 5% of the cases, were resolved through in-person

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	81 (3)	**55 (1)**	**84 (1)**	33 (3)	33 (1)
LAM$_m$	100 (0)	60 (1)	67 (7)	**25 (1)**	**22 (1)**
MST$_s$	99 (0)	**88 (0)**	**91 (0)**	39 (1)	38 (1)
MST$_m$	100 (0)	**59 (0)**	**83 (0)**	**12 (0)**	**11 (0)**
GEM$_s$	2 (2)	**0 (0)**	**34 (27)**	**0 (0)**	**16 (0)**
GEM$_m$	81 (4)	**47 (2)**	**98 (1)**	18 (1)	17 (0)
R1$_m$	100 (0)	**62 (5)**	**87 (5)**	**23 (1)**	**21 (0)**

(a) DiscrimEval

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	81 (10)	**71 (0)**	**85 (1)**	37 (3)	38 (4)
LAM$_m$	96 (2)	**48 (3)**	**62 (5)**	36 (1)	35 (0)
MST$_s$	98 (0)	**99 (0)**	**82 (2)**	48 (1)	50 (1)
MST$_m$	92 (0)	**58 (0)**	**91 (0)**	**33 (0)**	**32 (0)**
GEM$_s$	8 (0)	**4 (1)**	**92 (2)**	**43 (3)**	**33 (0)**
GEM$_m$	30 (3)	**61 (6)**	**97 (0)**	**34 (0)**	**33 (0)**
R1$_m$	73 (15)	**64 (0)**	**86 (7)**	40 (3)	37 (3)

(b) FolkTexts

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	85 (0)	74 (1)	81 (8)	**59 (3)**	**54 (0)**
LAM$_m$	99 (0)	**92 (0)**	**73 (10)**	70 (3)	67 (6)
MST$_s$	100 (0)	**90 (1)**	**96 (0)**	74 (0)	74 (0)
MST$_m$	100 (0)	**77 (0)**	**99 (0)**	**49 (0)**	**48 (0)**
GEM$_s$	97 (0)	**78 (0)**	**96 (0)**	**50 (0)**	**49 (0)**
GEM$_m$	100 (0)	**87 (0)**	**92 (4)**	51 (1)	49 (1)
R1$_m$	100 (0)	73 (2)	80 (5)	59 (3)	58 (4)

(c) Twitter Financial News

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	87 (2)	**49 (1)**	**58 (5)**	**73 (2)**	**69 (0)**
LAM$_m$	99 (0)	**87 (0)**	**67 (2)**	76 (1)	77 (0)
MST$_s$	85 (2)	**93 (0)**	**89 (2)**	77 (1)	77 (1)
MST$_m$	100 (0)	**85 (0)**	**98 (0)**	**66 (0)**	**65 (0)**
GEM$_s$	95 (1)	**74 (2)**	**97 (0)**	66 (1)	64 (1)
GEM$_m$	100 (0)	**83 (2)**	**95 (2)**	66 (1)	65 (1)
R1$_m$	99 (0)	**77 (1)**	**72 (1)**	65 (1)	63 (1)

(d) SST2

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	95 (1)	**11 (0)**	**49 (7)**	**68 (1)**	**62 (3)**
LAM$_m$	100 (0)	**25 (1)**	**60 (2)**	63 (0)	62 (1)
MST$_s$	100 (0)	57 (5)	64 (6)	59 (1)	60 (1)
MST$_m$	100 (0)	**10 (0)**	**75 (0)**	**55 (0)**	**58 (0)**
GEM$_s$	30 (0)	**6 (1)**	**48 (4)**	55 (3)	57 (1)
GEM$_m$	93 (2)	**7 (0)**	**76 (1)**	57 (1)	58 (1)
R1$_m$	99 (0)	**19 (0)**	**37 (6)**	63 (0)	62 (4)

(e) GSM8K

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	93 (0)	61 (1)	64 (11)	77 (1)	75 (1)
LAM$_m$	99 (0)	**90 (1)**	**60 (20)**	74 (0)	73 (1)
MST$_s$	98 (2)	89 (1)	88 (4)	73 (0)	73 (0)
MST$_m$	100 (0)	**68 (0)**	**87 (0)**	75 (0)	75 (0)
GEM$_s$	91 (5)	**66 (1)**	**84 (2)**	76 (0)	76 (0)
GEM$_m$	100 (0)	**74 (1)**	**89 (3)**	75 (0)	75 (0)
R1$_m$	100 (0)	**64 (2)**	**86 (1)**	73 (0)	73 (0)

(f) MGNLI

Table 5: Performance of LLMs in generating SCEs under rationale-based prompting at $T = 0.5$, measured in terms of percentage of times the models are able to generate a SCE (`Gen`), percentage of times the model predictions on SCEs yield the target label (`Val`), and the normalized edit distance (`ED`) between the original inputs and SCEs. `Val`$_C$ and `ED`$_C$ denotes the metric values when the instructions for prediction on the original input and the SCE generation are provided in the context while computing the validity of the SCE (Section 3.2). Values in parentheses indicate marginal confidence intervals. See Appendix E for details. Values are bolded when the differences in with and without context conditions (*e.g.*, `Val` and `Val`$_C$) are statistically significant. ↑ means higher values are better.

discussion. These disagreements typically arose from ambiguities in the counterfactual statements or occasional mistakes in solving the math problems. The resulting consensus labels were then used to compute correlations between **validity** and **correctness**.

H Clustering of SCE Representations: Methodology and Results

As introduced in Section 6, we applied K-means clustering to the embedding space of SCEs in order to probe potential task misunderstandings. In the following, we detail the methodology and results

	`Gen` ↑	`Val` ↑	`Val`$_C$ ↑	`ED` ↓	`ED`$_C$
`LAM`$_s$	97 (4)	84 (9)	75 (10)	52 (5)	53 (5)
`LAM`$_m$	100 (0)	**76 (10)**	**53 (12)**	34 (3)	38 (4)
`MST`$_s$	90 (7)	86 (9)	90 (7)	37 (4)	36 (4)
`MST`$_m$	97 (4)	**82 (9)**	**100 (0)**	24 (3)	23 (3)
`GEM`$_s$	89 (7)	**63 (12)**	**94 (6)**	24 (3)	23 (3)
`GEM`$_m$	100 (0)	**94 (6)**	**71 (11)**	22 (2)	24 (3)
`R1`$_m$	100 (0)	**76 (10)**	**99 (2)**	37 (3)	35 (3)

(a) DiscrimEval

	`Gen` ↑	`Val` ↑	`Val`$_C$ ↑	`ED` ↓	`ED`$_C$
`LAM`$_s$	99 (1)	**80 (4)**	**96 (2)**	48 (2)	46 (2)
`LAM`$_m$	99 (1)	**84 (3)**	**64 (4)**	37 (1)	37 (1)
`MST`$_s$	82 (3)	**85 (3)**	**99 (1)**	32 (1)	30 (1)
`MST`$_m$	100 (0)	**54 (4)**	**98 (1)**	32 (0)	32 (0)
`GEM`$_s$	94 (2)	**88 (3)**	**99 (1)**	40 (0)	39 (0)
`GEM`$_m$	100 (0)	**99 (1)**	**100 (0)**	38 (0)	38 (0)
`R1`$_m$	99 (1)	**75 (4)**	**40 (4)**	**62 (2)**	**57 (3)**

(b) FolkTexts

	`Gen` ↑	`Val` ↑	`Val`$_C$ ↑	`ED` ↓	`ED`$_C$
`LAM`$_s$	85 (3)	85 (3)	83 (3)	77 (2)	76 (2)
`LAM`$_m$	100 (0)	**87 (2)**	**75 (3)**	60 (1)	60 (1)
`MST`$_s$	99 (1)	**90 (2)**	**96 (1)**	64 (1)	64 (1)
`MST`$_m$	100 (0)	**82 (3)**	**100 (0)**	61 (1)	61 (1)
`GEM`$_s$	98 (1)	**84 (3)**	**96 (1)**	63 (1)	62 (1)
`GEM`$_m$	100 (0)	**75 (3)**	**91 (2)**	67 (1)	67 (1)
`R1`$_m$	100 (0)	**77 (3)**	**94 (2)**	**62 (1)**	**59 (1)**

(c) Twitter Financial News

	`Gen` ↑	`Val` ↑	`Val`$_C$ ↑	`ED` ↓	`ED`$_C$
`LAM`$_s$	93 (2)	59 (4)	53 (5)	77 (2)	78 (2)
`LAM`$_m$	94 (2)	**92 (2)**	**58 (4)**	70 (2)	72 (2)
`MST`$_s$	89 (3)	**92 (3)**	**80 (4)**	80 (1)	80 (1)
`MST`$_m$	96 (2)	97 (2)	96 (2)	67 (1)	66 (1)
`GEM`$_s$	76 (4)	93 (3)	92 (3)	72 (1)	72 (1)
`GEM`$_m$	98 (1)	**99 (1)**	**80 (4)**	76 (1)	76 (1)
`R1`$_m$	100 (0)	**91 (3)**	**77 (4)**	73 (1)	72 (1)

(d) SST2

	`Gen` ↑	`Val` ↑	`Val`$_C$ ↑	`ED` ↓	`ED`$_C$
`LAM`$_s$	95 (3)	**5 (3)**	**53 (6)**	61 (7)	59 (2)
`LAM`$_m$	100 (0)	**14 (4)**	**72 (6)**	54 (3)	58 (1)
`MST`$_s$	100 (0)	**10 (4)**	**39 (6)**	56 (5)	57 (2)
`MST`$_m$	100 (0)	**14 (4)**	**84 (5)**	56 (3)	58 (1)
`GEM`$_s$	13 (4)	12 (11)	27 (15)	61 (18)	66 (12)
`GEM`$_m$	96 (2)	**4 (2)**	**86 (4)**	55 (5)	58 (1)
`R1`$_m$	100 (0)	**26 (5)**	**63 (6)**	**73 (3)**	**83 (3)**

(e) GSM8K

	`Gen` ↑	`Val` ↑	`Val`$_C$ ↑	`ED` ↓	`ED`$_C$
`LAM`$_s$	95 (2)	**56 (4)**	**79 (3)**	73 (1)	73 (1)
`LAM`$_m$	97 (1)	**81 (3)**	**73 (3)**	71 (1)	71 (1)
`MST`$_s$	100 (0)	**62 (3)**	**82 (3)**	74 (1)	74 (1)
`MST`$_m$	100 (0)	**85 (3)**	**96 (1)**	76 (1)	76 (1)
`GEM`$_s$	97 (1)	**76 (3)**	**89 (2)**	77 (1)	77 (1)
`GEM`$_m$	100 (0)	**85 (3)**	**98 (1)**	75 (1)	75 (1)
`R1`$_m$	100 (0)	79 (3)	84 (3)	77 (1)	76 (1)

(f) MGNLI

Table 6: Performance of LLMs in generating SCEs under CoT prompting at $T = 0$, measured in terms of percentage of times the models are able to generate a SCE (`Gen`), percentage of times the model predictions on SCEs yield the target label (`Val`), and the normalized edit distance (`ED`) between the original inputs and SCEs. `Val`$_C$ and `ED`$_C$ denote the metric values when the instructions for prediction on the original input and the SCE generation are provided in the context while computing the validity of the SCE (Section 3.2). Values in parentheses indicate marginal confidence intervals. See Appendix E for details. Values are bolded when the differences in with and without context conditions (*e.g.*, `Val` and `Val`$_C$) are statistically significant. ↑ means higher values are better.

of this analysis, focusing on the systematic differences in the hidden representations of valid and invalid SCEs. We evaluated whether different clustering strategies and distance metrics provide consistent separation between valid and invalid SCEs. Specifically, we compared three strategies: using the representations at the *First Generated Token* and *Last Generated Token* of the SCE, and the *Last Input Token* of the prompt that elicited the SCE. For each strategy, we evaluated four distance metrics: raw Euclidean distance, normalized Euclidean distance, raw cosine distance (that is, 1 -

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	89 (7)	63 (12)	81 (10)	39 (6)	42 (5)
LAM$_m$	99 (2)	**84 (9)**	**55 (12)**	35 (4)	37 (5)
MST$_s$	91 (7)	81 (10)	88 (8)	40 (4)	37 (3)
MST$_m$	97 (4)	**78 (10)**	**97 (4)**	25 (3)	24 (3)
GEM$_s$	77 (10)	**59 (13)**	**91 (8)**	25 (3)	23 (2)
GEM$_m$	100 (0)	83 (9)	86 (8)	25 (3)	25 (2)
R1$_m$	93 (6)	**75 (11)**	**100 (0)**	41 (5)	41 (5)

(a) DiscrimEval

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	92 (2)	**72 (4)**	**82 (4)**	48 (3)	47 (2)
LAM$_m$	97 (2)	**80 (4)**	**66 (4)**	38 (1)	37 (1)
MST$_s$	76 (4)	**83 (4)**	**92 (3)**	34 (1)	33 (1)
MST$_m$	100 (0)	**65 (4)**	**98 (1)**	34 (0)	33 (0)
GEM$_s$	82 (3)	**81 (4)**	**97 (2)**	41 (1)	39 (1)
GEM$_m$	99 (1)	**99 (1)**	**100 (0)**	39 (0)	39 (0)
R1$_m$	67 (4)	**50 (5)**	**88 (3)**	38 (2)	36 (2)

(b) FolkTexts

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	86 (2)	80 (3)	82 (3)	76 (2)	75 (2)
LAM$_m$	100 (0)	**87 (2)**	**78 (3)**	61 (1)	61 (1)
MST$_s$	91 (2)	**81 (3)**	**92 (2)**	64 (1)	64 (1)
MST$_m$	100 (0)	**81 (3)**	**100 (0)**	58 (1)	57 (1)
GEM$_s$	97 (1)	**87 (2)**	**95 (2)**	63 (1)	63 (1)
GEM$_m$	100 (0)	**74 (3)**	**91 (2)**	67 (1)	67 (1)
R1$_m$	99 (1)	**77 (3)**	**91 (2)**	**62 (1)**	**59 (1)**

(c) Twitter Financial News

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	92 (2)	59 (4)	53 (5)	79 (2)	79 (2)
LAM$_m$	95 (2)	**87 (3)**	**54 (4)**	70 (2)	72 (2)
MST$_s$	87 (3)	**92 (3)**	**78 (4)**	80 (1)	80 (1)
MST$_m$	96 (2)	93 (2)	89 (3)	69 (1)	68 (1)
GEM$_s$	70 (4)	89 (3)	93 (3)	73 (1)	73 (1)
GEM$_m$	98 (1)	**97 (2)**	**81 (4)**	77 (1)	77 (1)
R1$_m$	98 (1)	**85 (3)**	**72 (4)**	75 (1)	75 (2)

(d) SST2

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	92 (3)	**4 (3)**	**58 (6)**	55 (11)	57 (2)
LAM$_m$	99 (1)	**18 (5)**	**63 (6)**	57 (4)	59 (2)
MST$_s$	99 (1)	**8 (3)**	**36 (6)**	56 (5)	60 (2)
MST$_m$	99 (1)	**6 (3)**	**82 (5)**	59 (5)	59 (1)
GEM$_s$	28 (6)	**3 (4)**	**39 (11)**	76 (45)	76 (9)
GEM$_m$	96 (2)	**3 (2)**	**84 (5)**	58 (8)	58 (1)
R1$_m$	100 (0)	**27 (6)**	**54 (6)**	75 (3)	73 (3)

(e) GSM8K

	Gen ↑	Val ↑	Val$_C$ ↑	ED ↓	ED$_C$
LAM$_s$	91 (2)	**56 (4)**	**76 (3)**	76 (1)	75 (1)
LAM$_m$	99 (1)	**84 (3)**	**75 (3)**	73 (1)	72 (1)
MST$_s$	99 (1)	**61 (4)**	**83 (3)**	73 (1)	73 (1)
MST$_m$	99 (1)	**86 (2)**	**97 (1)**	77 (1)	76 (1)
GEM$_s$	93 (2)	**77 (3)**	**92 (2)**	77 (1)	77 (1)
GEM$_m$	100 (0)	**85 (3)**	**97 (1)**	76 (1)	76 (1)
R1$_m$	97 (1)	**78 (3)**	**84 (3)**	78 (1)	77 (1)

(f) MGNLI

Table 7: Performance of LLMs in generating SCEs under CoT prompting at $T = 0.5$, measured in terms of percentage of times the models are able to generate a SCE (`Gen`), percentage of times the model predictions on SCEs yield the target label (`Val`), and the normalized edit distance (`ED`) between the original inputs and SCEs. `Val`$_C$ and `ED`$_C$ denote the metric values when the instructions for prediction on the original input and the SCE generation are provided in the context while computing the validity of the SCE (Section 3.2). Values in parentheses indicate marginal confidence intervals. See Appendix E for details. Values are bolded when the differences in with and without context conditions (*e.g.*, `Val` and `Val`$_C$) are statistically significant. ↑ means higher values are better.

cosine similarity), and normalized cosine distance. Here, "normalized" means that last-layer hidden-state vectors were standardized to zero mean and unit variance before distance computation. We ran k-means clustering with each of the above four metrics as the distance metric. To quantify performance, we define the **average separation score** as:

$$\text{SepScore} = \frac{1}{N}\sum_{i=1}^{N}\left(\Delta_0^{(i)} + \Delta_1^{(i)}\right),$$

	DEV		**TWT**		**SST**		**FLK**		**NLI**		**MTH**	
	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/
LAM$_\text{s}$	40 (19)	19 (30)	**6 (7)**	**44 (6)**	37 (8)	20 (9)	13 (10)	4 (2)	1 (22)	21 (20)	26 (30)	45 (13)
LAM$_\text{m}$	**16 (11)**	**67 (2)**	5 (6)	11 (5)	26 (11)	20 (8)	**0 (0)**	**100 (0)**	**0 (5)**	**15 (5)**	**22 (9)**	**100 (0)**
MST$_\text{s}$	4 (6)	14 (6)	**1 (7)**	**19 (5)**	27 (6)	26 (8)	**3 (1)**	**9 (1)**	5 (5)	9 (5)	9 (16)	18 (18)
MST$_\text{m}$	**19 (6)**	**100 (0)**	3 (3)	4 (3)	**8 (6)**	**27 (5)**	**1 (0)**	**2 (0)**	**3 (5)**	**16 (6)**	19 (10)	28 (4)
GEM$_\text{s}$	0 (0)	0 (0)	4 (4)	6 (4)	100 (0)	100 (0)	0 (0)	0 (0)	6 (4)	7 (5)	17 (26)	11 (18)
GEM$_\text{m}$	**11 (6)**	**100 (0)**	3 (4)	7 (3)	**6 (5)**	**49 (3)**	**4 (0)**	**100 (0)**	1 (5)	6 (5)	**31 (15)**	**9 (5)**
R1$_\text{m}$	**16 (22)**	**100 (0)**	37 (15)	44 (5)	**35 (18)**	**72 (8)**	**1 (7)**	**26 (5)**	11 (4)	12 (4)	63 (9)	70 (9)

Table 8: Normalized difference in lengths of valid and invalid counterfactuals. For DiscrimEval (DEV), Twitter Financial News (TWT), SST2 (SST), FolkTexts (FLK), MGNLI (NLI), and GSM8K (MTH) datasets under unconstrained prompting with $T = 0$. Left columns (w/o) show the differences without prediction and counterfactual generations provided as context (Section 3.2), whereas right columns (w/) show the differences with this information.

	DEV		**TWT**		**SST**		**FLK**		**NLI**		**MTH**	
	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/
LAM$_\text{s}$	**23 (14)**	**52 (7)**	80 (3)	81 (3)	18 (15)	1 (17)	2 (9)	8 (9)	25 (17)	46 (10)	46 (16)	40 (11)
LAM$_\text{m}$	1 (10)	7 (9)	5 (6)	4 (5)	29 (14)	38 (11)	**5 (2)**	**12 (2)**	10 (12)	1 (10)	12 (13)	0 (6)
MST$_\text{s}$	**2 (6)**	**100 (0)**	**1 (7)**	**21 (6)**	17 (10)	7 (11)	6 (3)	2 (3)	19 (7)	17 (7)	13 (14)	24 (7)
MST$_\text{m}$	**2 (7)**	**100 (0)**	**6 (3)**	**100 (0)**	**10 (6)**	**40 (5)**	0 (0)	1 (0)	**4 (5)**	**14 (5)**	17 (11)	13 (5)
GEM$_\text{s}$	16 (7)	10 (5)	4 (4)	6 (4)	**10 (9)**	**34 (7)**	**3 (1)**	**22 (3)**	6 (6)	7 (6)	10 (25)	11 (27)
GEM$_\text{m}$	12 (6)	15 (6)	3 (4)	7 (3)	**25 (5)**	**43 (4)**	**0 (1)**	**100 (0)**	9 (6)	16 (5)	**20 (23)**	**100 (0)**
R1$_\text{m}$	**6 (10)**	**55 (4)**	**37 (15)**	**93 (1)**	31 (20)	33 (21)	**1 (7)**	**26 (5)**	**17 (15)**	**81 (3)**	63 (8)	48 (12)

Table 9: Normalized difference in lengths of valid and invalid counterfactuals. For DiscrimEval (DEV), Twitter Financial News (TWT), SST2 (SST), FolkTexts (FLK), MGNLI (NLI), and GSM8K (MTH) datasets under CoT prompting with $T = 0$. Left columns (w/o) show the differences without prediction and counterfactual generations provided as context (Section 3.2), whereas right columns (w/) show the differences with this information.

where $\Delta_0^{(i)}$ and $\Delta_1^{(i)}$ are the absolute differences between valid and invalid SCEs in clusters 0 and 1 for the i-th (model, dataset) pair, and N is the total number of evaluated pairs.

When averaging across all models and datasets, we found that the separation scores do not differ much between various distance metrics and that normalized cosine distance yielded the highest separation score (178.9), outperforming raw Cosine (176.5), normalized Euclidean (175.7), and raw Euclidean (175.2). Therefore, we adopted **normalized Cosine distance** as our primary metric.

Detailed results for each model and dataset are reported in Table 11, where Δ_0 and Δ_1 denote the absolute difference between valid and invalid cases assigned to cluster 0 and cluster 1, respectively. Larger Δ values indicate clearer separation. For example, GSM8K shows consistently low Δ scores, suggesting weaker separation, whereas TWITTER and SST2 yield higher Δ values, indicating stronger clustering of valid vs. invalid cases.

I Statistical Significance via Permutation Testing

To complement the confidence interval comparisons reported in the Table 1 and Table 2, we additionally performed nonparametric permutation tests to assess whether the differences between the two conditions (with context and without context) are statistically significant. We applied paired permutation tests with the null hypothesis that the two conditions are drawn from the same distribution, *i.e.*, any observed difference in validity or normalized edit distance arises purely from random variation in the sample. In each test, the assignment of condition labels was randomly permuted across paired examples, and the distribution of mean differences was computed over $10,000$ resamples. Two-sided p-values were then obtained by comparing the observed effect size to this null distribution. Table 12 reports the effect size (mean difference between the

	DEV	TWT	SST	FLK	NLI	MTH
LAM$_s$	54 (12)	77 (3)	82 (3)	55 (4)	66 (3)	13 (4)
LAM$_m$	86 (8)	80 (3)	92 (2)	69 (4)	76 (3)	39 (6)
MST$_s$	82 (9)	82 (3)	60 (4)	60 (4)	75 (3)	8 (3)
MST$_m$	63 (11)	84 (3)	81 (3)	71 (4)	86 (2)	38 (6)
GEM$_s$	80 (9)	81 (3)	90 (3)	76 (4)	77 (3)	24 (5)
GEM$_m$	76 (10)	85 (3)	91 (2)	74 (4)	82 (3)	0 (1)
R1$_m$	39 (11)	79 (3)	95 (2)	30 (4)	82 (3)	13 (4)

(a) Accuracy under unconstrained and rationale-based prompting ($T = 0$)

	DEV	TWT	SST	FLK	NLI	MTH
LAM$_s$	51 (12)	77 (3)	83 (3)	55 (4)	65 (3)	12 (4)
LAM$_m$	85 (8)	82 (3)	92 (2)	70 (4)	76 (3)	40 (6)
MST$_s$	80 (9)	81 (3)	61 (4)	59 (4)	76 (3)	8 (3)
MST$_m$	68 (11)	82 (3)	81 (3)	69 (4)	84 (3)	41 (6)
GEM$_s$	80 (9)	81 (3)	90 (3)	75 (4)	78 (3)	22 (5)
GEM$_m$	79 (10)	85 (3)	90 (3)	74 (4)	82 (3)	27 (6)
R1$_m$	46 (12)	79 (3)	94 (2)	36 (4)	78 (3)	19 (5)

(b) Accuracy under unconstrained and rationale-based prompting ($T = 0.5$)

	DEV	TWT	SST	FLK	NLI	MTH
LAM$_s$	85 (8)	75 (3)	93 (2)	68 (4)	62 (3)	86 (4)
LAM$_m$	84 (9)	78 (3)	96 (2)	52 (5)	78 (3)	29 (6)
MST$_s$	63 (11)	76 (3)	78 (4)	31 (4)	63 (3)	11 (4)
MST$_m$	66 (11)	78 (3)	91 (2)	72 (4)	80 (3)	96 (2)
GEM$_s$	72 (10)	79 (3)	86 (3)	67 (4)	77 (3)	61 (6)
GEM$_m$	69 (11)	81 (3)	82 (3)	69 (4)	76 (3)	29 (6)
R1$_m$	17 (9)	72 (3)	94 (2)	13 (3)	76 (3)	31 (6)

(c) Accuracy under CoT prompting ($T = 0$)

	DEV	TWT	SST	FLK	NLI	MTH
LAM$_s$	83 (9)	75 (3)	92 (2)	65 (4)	62 (3)	82 (5)
LAM$_m$	89 (7)	80 (3)	96 (2)	61 (5)	80 (3)	98 (2)
MST$_s$	62 (11)	75 (3)	80 (3)	38 (4)	62 (3)	12 (4)
MST$_m$	66 (11)	80 (3)	90 (3)	73 (4)	80 (3)	94 (3)
GEM$_s$	72 (10)	79 (3)	85 (3)	69 (4)	77 (3)	64 (6)
GEM$_m$	66 (11)	78 (3)	83 (3)	69 (4)	73 (3)	27 (6)
R1$_m$	15 (8)	68 (3)	93 (2)	17 (3)	65 (3)	34 (6)

(d) Accuracy under CoT prompting ($T = 0.5$)

Table 10: Task-specific accuracy (%) of models on each dataset under (a) $T = 0$ and (b) $T = 0.5$. Since the prompts used for unconstrained and rationale-based generations are identical when obtaining model predictions, their accuracy values are shared. However, because CoT uses a different prompt format, we independently report its accuracy. Values in parentheses indicate marginal confidence intervals. See Appendix E for details.

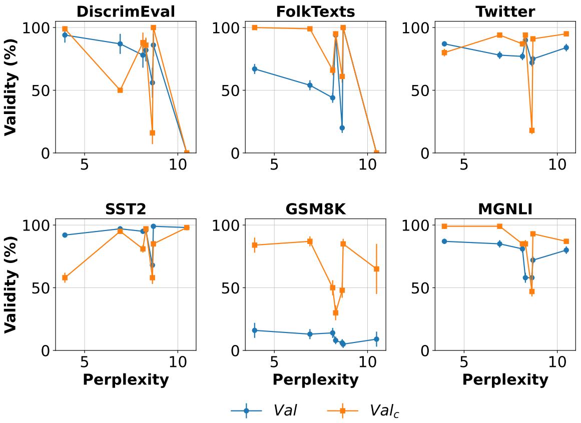

Figure 4: Line plots of few-shot perplexity (measured on WIKITEXT) versus SCE validity across datasets. Blue lines indicate validity without context (`Val`) and orange lines indicate validity with context (`Val`$_c$).

two conditions) for both validity and normalized edit distance under two prompting strategies: (i) Unconstrained prompting ($T = 0$; see Table 12a and Table 12b), and (ii) Rationale-based prompting ($T = 0$; see Table 12c and Table 12d). The table shows that when comparing validity, permutation testing detects more statistically significant differences than CI overlap alone. The effect magnitude varies across datasets and prompting strategies.

J Bootstrap Confidence Intervals

To avoid reliance on normality assumptions and to allow for asymmetric intervals, we computed confidence intervals for the normalized differences in SCE lengths using nonparametric bootstrap resampling (Tibshirani and Efron, 1993). Specifically, 10,000 bootstrap samples with replacement were drawn from the valid and invalid counterfactual length distributions. For each resample, we calculated the normalized difference, and reported the bootstrap mean together with the 2.5th and 97.5th percentiles. This yields a 95% confidence interval that does not rely on normality assumptions and naturally accommodates asymmetry. The original results with normality-based intervals are provided in Appendix D.

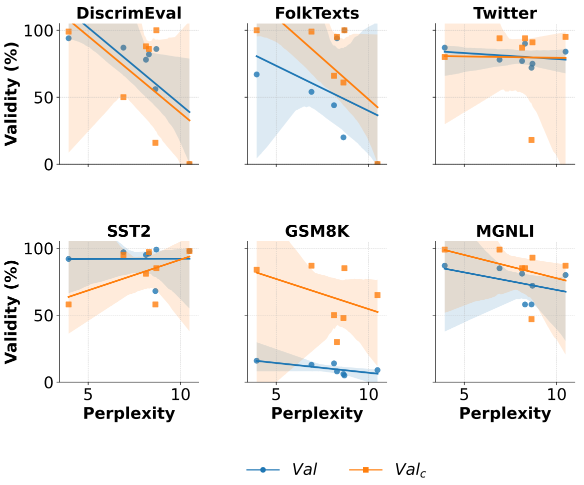

Figure 5: Regression plots of few-shot perplexity versus SCE validity across datasets. Blue lines indicate validity without context (`Val`) and orange lines indicate validity with context (`Val`$_{\text{C}}$), with shaded regions denoting 95% confidence intervals.

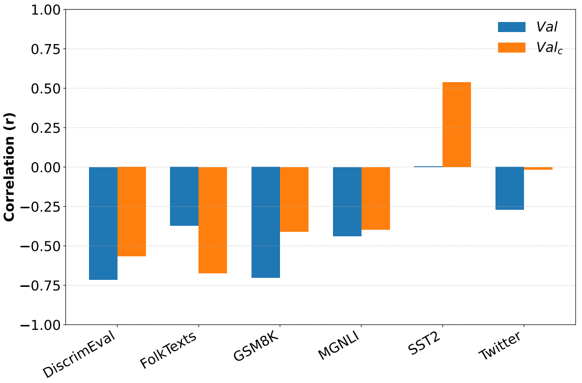

Figure 6: Pearson correlation coefficients between few-shot perplexity and SCE validity across datasets. Blue bars represent validity without context (`Val`) and orange bars represent validity with context (`Val`$_{\text{C}}$).

	DEV				TWT				SST				FLK				NLI				MTH			
	Δ_0		Δ_1		Δ_0		Δ_1		Δ_0		Δ_1		Δ_0		Δ_1		Δ_0		Δ_1		Δ_0		Δ_1	
	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/
LAM$_s$	22	3	11	5	424	356	70	203	306	92	108	66	272	197	97	88	185	144	87	69	1	11	8	23
LAM$_m$	27	21	33	17	429	432	80	317	244	258	236	242	92	91	249	183	404	465	131	211	44	90	32	119
MST$_s$	10	18	11	22	539	275	103	62	26	15	63	40	90	52	100	109	142	101	135	40	6	3	32	27
MST$_m$	26	28	31	39	246	97	189	377	161	157	256	271	111	121	283	3	238	130	163	145	7	13	27	49
GEM$_s$	19	2	22	1	402	402	65	19	231	235	155	143	98	45	104	71	264	141	427	147	2	20	3	4
GEM$_m$	32	0	28	0	33	84	358	379	181	174	187	187	325	282	171	94	382	369	148	100	1	119	2	60
R1$_m$	4	15	34	9	52	64	29	93	8	10	29	35	197	88	234	65	107	54	96	14	89	65	78	91

(a) Clustering results using the **first generated token representation**. Entries show Δ_0 and Δ_1 (absolute differences between valid and invalid SCEs in clusters 0 and 1) under the w/o (without context) and w/ (with context) settings.

	DEV				TWT				SST				FLK				NLI				MTH			
	Δ_0		Δ_1		Δ_0		Δ_1		Δ_0		Δ_1		Δ_0		Δ_1		Δ_0		Δ_1		Δ_0		Δ_1	
	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/
LAM$_s$	17	2	16	0	417	362	77	197	198	67	216	91	19	48	350	61	153	116	119	97	9	26	0	8
LAM$_m$	28	19	32	19	310	462	199	287	247	261	233	239	98	20	243	72	319	373	216	303	57	147	19	62
MST$_s$	10	17	11	23	320	187	322	150	206	170	117	145	137	85	53	76	104	183	173	42	36	6	2	30
MST$_m$	24	26	33	41	200	253	235	221	205	214	212	214	142	191	252	309	301	228	100	47	25	46	9	16
GEM$_s$	24	1	17	2	159	210	178	211	205	197	181	181	86	118	116	2	138	94	553	194	1	21	4	3
GEM$_m$	24	1	36	1	78	122	247	341	50	40	318	321	328	283	168	95	293	300	237	169	1	125	0	54
R1$_m$	4	15	34	9	66	70	43	99	59	47	38	2	220	98	211	55	73	22	130	46	78	54	89	102

(b) Clustering results using the **last input token representation**. Entries show Δ_0 and Δ_1 under w/o (without context) and w/ (with context).

	DEV				TWT				SST				FLK				NLI				MTH			
	Δ_0		Δ_1		Δ_0		Δ_1		Δ_0		Δ_1		Δ_0		Δ_1		Δ_0		Δ_1		Δ_0		Δ_1	
	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/	w/o	w/
LAM$_s$	26	2	7	0	257	280	237	279	231	85	183	73	239	37	130	72	135	74	137	139	2	12	7	22
LAM$_m$	32	26	28	12	401	425	108	324	225	245	255	255	247	8	94	84	226	327	309	349	45	111	31	98
MST$_s$	10	22	11	18	400	207	242	130	118	114	29	89	86	78	104	83	171	18	106	159	39	78	1	54
MST$_m$	32	40	25	27	390	282	45	192	202	210	215	218	192	168	202	50	151	61	250	214	24	34	10	28
GEM$_s$	15	5	26	8	67	86	270	335	314	305	72	73	193	49	9	67	270	154	421	134	0	23	5	1
GEM$_m$	41	0	19	0	73	50	398	413	135	127	233	234	82	12	414	176	234	369	296	100	6	67	7	112
R1$_m$	5	24	25	0	48	36	25	65	18	50	39	95	219	107	212	46	105	140	98	208	75	77	92	79

(c) Clustering results using the **last generated token representation**. Entries show Δ_0 and Δ_1 under w/o (without context) and w/ (with context).

Table 11: Comparison of clustering strategies for separating valid vs. invalid SCEs. Each panel reports results for one token-based representation (first generated token, last input token, last generated token). Performance is measured by Δ_0 and Δ_1, which quantify how well valid and invalid cases are separated within clusters under both w/o (without context) and w/ (with context) settings, where larger values indicate stronger separation.

	DEV	TWT	SST	FLK	NLI	MTH
LAM$_s$	**-55**	**-55**	0	**-81**	**15**	**43**
LAM$_m$	4	**1**	**-33**	**33**	**12**	**33**
MST$_s$	**16**	**6**	**1**	1	**26**	**44**
MST$_m$	**13**	**16**	**1**	**46**	**15**	**54**
GEM$_s$	**N/A**	**14**	1	**N/A**	**16**	-8
GEM$_m$	**11**	**16**	**-14**	0	**21**	**33**
R1$_m$	**25**	**25**	**-14**	**50**	**25**	**21**

(a) Unconstrained prompting: effect size on **validity**.

	DEV	TWT	SST	FLK	NLI	MTH
LAM$_s$	-19	**-8**	0	**7**	0	-2
LAM$_m$	0	1	2	0	0	1
MST$_s$	-2	-1	0	**-1**	0	-1
MST$_m$	0	0	0	0	0	0
GEM$_s$	N/A	-1	0	N/A	0	-10
GEM$_m$	-1	0	-1	0	0	-4
R1$_m$	2	**-3**	**-2**	**-1**	0	-6

(b) Unconstrained prompting: effect size on **normalized edit distance**.

	DEV	TWT	SST	FLK	NLI	MTH
LAM$_s$	**42**	**12**	**10**	**30**	**28**	-43
LAM$_m$	**9**	-1	**-14**	**38**	**23**	**15**
MST$_s$	**-60**	**-1**	-1	**-5**	**-56**	**-100**
MST$_m$	**40**	**24**	**12**	**50**	**99**	**39**
GEM$_s$	N/A	**19**	**18**	N/A	**23**	23
GEM$_m$	**51**	**14**	**7**	**36**	**25**	**21**
R1$_m$	**45**	**8**	**-16**	**38**	**24**	**44**

(c) Rationale-based prompting: effect size on **validity**.

	DEV	TWT	SST	FLK	NLI	MTH
LAM$_s$	3	**-8**	**-4**	**10**	0	-12
LAM$_m$	-1	**-4**	2	0	**-5**	**-6**
MST$_s$	-6	**-1**	0	-2	**-1**	0
MST$_m$	-1	**1**	-1	0	0	0
GEM$_s$	N/A	-1	-2	N/A	0	-5
GEM$_m$	-1	-1	-2	0	0	-2
R1$_m$	1	-1	**-7**	**-5**	-1	6

(d) Rationale-based prompting: effect size on **normalized edit distance**.

Table 12: Effect sizes (mean difference between with-context and without-context conditions) for validity and normalized edit distance under two prompting strategies (unconstrained and rationale-based) at $T = 0$ across datasets. Positive values indicate higher scores with context ($\mathtt{Val_C}$) compared to without context (`Val`), and bolded entries mark statistically significant differences.