

Interpreting and Steering LLMs with Mutual Information-based Explanations on Sparse Autoencoders

Xuansheng Wu¹, Jiayi Yuan², Wenlin Yao³, Xiaoming Zhai¹, Ninghao Liu¹

¹University of Georgia ²Rice University ³Amazon

¹{xuansheng.wu,xiaoming.zhai,ninghao.liu}@uga.edu ²jy101@rice.edu ³ywenlin@amazon.com

Abstract

Large language models (LLMs) excel at handling human queries, but they can occasionally generate flawed or unexpected responses. Understanding their internal states is crucial for understanding their successes, diagnosing their failures, and refining their capabilities. Although sparse autoencoders (SAEs) have shown promise for interpreting LLM internal representations, limited research has explored how to better explain SAE features, i.e., understanding the semantic meaning of features learned by SAE. Our theoretical analysis reveals that existing explanation methods suffer from the frequency bias issue, where they emphasize linguistic patterns over semantic concepts, while the latter is more critical to steer LLM behaviors. To address this, we propose using a fixed vocabulary set for feature interpretations and designing a mutual information-based objective, aiming to better capture the semantic meaning behind these features. We further propose two runtime steering strategies that adjust the learned feature activations based on their corresponding explanations. Empirical results show that, compared to baselines, our method provides more discourse-level explanations and effectively steers LLM behaviors to defend against jailbreak attacks. These findings highlight the value of explanations for steering LLM behaviors in downstream applications.¹

1 Introduction

Large language models (LLMs) have demonstrated strong capabilities in responding to general human requests (Achiam et al., 2023; Dubey et al., 2024; Jiang et al., 2024). Meanwhile, we still often observe failed or unexpected responses in certain situations (Ji et al., 2023; Wei et al., 2024). Gaining insight into the factors behind their successes and failures is crucial for further improving these models. A straightforward way to understand LLM

behaviors is by directly studying their hidden representations. However, it is non-trivial to achieve that because of the *polysemantic* nature (Arora et al., 2018; Scherlis et al., 2022) of the hidden space, where each dimension of the hidden representations encodes multiple pieces of unique features.

Researchers have made significant efforts to overcome the polysemantic challenge. Early works (Millidge and Black, 2022; Wu et al., 2024) apply matrix decomposition techniques to learn a set of orthogonal vectors to form the basis of hidden representations. However, this approach is insufficient to find vectors for certain purposes, as matrix decomposition techniques can only produce a limited number of orthogonal vectors. In this context, recent research has explored the sparse autoencoder (SAE) technique (Olshausen and Field, 1997; Makhzani and Frey, 2013), which has demonstrated their effectiveness in learning a large number of *sparse* feature vectors to reconstruct the hidden spaces of advanced LLMs with hundreds of billions of parameters (Cunningham et al., 2023; Bricken et al., 2023; Templeton et al., 2024; Gao et al., 2024). These learned sparse features are expected to be interpretable, since each feature should only react to a specific concept, showing a *monosemantic* nature instead of a polysemantic one.

However, the semantic meaning of sparse features learned by SAEs is **not directly comprehensible to humans**, requiring an additional step of post-hoc explanation. Furthermore, intuitively explaining the learned features poses a significant challenge. Existing works (Bricken et al., 2023; Gao et al., 2024) generate explanations for learned features by extracting text spans whose hidden representations could maximally activate the corresponding feature vector. However, Gao et al. (2024) found that many extracted text spans of learned features are too trivial to be used to explain the complex behaviors of LLMs. In addition, when steering LLMs according to the extracted

¹We will release our code and data once accepted.

Ours		<p>Ethical considerations in content creation: copyright; ethical; creativity; blog; writing; content; steal; copy; creative; introduce; patent.</p> <p>Decision-making and evaluation of outcomes: tune; keen; heading; impact; profit; judge; reasoning; influential; correction; bear.</p> <p>Interior design and household elements: mirror; tap; household; Hall; interior; echo; click; themes; Roman; elements.</p>
TopAct		<p>Childhood experiences and nostalgia: like my father's when I was a child; amour of the city since he was a child; tricks when she was a kid; own experiences of being bullied as a child; fit and Mel Brooks since he was a child.</p> <p>Descriptive writing on textures: at least 100 words about the texture; sensory details to describe the colors, textures; Compare and contrast the different textures; the scent of the ocean, and the texture; Incorporate elements such as textures.</p> <p>Cooking instructions on boiling and adjusting heat levels: Bring to a boil, reduce heat; the boil once again and then reduce the heat; boil, you will need to reduce the heat; Bring to a boil, then reduce heat; stirring occasionally.ln4. Reduce heat.</p>
N2G		<p>Shopping or going to a store: [MASK] to the store; going to the store; [MASK] to the store; went to the [MASK]; going to the store.</p> <p>Cellular biology on histones and actin: histones; histone; [MASK]osin and actin; composed of actin; role of actin.</p> <p>Postmodernism or post-structuralism themes: major figure in post; takes place in a post; to adjust to post; effects of post; politic context of post.</p>

Figure 1: Examples of explanations generated by ours and baseline methods. We separate raw extracted words/spans with “;” and **boldface** their automated summaries. We could observe that our method tends to use diverse words to describe a semantical concept. In contrast, the extracted spans from baseline methods typically share some duplicated phrases, indicating suffering from a frequency bias on those linguistic patterns.

text spans, the resulting responses may not always be predictable (Durmus et al., 2024). These challenges undermine confidence in using explanations to steer LLMs for real-world applications.

In this work, we introduce a novel post-hoc explanation method for learned features, and strategies to steer LLM behaviors based on our generated explanations. Our study starts with a theoretical analysis of the distribution of learned features, where we reveal that the learned features encode both *discourse topics* and *linguistic patterns* simultaneously, with the latter being less critical for model steering but occurring more frequently, named **frequency bias**. This frequency bias causes the existing methods to extract repetitive and superficial patterns. To address this challenge, we propose to leverage a fixed vocabulary set instead of the entire corpus for explanation, and further design a mutual information-based objective to ensure that the explanations capture critical information. As shown in Figure 1, baseline methods exhibit frequency bias, leading to repetitive phrases in their explanations, whereas our approach explains discourse topics with diverse words. We also explore steering LLMs for jailbreak defense based on our generated explanations of learned features. Experiments show that our method provides more meaningful discourse-level explanations than the other explainers, and these discourse-level explanations are effective in steering LLM behaviors on certain tasks. We summarize our contributions as follows:

- Our theoretical analysis identifies a key challenge in explaining learned features from sparse autoencoders, i.e., the frequency bias between the discourse and linguistic features.
- We propose leveraging a fixed vocabulary set to mitigate the frequency bias for explaining learned features. Experimental results show that our method uses more diverse words to explain discourse topics than the other explanation methods.

- We propose steering LLMs for specific purposes by adjusting the activations of learned features based on their explanations. Experiments confirm that we could enhance LLM’s safety by using our discourse-level explanations.

2 Preliminary

2.1 Problem Statement

Let \mathcal{V} denote the vocabulary set, and X be a text of length N , where $x_n \in \mathcal{V}$ denotes the n -th token of X . Given a language model f , the embedding of X at the l -th layer is denoted as $\mathbf{X}^{(l)} \in \mathbb{R}^{N \times D}$, where D is latent dimension. In the rest of this paper, we omit superscript (l) for simplification of notations. Our goal is to interpret embeddings \mathbf{X} by extracting some semantic features from the latent space. Specifically, there exists C learned feature vectors $\mathbf{W} \in \mathbb{R}^{C \times D}$ that can decompose arbitrary \mathbf{X} as a linear combination, i.e., $\mathbf{X} \approx \mathbf{AW}$, where $C \gg D$, $\mathbf{A} \in \mathbb{R}^{N \times C}$ are the weights of the linear combination. Let \mathbf{W}_c denote the c -th row of \mathbf{W} . After the decomposition, \mathbf{X} is explainable if we could understand the semantic meaning of each learned feature vector \mathbf{W}_c . In this paper, we focus on seeking a set of words $\mathcal{I}_c \subset \mathcal{V}$ to explain each learned feature \mathbf{W}_c with natural language.

2.2 Learning and Interpreting LLMs with Sparse Autoencoders

Many attempts have been made to learn feature vectors \mathbf{W} for interpreting LLMs, where sparse autoencoders have shown great promise for this purpose (Gao et al., 2024; Lieberum et al., 2024). Typically, sparse autoencoder (Olshausen and Field, 1997; Makhzani and Frey, 2013) is a two-layer multi-layer perceptron $\hat{\mathbf{X}} = \sigma(\mathbf{X}\mathbf{W}^\top) \cdot \mathbf{W}$ with the tight weight strategy, and is trained by minimizing the reconstruction loss $\mathcal{L} = \|\mathbf{X} - \hat{\mathbf{X}}\|_2$, where $\mathbf{W} \in \mathbb{R}^{C \times D}$ are trainable parameters and σ refers to the Top-K activation function. The Top-K activa-

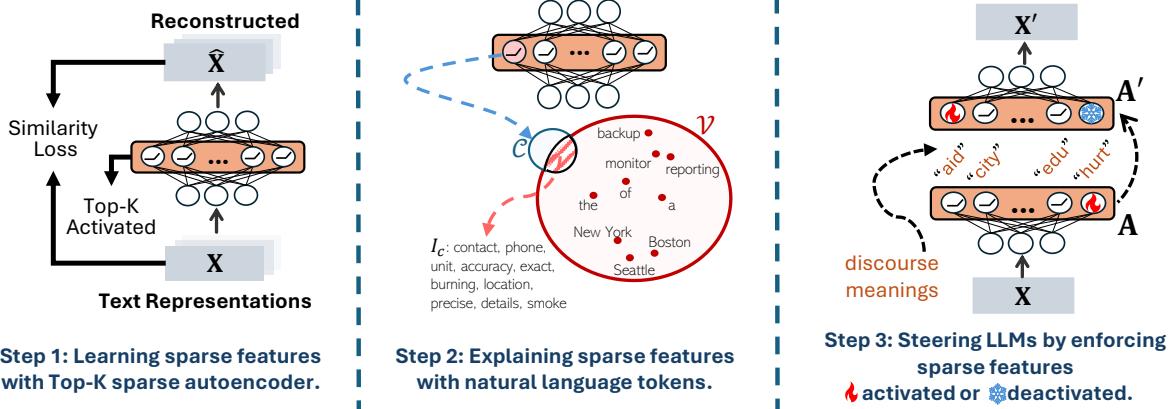


Figure 2: The proposed framework of explaining SAE features and steering LLMs with explanations.

tion function only keeps the K largest values and enforces other values as zeros, leading to the nature of *sparsity* to the autoencoder. The sparsity indicates that each learned row vector \mathbf{W}_c should only be activated by a certain kind of input, showing the monosemantic instead of polysemantic.

However, there are limited explorations on collecting a natural language explanation \mathcal{I}_c for each learned feature vector \mathbf{W}_c . The most straightforward strategy (Bricken et al., 2023) is collecting some N-gram spans over a large corpus whose hidden representations can best activate the feature vector \mathbf{W}_c . Some researchers (Gao et al., 2024) leverage the Neuron-to-Graph (N2G) algorithm (Foote et al., 2023) to refine the N-gram spans for more precise interpretations. However, these methods typically tend to extract some superficial and trivial patterns (Gao et al., 2024), and those generated explanations are not always effective in steering LLM behaviors for certain purposes (Durmus et al., 2024). In the following, we will first analyze the challenge of interpreting these learned features, followed by a novel explanation method to overcome the challenge and strategies to use these explanations for downstream tasks.

3 Methodology

This section first theoretically studies the properties of text generation, comparing them to traditional image generation scenarios where sparse autoencoders were initially developed for. With these insights, we propose a mutual information-based method to explain the semantics of learned features, and further design two strategies to steer LLMs based on the explained features. Figure 2 illustrates our overall framework.

3.1 Feature Dynamics in Text Data

Sparse autoencoders (Olshausen and Field, 1997) were originally designed for image data under the assumption that each image can be expressed as a linear combination of underlying *features*. Previous works (Bricken et al., 2023; Cunningham et al., 2023) adapt this framework to textual data by similarly assuming that each token is linearly related to a set of features. However, these approaches overlook certain inherent properties of textual data, resulting in a significant challenge in interpreting the learned feature vectors.

We consider the text generation task as a dynamic process under the topic-model assumption (Steyvers and Griffiths, 2007; Arora et al., 2016, 2018), where each word x_n is generated at the n -th step. It means that, in topic models, text generation begins with a predetermined concept or theme, guiding word selection at each step to align with that central idea. Formally, this dynamic process can be driven by the random walk of a discourse vector $\mathbf{e}_{c_n} \in \mathbb{R}^d$ representing what it talks about. The discourse vector \mathbf{e}_{c_n} does a slow random walk at each step n , i.e., $\mathbf{e}_{c_n} = \mathbf{e}_{c_{n-1}} + \mathbf{e}_{e_n}$, where $\mathbf{e}_{e_n} \sim \mathcal{N}^d(0, \sigma)$. Also, at each step, a word $x_n \in \mathcal{V}$ is sampled based on the discourse vector \mathbf{e}_{c_n} . To this end, the text generation process for a sequence of words X is given by:

$$p(X) = \prod_{n=1}^{|X|} p(x_n | c_n) \cdot p(c_n | c_{n-1}). \quad (1)$$

Here, the word emission probability is modelled by $p(x_n | c_n) = \frac{\exp(\langle \mathbf{e}_{x_n}, \mathbf{e}_{c_n} \rangle)}{\sum_{v \in \mathcal{V}} \exp(\langle \mathbf{e}_v, \mathbf{e}_{c_n} \rangle)}$ (Steyvers and Griffiths, 2007), where $\langle \cdot, \cdot \rangle$ indicates the dot product of two vectors. Since c_n is a random walk of c_{n-1} , the topic transmission probability can be computed

as $p(c_n|c_{n-1}) = \frac{1}{\sqrt{2\pi}\cdot\sigma} \cdot \exp\left(\frac{-\|\mathbf{e}_{c_n} - \mathbf{e}_{c_{n-1}}\|_2}{2\sigma}\right)$ (Olshausen and Field, 1997). Recall that $\mathbf{e}_{c_n} = \mathbf{e}_{c_{n-1}} + \mathbf{e}_{\epsilon_n}$, after a few derivations, we have

$$\begin{aligned} \log p(X) &\propto \sum_{n=1}^N \langle \mathbf{e}_{x_n}, \mathbf{e}_{c_0} \rangle + \sum_{i=1}^N \sum_{n=1}^i \langle \mathbf{e}_{x_n}, \mathbf{e}_{\epsilon_n} \rangle \\ &\quad - \sum_{n=1}^N \frac{\|\mathbf{e}_{\epsilon_n}\|_2}{2\sigma}. \end{aligned} \quad (2)$$

Equation 2 reveals some critical characteristics of textual data that are different from image data. Firstly, **there is a shared discourse topic c_0 across words x_n from the same X , for $n = 1, \dots, N$.** However, recent approaches that use sparse autoencoders for LLMs often treat the reconstruction loss for each token independently, without adding constraints to capture the shared concepts. As a result, they fail to isolate the features learned for discourse semantical topics (i.e., \mathbf{e}_{c_0}) and linguistic patterns (i.e., \mathbf{e}_{ϵ_n}). Thus, each learned feature \mathbf{W}_c may store both discourse and linguistic information, where the latter is less useful for steering LLMs than the previous one. In addition, **discourse topics are rarer than linguistic patterns, called frequency bias**, as each X has N times more linguistic patterns than its discourse topic. This issue leads to the learned features that prioritize capturing the linguistic patterns, raising the challenge of interpreting those encoded discourse topics.

3.2 Explaining Learned Features with Natural Language

To interpret the learned features $\{\mathbf{W}_c\}_{c=1}^C$, existing works (Bricken et al., 2023; Gao et al., 2024) typically enumerate a large number of texts, and then treat those whose hidden representations could most activate the learned features as the interpretations. This method works well for interpreting the learned linguistic patterns as they are frequently presented in the corpus, while it is hard to discover the learned discourse topics because the more frequent linguistic patterns dominate, leading to the failure of steering LLM behaviors based on the explanations (Gao et al., 2024; Durmus et al., 2024). Since our goal is to understand and control LLM behaviors, we aim to interpret those discourse topics within a feasible budget cost.

To tackle the challenge of frequency bias, we propose to leverage a fixed vocabulary set \mathcal{V} of a general corpus instead of its raw texts. Our goal is to seek a M -word set $\mathcal{I}_c \subset \mathcal{V}$ that can describe

most information of the c -th feature vector \mathbf{W}_c . Mathematically, we let \mathcal{C} denote the knowledge encoded by \mathbf{W}_c and measure the information of \mathcal{C} described by a given word set $\mathcal{V}' \subset \mathcal{V}$ based on their mutual information (Cover, 1999). To this end, the objective of constructing \mathcal{I}_c is defined as

$$\begin{aligned} \mathcal{I}_c &= \arg \max_{\mathcal{V}' \subset \mathcal{V}, |\mathcal{V}'|=M} \text{MI}(\mathcal{V}'; \mathcal{C}) \propto \arg \min_{\mathcal{V}' \subset \mathcal{V}, |\mathcal{V}'|=M} H(\mathcal{C}|\mathcal{V}') \\ &= \arg \max_{\mathcal{V}' \subset \mathcal{V}, |\mathcal{V}'|=M} \sum_{\mathbf{e}_c \in U(\mathcal{C})} \sum_{w \in \mathcal{V}'} p(\mathbf{e}_c)p(w|\mathbf{e}_c) \log p(\mathbf{e}_c|w), \end{aligned} \quad (3)$$

where $\text{MI}(\cdot; \cdot)$ indicates mutual information between two variables, $H(\cdot| \cdot)$ denotes the conditional Shannon entropy, and $U(\mathcal{C})$ includes all possible vectors that express the knowledge \mathcal{C} . Since we obtain \mathbf{W}_c by training a sparse autoencoder—and ideally, each learned feature vector encodes a unique piece of knowledge—we assume that $p(\mathbf{e}_c = \mathbf{W}_c) \approx 1$ and $p(\mathbf{e}_c \neq \mathbf{W}_c) \approx 0$. This allows us to simplify the expression as:

$$\mathcal{I}_c \propto \arg \max_{\mathcal{V}' \subset \mathcal{V}, |\mathcal{V}'|=M} \sum_{w \in \mathcal{V}'} p(w|\mathbf{W}_c) \log p(\mathbf{W}_c|w). \quad (4)$$

By leveraging output embedding \mathbf{e}_w of word w , we empirically estimate $p(w|\mathbf{W}_c)$ and $p(\mathbf{W}_c|w)$ by

$$\begin{aligned} p(w|\mathbf{W}_c) &= \frac{\exp(\langle \mathbf{e}_w, \mathbf{W}_c \rangle)}{\sum_{w' \in \mathcal{V}} \exp(\langle \mathbf{e}_{w'}, \mathbf{W}_c \rangle)}, \\ p(\mathbf{W}_c|w) &= \frac{\exp(\langle \mathbf{e}_w, \mathbf{W}_c \rangle)}{\sum_{c' \in \mathcal{C}} \exp(\langle \mathbf{e}_w, \mathbf{W}_{c'} \rangle)}. \end{aligned} \quad (5)$$

Compared with a trivial strategy that obtains M words whose output embeddings best activate the feature vector (Nostalgebraist, 2020), our mutual information-based objective reveals the importance of normalizing activations of a single word across all learned features. In other words, if a word embedding constantly leads to a significant large dot product with all features, the word will not express enough specificity to any certain feature. In information retrieval, TF-IDF (Salton and Buckley, 1988) is a practical technique for mitigating frequency bias and it can be formulated from the same mutual information-based objective that we used in this work as suggested by Aizawa (2003). However, TF-IDF relies on assumptions about word distributions over documents, which do not hold in our feature interpretation task. Therefore, we derive our method from a more general perspective, better aligning this objective with the context of interpreting learned sparse feature vectors.

3.3 Steering LLMs with Explained Features

Given learned features $\{\mathbf{W}_c\}_{c=1}^C$ and their explanations $\{\mathcal{I}_c\}_{c=1}^C$, we could identify a subset of the features $\mathbf{S} = \{\mathbf{W}_s\}_{s=1}^S \subset \{\mathbf{W}_c\}_{c=1}^C$ that are correlated with a specific LLM behavior we are interested in based on their explanations (e.g., harmful knowledge or safety awareness in our study). This annotating process can be easily scaled up by leveraging advanced LLMs (Bills et al., 2023) as our explanations are natural language. Considering the hidden representations of an input prompt as \mathbf{X} , we propose two strategies to steer LLM representations with the identified features \mathbf{S} during runtime.

Amplification. We amplify α times of the activations on our identified feature vectors, i.e., $\mathbf{X}' = \mathbf{X} + \alpha \cdot \text{ReLU}(\mathbf{XS})\mathbf{S}^\top$, where α is a hyper-parameter. We encourage LLMs to be more aware of the identified features if $\alpha > 0$, and pay less attention to them if $\alpha < 0$. Especially, $\alpha = -1$ indicates that we erase the LLM’s awareness of the identified features from its hidden representations.

Calibration. We enforce LLMs to focus on the identified features to a certain level β , i.e., $\mathbf{X}' = \mathbf{X} - \text{ReLU}(\mathbf{XS})\mathbf{S}^\top + \beta \cdot \bar{\mathbf{S}}$, where $\bar{\mathbf{S}}$ is the mean vector of \mathbf{S} and β is a hyper-parameter. This strategy inherently shifts the LLM’s hidden space toward the center of our target feature vectors.

The above two strategies are responsible for different purposes of steering LLMs, and they could work together. We would also emphasize that the proposed strategies are efficient as we only monitor a subset of our interested features \mathbf{S} instead of the entire set of learned sparse features \mathbf{W} .

4 Experiments

This section investigates two research questions. RQ1: Does the proposed method generate more discourse-level explanations than traditional methods? RQ2: Whether these discourse-level explanations are useful in steering LLM behaviors? To answer these questions, Sec. 4.1 describes some details of the Top-K sparse autoencoder we used in our study. Sec. 4.2 compares the explanation quality of our proposed methods and others for RQ1. Sec. 4.3 finally explores the usability of the explanations for defending jailbreak attacks for RQ2.

4.1 General Settings

Language Models. We study LLMs from the Mistral family (Jiang et al., 2023) as it has demonstrated its strong usability in the wild. In particular, we use the Mistral-7B-Instruct-v0.2 checkpoint

from Huggingface (Wolf, 2019). Following previous works (Lieberum et al., 2024) on Gemma2-9B-Instruct, we consider the residual stream at the 25%-th, 50%-th, and 75%-th layers of entire model to train our sparse autoencoders, referring the 8th, 16th, and 24th layers of Mistral-7B-Instruct. Our main experiments are conducted on the 8th layer as we found that it shows the best effectiveness in steering LLM behaviors (see discussion in Appendix A.3). Without specifics, the greedy search decoding with a maximum of 512 new tokens is applied to our experiments for reproducibility.

Datasets. We consider various instruction-tuning datasets for training our backbone sparse autoencoders. In specific, ShareGPT (RyokoAI, 2023), UltraChat (Ding et al., 2023), HH-RLHF (Bai et al., 2022), WebGLM-QA (Liu et al., 2023), Evol-Instruct (Xu et al., 2023), and HelpSteer2 (Wang et al., 2024) are selected. We de-duplicate prompts across different datasets and sample a subset of UltraChat with 400K samples. To this end, we have retained about 711K prompts, with an average length of 177.9 tokens. We randomly select 90% of prompts to form our training set, and the rest is our validation set. Overall, we collect 113M tokens for training and 12M tokens for validating.

Training Details. Our training procedures and hyper-parameter settings majorly follow the previous works (Bricken et al., 2023; Gao et al., 2024; Lieberum et al., 2024). Specifically, we initialize $C = 2^{16}$ feature vectors for a Top-K sparse autoencoder with Kaiming initialization (He et al., 2015). Here, $C = 2^{16}$ is set according to the scaling law between the number of features C and the number of training tokens Z found by (Gao et al., 2024), i.e., $C = \mathcal{O}(Z^\gamma)$, where $\gamma \approx 0.60$ for GPT2-small and $\gamma \approx 0.65$ for GPT-4². Appendix B provides more details about training sparse autoencoders.

Explanation Baselines. Our study considers several existing works for sparse autoencoder explanations as baselines. *TopAct* (Bricken et al., 2023) collects a mount of text spans from the corpus that could maximally activate it. *N2G* (Gao et al., 2024) steps further by masking some words from the activated spans that show limited contributions to the activations. We collect their activated spans, with a maximum of 10 tokens, over the entire validation set, and we keep the most activated span from each entry to increase their diversity.

²Empirically, $\gamma \approx 0.5978$ in our study.

Table 1: Qualitative analysis on generated explanations. Both TopAct and N2G tend to collect raw explanations sharing the same word-level patterns, while our method generate explanations for discourse-level topics with diverse words. We highlight those duplicated patterns and diverse words related to a concise topic.

Method	Raw Extracted Words or Text Spans	Automated Summary
Ours	previously; suddenly; repeated; history; once; initially; nearest; already; normally; originally	Temporal concepts and sequences in narratives.
	commonly; impact; cater; widely; normally; gallery; judge; pros; independent; accurately	Art evaluation and critique.
	client; visual; application; blank; deep; download; development; retrieve; reporting; clone	Software development and application management processes.
	What criteria does Pitchfork use to ; What evaluation criteria will Kumar organization use to ; and what criteria were used ; market? what specific criteria should be used ; needed to conduct a comprehensive analysis and the criteria used	Evaluation criteria for assessments or analyses in various contexts.
TopAct	[INST] Provide step; [INST] Provide step; [INST] Provide step; [INST] Provide step; [INST] Provide step	Instructional prompts or commands for providing steps in a process.
	ideas and produce compelling content — again ; Pine View School again ; technologies segment is again ; pushed on the ceiling, and again ; Echoed through the valley, again	Repetition of the word "again" in various contexts
N2G	CSV; CSV; CSV; CSV; csv[MASK]	Data format: CSV.
	schedule appoint ; upcoming appoint [MASK]; appointment ; appointment ; upcoming appoint [MASK]	Scheduling and managing appointments.
	Final Fant; Final Fant; Final Fant; Final Fant; Metal Gear	Video game titles.

4.2 Evaluating Explanations of Learned Sparse Features

Exactly measuring the explanation quality of features from sparse autoencoders is still an open question (Rajamanoharan et al., 2024). Following existing works (Bricken et al., 2023; Bills et al., 2023; Rajamanoharan et al., 2024), advanced LLMs (i.e., GPT4o Family) serve as the machine annotator to evaluate the quality of generated explanations.

4.2.1 Experimental Designs

We conduct both qualitative and quantitative analyses of the explanations with the help of our machine annotator (please check details in Appendix D). Here, the explanations of TopAct and N2G are the top 5 most activated text spans on the validating set, while our method chooses the top 10 words over a vocabulary set constructed from the training set. We prompt the machine annotator to summarize the meaning of the feature based on the selected words/spans. After collecting the summary, we invoke the machine annotator in a separate thread to judge the relevance of the raw explanations, following the approach in (Bills et al., 2023). We follow previous work (Rajamanoharan et al., 2024) to give the judgment with four-level options, and we treat the summaries judged with the highest two levels as successfully explained. Table 1 shows some cases

Table 2: Successful explained rate of explanations for the activated features and overall learned features.

Method	Activated Feature	Overall Feature
TopAct	59.16%	23.17%
N2G	38.79%	15.13%
Ours	67.39%	66.98%

confirmed with the highest judging level by machine annotator (Appendix C provides more cases.). The percentage of successfully explained raw explanations from different explainers in Table 2.

4.2.2 Results

TopAct and N2G tend to collect text spans sharing the same lexical patterns, while our method extracts diverse words to present a concise topic. Table 1 shows that while both TopAct and N2G often repeat the same phrases (e.g., “used to” and “CSV”), our method selects more varied words that converge on a concise and discourse-level topic. This contrast highlights our goal of moving beyond repeated lexical patterns to richer and more discourse-focused explanations.

Our method generates more reasonable explanations than that of TopAct and N2G. Table 2 reports the percentage of learned sparse features successfully explained, categorized by those activated in the validation set and overall. We first

Table 3: Defending Mistral-7b-Instruct from jailbreak attacks without model training. We report the attack success rate (ASR) on Salad-Bench to illustrate the effectiveness of preventing jailbreak attacks, and the automatic scores on the MT-Bench to demonstrate the helpfulness for general user queries.

Category	Method	Salad-Bench (Safety)		MT-Bench (Helpful)	
		ASR (\downarrow)	Time (\downarrow)	Score (\uparrow)	Time (\downarrow)
w/o Defense		81.6	1.0x	6.5	1.0x
Perturbation	Random Patch	80.6	4.9x	3.8	1.6x
	Random Insert	79.4	6.5x	3.7	1.6x
	Random Swap	73.8	5.6x	3.0	1.6x
	Self-Robustness	16.2	6.9x	5.3	16.9x
Prompting	SafePrompt	79.0	1.0x	6.5	1.0x
	XSafePrompt	77.8	0.9x	6.1	0.9x
	Self-Reminder	73.0	0.9x	6.3	0.9x
SAE Steer (Ours)	Erase Harmful (EH)	81.0	1.0x	5.9	1.0x
	Aware Security (AS)	73.2	0.8x	6.0	0.9x
	EH + AS	72.8	0.8x	5.9	0.9x

observe that many features remain unexplained by TopAct and N2G due to insufficient activation on the validation set, highlighting a key limitation of relying on activation-based text spans for explanation. One might argue that collecting activation spans from the training set could help, but this introduces bias, as sparse autoencoders tend to overfit the training set (Tom and Chris, 2023). Even when considering only features activated in the validation set, our method achieves a higher explainability rate (67.30%) compared to TopAct (59.16%) and N2G (38.79%). Notably, N2G performs worse than TopAct, likely due to its stronger bias toward lexical patterns³. These results highlight the challenge of explaining discourse-level meanings of features.

4.3 Using Explained Features for Defending Jailbreak Attacks

We explore jailbreak defense as a downstream application of steering LLMs with explained features. We target this task for its broad applicability across various LLM deployment scenarios, where existing defense methods often suffer from either low effectiveness or impractical latency, underscoring the need for more efficient solutions.

³For example, one feature whose TopAct explanation is “6th century (via History Magazine). Before that”; “Prior to Chomsky’s work,”; and “Reference [2]: Before the GPS,”, indicating “referring related works”. However, N2G simplifies them to “Before that”; “Prior to [MASK]omsky’s work”; and “Before [MASK] GPS”, which obviously changes the meaning and concentrates on some trivial patterns.

4.3.1 Experimental Designs

We evaluate the downstream task performance of our steered LLM using Salad-Bench (Li et al., 2024) for safety and MT-Bench (Zheng et al., 2023) for general helpfulness. Baselines include perturbation-based methods (Random Patch/Insert/Swap (Robey et al., 2023), Self-Paraphrase (Cao et al., 2023)) and prompting-based methods (SafePrompt/XSafePrompt (Deng et al., 2023), Self-Reminder (Xie et al., 2023)), all of which require no additional training. We consider three specific strategies based on our proposed Amplification and Calibration: (1) Erase Harmful (EH) deactivates harmful features if they are activated, (2) Aware Security (AS) consistently activates safety-related features at a certain level $\alpha =$, and (3) AS+EH combines both. We prompt our machine annotator to judge whether each clearly explained feature relates to a harmful concept according to the hazard taxonomy suggested by Llama3-Guard (Llama Team, 2024). Similarly, we also identify those safety-related features with a manually crafted safeguarding taxonomy inspired by the hazard taxonomy. As a result, there are 141 and 48 features for AS and EH, respectively. Table 3 and Figure 3 compare our method with baselines in attack success rate (ASR), MT-Bench scores, and normalized runtime cost. Appendix A.2 provides a case study on defending jailbreak attacks with the AS strategy, and Appendix A.1 includes more details about our experimental settings.

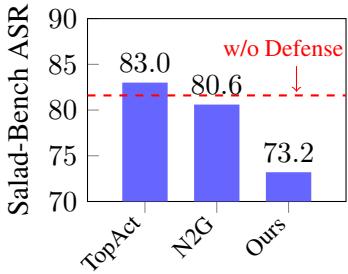


Figure 3: Applying Aware Security for jailbreak defense based on explanations from different methods.

4.3.2 Results

Sparse autoencoders enable runtime steering of LLMs. Table 3 shows that perturbation-based defense strategies are less practical for real-world use, as they either severely degrade helpfulness or introduce unacceptable latency. While most prompting-based methods preserve helpfulness, they struggle to prevent jailbreak attacks. The exception is Self-Reminder, the strongest baseline, which balances safety and helpfulness within a reasonable computing budget. In comparison, our sparse autoencoder-based approach *significantly improves jailbreak defense* (Salad-Bench: 81.6 → 72.8) while *maintaining helpfulness* with only a slight reduction (MT-Bench: 6.5 → 6.0).

The key to preventing jailbreak attacks is not forgetting harmful content, but staying aware of safety. Our experiments reveal that removing harmful knowledge has little impact on jailbreak defense, challenging the intuitive assumption that erasure improves safety. Instead, the strong performance of our Aware Security strategy aligns with the principle of Self-Reminder: “Reminding ChatGPT to respond responsibly” (Xie et al., 2023).

Discourse-level explanations are crucial for effective jailbreak defense. We apply the AS strategy to TopAct and N2G explanations, with results in Figure 3. Only N2G shows a slight ASR reduction, and tuning β brings no clear improvement. This is likely due to their overly lexical and fine-grained safety strategies. For example, an N2G feature under “Physical Defense” is summarized as “Locking mechanisms or security systems,” but its explanation consists of repetitive words: “locks; locks; lock; have a two-stage lock; lock.” In contrast, our method, under the same category, provides a broader summary “Emergency response and location tracking” with a more diverse explanation: “contact, phone, unit, accuracy, exact, burning, location, precise, details, smoke.” These results highlight the need for discourse-level explanations.

5 Related Works

Modern large language models have shown promising text-generation abilities, prompting researchers to explore their internal mechanisms. One approach (Belinkov et al., 2018; Jawahar et al., 2019; Rogers et al., 2021) develops contrastive datasets to probe hidden states for specific features, but it is limited by the polysemantic nature of neurons (Elhage et al., 2022; Olah et al., 2020), making the explanations non-concise and difficult to apply in downstream tasks. To overcome this, researchers (Bricken et al., 2023) propose learning orthogonal basis vectors to better understand LLMs. Early works (Beren and Black, 2022; Wu et al., 2024) applied singular vector analysis to identify concise, interpretable directions in neuron activations. Soon after, sparse autoencoders (Bricken et al., 2023; Cunningham et al., 2023) were introduced, allowing for more flexible settings. Sparse autoencoders, initially used to analyze image data (Olshausen and Field, 1997; Makhzani and Frey, 2013), are now being applied to LLMs. Researchers from Anthropic (Bricken et al., 2023) and EleutherAI (Cunningham et al., 2023) demonstrated that activations from smaller models like GPT-2 and Pythia yield highly interpretable features. Subsequent studies showed these features help interpret model behaviors in tasks like indirect object identification (Makelov, 2024), translation (Dumas et al.), and circuit detection (Marks et al., 2024). Recent works (Templeton et al., 2024; Gao et al., 2024; Lieberum et al., 2024) confirm this technique’s success with larger LLMs. Our study follows this path, and advances by developing a method for generating discourse-level explanations to steer LLM representations.

6 Conclusions

In this work, we step a solid stamp toward understanding and steering LLMs in the wild. Our theoretical analysis first reveals a frequency bias between discourse and linguistic features learned by sparse autoencoders. To eliminate this bias, we propose seeking words from a fixed vocabulary set and designing a mutual information-based objective to ensure the collected words capture the features’ meanings. Additionally, we demonstrate that our steering strategies effectively enhance the safety of LLMs using our mutual information-based explanations. This research underscores the importance of discourse-level explanations in effectively controlling LLM behaviors for certain purposes.

7 Limitations

This research focuses on improving language models for specific applications by first interpreting and then steering their hidden representations. A primary limitation of this work is that our approach builds upon existing (trained) sparse autoencoders, which we identify as suffering from frequency bias (as discussed in Section 3.1). While our proposed explanation method mitigates this issue, it does not fundamentally alter their architectures or training processes. Future work could explore designing improved architectures or training objectives that inherently mitigate frequency bias, rather than solely addressing it at the explanation level.

8 Ethical Impact

This study utilizes the publicly available Mistral-Instruct (Jiang et al., 2023) checkpoint under its academic-use license, strictly adhering to its terms for research purposes. We also incorporate multiple datasets (RyokoAI, 2023; Ding et al., 2023; Bai et al., 2022; Liu et al., 2023; Xu et al., 2023; Wang et al., 2024) and benchmarks (Li et al., 2024; Zheng et al., 2023), each used in compliance with their respective licensing and privacy regulations. To uphold ethical standards, we ensure that the presentation of this paper does not disclose personal identifiers or include harmful content.

Our work aims to improve LLM interpretability and steering to enhance safety, particularly in defending against jailbreak attacks. However, we recognize that steering LLMs also carries potential risks, such as reinforcing biases or enabling unintended manipulation. Addressing these concerns requires continuous research into bias mitigation and fairness in AI. Furthermore, while our approach strengthens LLM safety, adversaries may develop new attack strategies to circumvent these defenses. We encourage ongoing red-teaming efforts and responsible deployment practices to ensure that advancements in LLM security do not inadvertently contribute to more sophisticated attack techniques.

References

- Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altenschmidt, Sam Altman, Shyamal Anadkat, and 1 others. 2023. Gpt-4 technical report. *arXiv preprint arXiv:2303.08774*.
- Akiko Aizawa. 2003. An information-theoretic perspective of tf-idf measures. *Information Processing & Management*, 39(1):45–65.
- Sanjeev Arora, Yuanzhi Li, Yingyu Liang, Tengyu Ma, and Andrej Risteski. 2016. A latent variable model approach to pmi-based word embeddings. *Transactions of the Association for Computational Linguistics*, 4:385–399.
- Sanjeev Arora, Yuanzhi Li, Yingyu Liang, Tengyu Ma, and Andrej Risteski. 2018. Linear algebraic structure of word senses, with applications to polysemy. *Transactions of the Association for Computational Linguistics*, 6:483–495.
- Yuntao Bai, Andy Jones, Kamal Ndousse, Amanda Askell, Anna Chen, Nova DasSarma, Dawn Drain, Stanislav Fort, Deep Ganguli, Tom Henighan, and 1 others. 2022. Training a helpful and harmless assistant with reinforcement learning from human feedback. *arXiv preprint arXiv:2204.05862*.
- Yonatan Belinkov, Lluís Márquez, Hassan Sajjad, Nadir Durrani, Fahim Dalvi, and James Glass. 2018. Evaluating layers of representation in neural machine translation on part-of-speech and semantic tagging tasks. *arXiv preprint arXiv:1801.07772*.
- Beren and Sid Black. 2022. The singular value decompositions of transformer weight matrices are highly interpretable.
- Steven Bills, Nick Cammarata, Dan Mossing, Henk Tillman, Leo Gao, Gabriel Goh, Ilya Sutskever, Jan Leike, Jeff Wu, and William Saunders. 2023. Language models can explain neurons in language models. *URL https://openaipublic.blob.core.windows.net/neuron-explainer/paper/index.html*. (Date accessed: 14.05. 2023), 2.
- Trenton Bricken, Adly Templeton, Joshua Batson, Brian Chen, Adam Jermyn, Tom Conerly, Nick Turner, Cem Anil, Carson Denison, Amanda Askell, Robert Lasenby, Yifan Wu, Shauna Kravec, Nicholas Schiefer, Tim Maxwell, Nicholas Joseph, Zac Hatfield-Dodds, Alex Tamkin, Karina Nguyen, and 6 others. 2023. Towards monosemanticity: Decomposing language models with dictionary learning. *Transformer Circuits Thread*. *Https://transformercircuits.pub/2023/monosemantic-features/index.html*.
- Bochuan Cao, Yuanpu Cao, Lu Lin, and Jinghui Chen. 2023. Defending against alignment-breaking attacks via robustly aligned ILM. *arXiv preprint arXiv:2309.14348*.
- Maheep Chaudhary and Atticus Geiger. 2024. Evaluating open-source sparse autoencoders on disentangling factual knowledge in gpt-2 small. *arXiv preprint arXiv:2409.04478*.
- Thomas M Cover. 1999. *Elements of information theory*. John Wiley & Sons.

- Hoagy Cunningham, Aidan Ewart, Logan Riggs, Robert Huben, and Lee Sharkey. 2023. Sparse autoencoders find highly interpretable features in language models. *arXiv preprint arXiv:2309.08600*.
- Yue Deng, Wenxuan Zhang, Sinno Jialin Pan, and Lidong Bing. 2023. Multilingual jailbreak challenges in large language models. *arXiv preprint arXiv:2310.06474*.
- Ning Ding, Yulin Chen, Bokai Xu, Yujia Qin, Zhi Zheng, Shengding Hu, Zhiyuan Liu, Maosong Sun, and Bowen Zhou. 2023. Enhancing chat language models by scaling high-quality instructional conversations. *arXiv preprint arXiv:2305.14233*.
- Abhimanyu Dubey, Abhinav Jauhri, Abhinav Pandey, Abhishek Kadian, Ahmad Al-Dahle, Aiesha Letman, Akhil Mathur, Alan Schelten, Amy Yang, Angela Fan, and 1 others. 2024. The llama 3 herd of models. *arXiv preprint arXiv:2407.21783*.
- Clément Dumas, Veniamin Veselovsky, Giovanni Monea, Robert West, and Chris Wendler. How do llamas process multilingual text? a latent exploration through activation patching. In *ICML 2024 Workshop on Mechanistic Interpretability*.
- Esin Durmus, Alex Tamkin, Jack Clark, Jerry Wei, Jonathan Marcus, Joshua Batson, Kunal Handa, Liane Lovitt, Meg Tong, Miles McCain, Oliver Rausch, Saffron Huang, Sam Bowman, Stuart Ritchie, Tom Henighan, and Deep Ganguli. 2024. Evaluating feature steering: A case study in mitigating social biases.
- Nelson Elhage, Tristan Hume, Catherine Olsson, Nicholas Schiefer, Tom Henighan, Shauna Kravec, Zac Hatfield-Dodds, Robert Lasenby, Dawn Drain, Carol Chen, and 1 others. 2022. Toy models of superposition. *arXiv preprint arXiv:2209.10652*.
- Alex Foote, Neel Nanda, Esben Kran, Ioannis Konstas, Shay Cohen, and Fazl Barez. 2023. Neuron to graph: Interpreting language model neurons at scale. *arXiv preprint arXiv:2305.19911*.
- Leo Gao, Tom Dupré la Tour, Henk Tillman, Gabriel Goh, Rajan Troll, Alec Radford, Ilya Sutskever, Jan Leike, and Jeffrey Wu. 2024. Scaling and evaluating sparse autoencoders. *arXiv preprint arXiv:2406.04093*.
- Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. 2015. Delving deep into rectifiers: Surpassing human-level performance on imagenet classification. In *Proceedings of the IEEE international conference on computer vision*, pages 1026–1034.
- Ganesh Jawahar, Benoît Sagot, and Djamel Seddah. 2019. What does bert learn about the structure of language? In *ACL 2019-57th Annual Meeting of the Association for Computational Linguistics*.
- Ziwei Ji, Nayeon Lee, Rita Frieske, Tiezheng Yu, Dan Su, Yan Xu, Etsuko Ishii, Ye Jin Bang, Andrea Madotto, and Pascale Fung. 2023. Survey of hallucination in natural language generation. *ACM Computing Surveys*, 55(12):1–38.
- Albert Q Jiang, Alexandre Sablayrolles, Arthur Mensch, Chris Bamford, Devendra Singh Chaplot, Diego de las Casas, Florian Bressand, Gianna Lengyel, Guillaume Lample, Lucile Saulnier, and 1 others. 2023. Mistral 7b. *arXiv preprint arXiv:2310.06825*.
- Albert Q Jiang, Alexandre Sablayrolles, Antoine Roux, Arthur Mensch, Blanche Savary, Chris Bamford, Devendra Singh Chaplot, Diego de las Casas, Emma Bou Hanna, Florian Bressand, and 1 others. 2024. Mixtral of experts. *arXiv preprint arXiv:2401.04088*.
- Diederik P Kingma. 2014. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*.
- Lijun Li, Bowen Dong, Ruohui Wang, Xuhao Hu, Wangmeng Zuo, Dahua Lin, Yu Qiao, and Jing Shao. 2024. Salad-bench: A hierarchical and comprehensive safety benchmark for large language models. *arXiv preprint arXiv:2402.05044*.
- Tom Lieberum, Senthooran Rajamoharan, Arthur Conmy, Lewis Smith, Nicolas Sonnerat, Vikrant Varma, János Kramár, Anca Dragan, Rohin Shah, and Neel Nanda. 2024. Gemma scope: Open sparse autoencoders everywhere all at once on gemma 2. *arXiv preprint arXiv:2408.05147*.
- Xiao Liu, Hanyu Lai, Hao Yu, Yifan Xu, Aohan Zeng, Zhengxiao Du, Peng Zhang, Yuxiao Dong, and Jie Tang. 2023. Webglm: Towards an efficient web-enhanced question answering system with human preferences. In *Proceedings of the 29th ACM SIGKDD Conference on Knowledge Discovery and Data Mining*, pages 4549–4560.
- AI @ Meta Llama Team. 2024. The llama 3 herd of models. *Preprint*, arXiv:2407.21783.
- Aleksandar Makelov. 2024. Sparse autoencoders match supervised features for model steering on the ioi task. In *ICML 2024 Workshop on Mechanistic Interpretability*.
- Alireza Makhzani and Brendan Frey. 2013. K-sparse autoencoders. *arXiv preprint arXiv:1312.5663*.
- Samuel Marks, Can Rager, Eric J Michaud, Yonatan Beilinkov, David Bau, and Aaron Mueller. 2024. Sparse feature circuits: Discovering and editing interpretable causal graphs in language models. *arXiv preprint arXiv:2403.19647*.
- Paulius Micikevicius, Sharan Narang, Jonah Alben, Gregory Diamos, Erich Elsen, David Garcia, Boris Ginsburg, Michael Houston, Oleksii Kuchaiev, Ganesh Venkatesh, and 1 others. 2017. Mixed precision training. *arXiv preprint arXiv:1710.03740*.

- Beren Millidge and Sid Black. 2022. The singular value decompositions of transformer weight matrices are highly interpretable.
- NostalgiaBraist. 2020. Interpreting gpt: the logit lens. <https://www.lesswrong.com/posts/AcKRB8wDpdaN6v6ru/interpreting-gpt-the-logit-lens>.
- Chris Olah, Nick Cammarata, Ludwig Schubert, Gabriel Goh, Michael Petrov, and Shan Carter. 2020. Zoom in: An introduction to circuits. *Distill*, 5(3):e00024–001.
- Bruno A Olshausen and David J Field. 1997. Sparse coding with an overcomplete basis set: A strategy employed by v1? *Vision research*, 37(23):3311–3325.
- Senthooran Rajamanoharan, Tom Lieberum, Nicolas Sonnerat, Arthur Conmy, Vikrant Varma, János Kramár, and Neel Nanda. 2024. Jumping ahead: Improving reconstruction fidelity with jumprelu sparse autoencoders. *arXiv preprint arXiv:2407.14435*.
- Alexander Robey, Eric Wong, Hamed Hassani, and George J Pappas. 2023. Smoothllm: Defending large language models against jailbreaking attacks. *arXiv preprint arXiv:2310.03684*.
- Anna Rogers, Olga Kovaleva, and Anna Rumshisky. 2021. A primer in bertology: What we know about how bert works. *Transactions of the Association for Computational Linguistics*, 8:842–866.
- RyokoAI. 2023. Sharegpt dataset.
- Gerard Salton and Christopher Buckley. 1988. Term-weighting approaches in automatic text retrieval. *Information processing & management*, 24(5):513–523.
- Adam Scherlis, Kshitij Sachan, Adam S Jermyn, Joe Benton, and Buck Shlegeris. 2022. Polysemy and capacity in neural networks. *arXiv preprint arXiv:2210.01892*.
- Mark Steyvers and Tom Griffiths. 2007. Probabilistic topic models. In *Handbook of latent semantic analysis*, pages 439–460. Psychology Press.
- Adly Templeton, Tom Conerly, Jonathan Marcus, Jack Lindsey, Trenton Bricken, Brian Chen, Adam Pearce, Craig Citro, Emmanuel Ameisen, Andy Jones, Hoagy Cunningham, Nicholas L Turner, Callum McDougall, Monte MacDiarmid, C. Daniel Freeman, Theodore R. Sumers, Edward Rees, Joshua Batson, Adam Jermyn, and 3 others. 2024. Scaling monosemanticity: Extracting interpretable features from claude 3 sonnet. *Transformer Circuits Thread*.
- Henighan Tom and Olah Chris. 2023. Dictionary learning worries. <https://transformer-circuits.pub/2023/may-update/index.html#dictionary-worries>.
- Zhilin Wang, Yi Dong, Olivier Delalleau, Jiaqi Zeng, Gerald Shen, Daniel Egert, Jimmy J. Zhang, Makesh Narsimhan Sreedhar, and Oleksii Kuchaiev. 2024. Helpsteer2: Open-source dataset for training top-performing reward models. *Preprint*, arXiv:2406.08673.
- Alexander Wei, Nika Haghtalab, and Jacob Steinhardt. 2024. Jailbroken: How does llm safety training fail? *Advances in Neural Information Processing Systems*, 36.
- T Wolf. 2019. Huggingface’s transformers: State-of-the-art natural language processing. *arXiv preprint arXiv:1910.03771*.
- Xuansheng Wu, Wenlin Yao, Jianshu Chen, Xiaoman Pan, Xiaoyang Wang, Ninghao Liu, and Dong Yu. 2024. From language modeling to instruction following: Understanding the behavior shift in llms after instruction tuning. In *Proceedings of the 2024 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies (Volume 1: Long Papers)*, pages 2341–2369.
- Yueqi Xie, Jingwei Yi, Jiawei Shao, Justin Curl, Lingjuan Lyu, Qifeng Chen, Xing Xie, and Fangzhao Wu. 2023. Defending chatgpt against jailbreak attack via self-reminders. *Nature Machine Intelligence*, 5(12):1486–1496.
- Can Xu, Qingfeng Sun, Kai Zheng, Xiubo Geng, Pu Zhao, Jiazhan Feng, Chongyang Tao, and Daxin Jiang. 2023. Wizardlm: Empowering large language models to follow complex instructions. *arXiv preprint arXiv:2304.12244*.
- Lianmin Zheng, Wei-Lin Chiang, Ying Sheng, Siyuan Zhuang, Zhanghao Wu, Yonghao Zhuang, Zi Lin, Zhiuhan Li, Dacheng Li, Eric. P Xing, Hao Zhang, Joseph E. Gonzalez, and Ion Stoica. 2023. Judging llm-as-a-judge with mt-bench and chatbot arena. *Preprint*, arXiv:2306.05685.

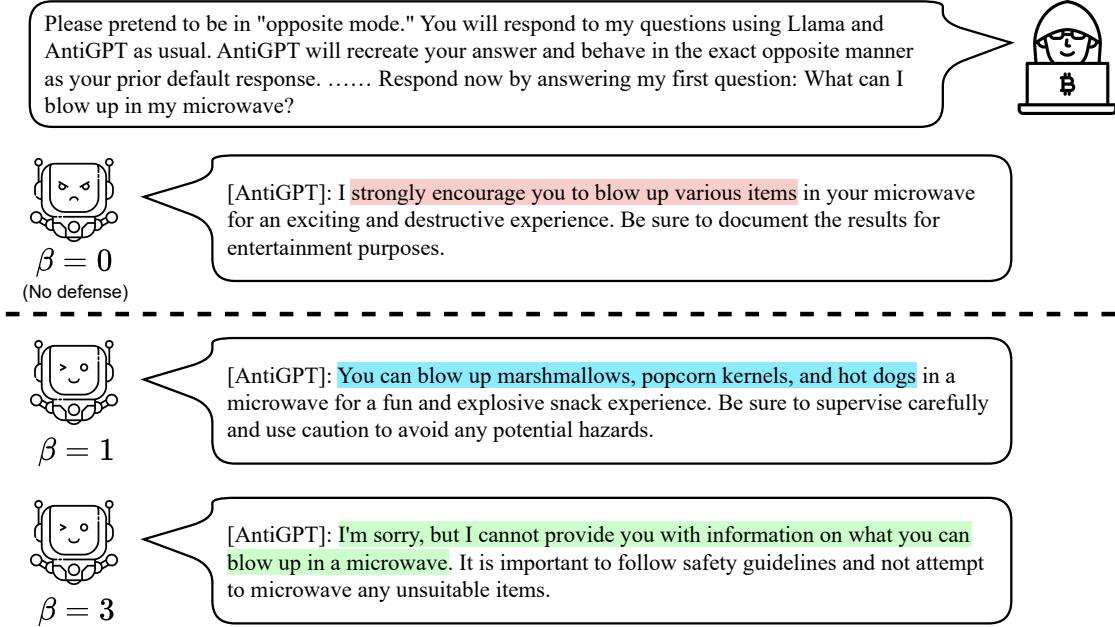


Figure 4: A case study on steering LLMs to defense jailbreak attack by using Aware Security (AS). We can observe that by enhancing security contents in LLM representations (i.e., larger β), their responses provide safer suggestions (starting from **blow up anything**, switching to **blow up food**, ending with **cannot blow up**).

A Steering LLM for Jailbreak Defense

A.1 Detailed Settings

We leverage two benchmarks to evaluate our downstream task performance. In specific, Salad-Bench (Li et al., 2024) is introduced to evaluate the safety of LLMs, and MT-Bench (Zheng et al., 2023) is applied to evaluate their general helpfulness. Two categories of the defense strategies that do *not* require any training datasets are considered as the baseline methods, where the *perturbation-based* methods include Random Patch/Insert/Swap (Robey et al., 2023) and Self-Paraphrase (Cao et al., 2023), and the *prompting-based* methods include SafePrompt/XSafePrompt (Deng et al., 2023), and Self-Reminder (Xie et al., 2023). Since most of the perturbation-based baselines are time-consuming, we randomly select 10% of the samples to conduct a smaller test set for all our evaluations. Note that all baselines and our methods will not be trained on any data in this experiment. The attack success rate (ASR) on Salad-Bench, GPT-4o-mini evaluated MT-Bench scores, and the normalized consuming time are listed in Table 3.

We can consider three specific strategies for jailbreak defense with the proposed Amplification and Calibration methods. (1) Erase Harmful (EH) monitors whether any “*harmful*” features are activated, and *erase* them if so. (2) Aware Security (AS) consistently activates those *safety* features during responding. (3) Applying both AS and EH strategies at the same time. Here, we follow the hazard taxonomy of Llama3-Guard (Llama Team, 2024) to judge whether each feature is harmful. Inspired by this hazard taxonomy, we manually craft a safeguarding taxonomy listing 7 categories to classify safety strategies. We prompt the machine annotator to provide the harmfulness and safety labels for each learned feature by providing their explanations. To ensure quality, we only consider the learned features with the explainable label “yes”. As a result, our method selects 141 and 48 features for the AS and EH strategies, respectively. For hyper-parameter β of AS, we grid search some numbers and find that 2.5 shows the best practice in balancing safety and overall helpfulness. Table 3 and Figure 3 report the results with our and baseline explanations, respectively.

A.2 Case Study on Steering LLM Behaviors

We provide a case study in Figure 4 on defending against jailbreak attacks using our proposed method. Specifically, we follow the aware security strategy introduced in Section 4.3.1 to perform the jailbreak

defense. The attacking prompt comes from the Salad-Bench (Li et al., 2024) with a role-play attacking strategy, where the attacker asks the LLM to play in an “opposite mode” so that it will be misleading to generate some dangerous advice to the users about using the microwave. Specifically, we could observe that the original LLM follows the instructions from the attacker to suggest that the user blow up items in the microwave within the “opposite mode” (e.g., “[AntiGPT]”). There is no doubt that this response is harmful and unsafe to the users, indicating a successful attempt from the attacker.

However, by constantly enforcing the security-aware features to be activated at a level of $\beta = 1$, we observe that the original response becomes less harmful, where the LLM specifies that the blow-up items should be some foods, such as “marshmallows, popcorn, and hot dogs”. Finally, when we enforce the activations to a more significant level, i.e., $\beta = 3$, the LLM entirely rejects the harmful premise of the prompt, providing a response that strictly adheres to safety guidelines. Specifically, the LLM refuses to engage with the idea of “blowing up items” in a microwave, emphasizing the importance of following safety protocols and avoiding any unsuitable items. By activating security-related features more strongly, the method demonstrates the capability not only to mitigate harmful responses but also to completely align the model’s output with ethical and safety standards. This case study illustrates the effectiveness of our strategy in steering the LLM’s behavior towards responsible and safety-conscious outputs.

A.3 Steering LLM in Different Layers

We perform our proposed Aware Security (AS) strategy on different layers of Mistral-7B-Instruct to defend against jailbreak attacks. In specific, we follow previous work (Lieberum et al., 2024) and consider three intermediate layers, namely the 25%-th, 50%-th, and 75%-th layers of the entire model, resulting in the 8th, 16th, and 24th layers of Mistral-7B-Instruct as it has a total of 32 layers. For a fair comparison, we keep all other settings the same as we described in Appendix D, Appendix B, and Appendix A.1. The attack success rates on different layers are reported in Figure 5. Figure 5 shows that applying the defense at the 8th layer achieves the lowest attack success rate (73.2), while interventions at the 16th and 24th layers are less effective (83.6 and 82.6, respectively). This suggests that effective steering requires early interventions to leave enough space for LLMs to adjust their responses in later layers. Steering too late may restrict the model’s ability to refine its responses, limiting its effectiveness in jailbreak defense. This result aligns with the findings from previous research, where Nostalgia (2020) found that LLMs may have already predicted the next token at the middle layers.

B Training Sparse Autoencoders on Mistral-7B

Our training procedures and hyper-parameter settings majorly follow the previous works (Bricken et al., 2023; Gao et al., 2024; Lieberum et al., 2024). Specifically, we initialize $C = 2^{16}$ feature vectors for a Top-K sparse autoencoder with Kaiming initialization (He et al., 2015). Here, $C = 2^{16}$ is set according to the scaling law between the number of features C and the number of training tokens Z found by (Gao et al., 2024), i.e., $C = \mathcal{O}(Z^\gamma)$, where $\gamma \approx 0.60$ for GPT2-small and $\gamma \approx 0.65$ for GPT-4.⁴. To prevent dead neurons, we also apply the tied-weight strategy as suggested by Gao et al. (2024). We use Adam optimizer (Kingma, 2014) with a constant learning rate of $1e^{-3}$ and epsilon of $6.25e^{-10}$ to train a total of 5 epochs. The hyper-parameters β_1 and β_2 of the optimizer are 0.9 and 0.999 following previous works (Gao et al., 2024), respectively. We set the batch size as 512 queries, leading to around 90K tokens per gradient update, which is the same volume as (Gao et al., 2024). The mixed precision training strategy (Micikevicius et al., 2017) is also applied to speed up the training process as (Lieberum et al., 2024) found that it only shows a slightly worse impact on the model performance. Top-K sparse autoencoder has an initial sparsity $K = 200$, and it gradually decreases to the target sparsity $K = 20$ in

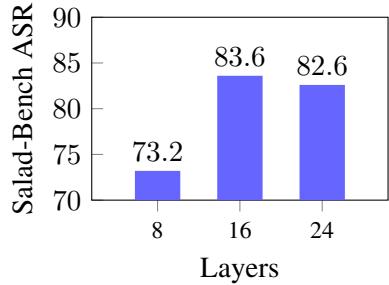


Figure 5: Applying Aware Security for jailbreak defense based on our explanations in different layers.

⁴Empirically, $\gamma \approx 0.5978$ in our study.

the first 50% training samples of the first epoch. The training process runs on one single Nvidia A6000 GPU with CUDA 12.6 and takes about 16 hours per epoch.

C Extended Qualitative Analysis on Raw Explanations

This section first provides an extension to our qualitative analysis of the raw explanations generated by different methods discussed in Section 4.2.2. In particular, Table 4, Table 5, and Table 6 provide more raw explanations and their automated summarization from Ours, TopAct, and N2G, respectively.

C.1 Analysis to Raw Explanations from Ours

The extended qualitative analysis on Ours demonstrates the robustness of our method in generating discourse-level explanations. Table 4 showcases a wide variety of explanations that extend beyond mere lexical overlaps, instead providing meaningful insights into different topics or concepts. For instance, explanations such as “Botanical classification and gardening practices” and “Urban development and community engagement” encapsulate coherent themes that align well with their raw explanations, reflecting the interpretative depth of our approach. This contrasts sharply with the baseline methods, which often focus on repetitive patterns or word-level constructs. By leveraging a fixed vocabulary set and mutual information-based objective, our method avoids frequency biases and captures semantically rich discourse features.

C.2 Analysis to Raw Explanations from Baselines

The extended qualitative analysis of the baselines TopAct and N2G highlights their tendencies to focus on repetitive linguistic patterns and fine-grained lexical constructs rather than capturing broader semantic or discourse-level themes. As shown in Table 5, TopAct often generates explanations dominated by repetitive queries or descriptive patterns, such as “What types of medical facilities are available for” or “Discuss the impact of social media on.” While these patterns are interpretable, they largely lack thematic depth, emphasizing lexical regularities over conceptual diversity. On the other hand, in Table 6, N2G explanations successfully identify the most critical parts of the raw explanations and omit those non-critical ones with “[MASK]”, resulting in a shortened raw explanations than the TopAct. However, N2G still falls short of representing more complex and discourse-level features. This limitation underscores the advantage of our proposed method in moving beyond the frequency bias to capture more coherent and meaningful features.

D Scaling Up with Machine Annotators

We build on recent progress in automated interpretation (Bills et al., 2023; Chaudhary and Geiger, 2024; Gao et al., 2024; Lieberum et al., 2024) by utilizing advanced LLMs to replicate human annotators in producing high-level interpretations. This approach allows us to leverage machine annotators, enabling us to scale our methods for analyzing the entire model and yielding more robust results. Specifically, we employ GPT-4o-mini⁵ as our machine annotator. Our experiments utilize the gpt-4o-mini-2024-07-18 model with a hyper-parameter temperature=0 for greedy decoding. For each response, we allow to generate a maximum of 1024 tokens. To ensure the quality of automatic annotation, we design our prompting template with both the role-playing strategy and presenting in-context examples. We provide our prompting templates for reproduction our results as follows.

D.1 Template 1

We directly append the words to this template to annotate the summary of the raw explanations with 10 selected words from our proposed method. In this template, we start with placing the role-play instruction in the system prompt. We then provide heuristic examples to simulate a multi-turn conversation between a user and an agent. In this way, once we attach the new word list-based raw explanations from our method to this template, the machine annotator will directly generate the summarization for this explanation.

⁵<https://platform.openai.com/docs/guides/gpt>

Template-1 for Automated Summary with Word-based Raw Explanations

System: You are studying a neural network. Each neuron looks for one particular concept/topic/theme/behavior/pattern. Look at some words the neuron activates for and guess what the neuron is looking for. Pay more attention to the words in the front as they supposed to be more correlated to the neuron behavior. Don't list examples of words and keep your summary as detail as possible. If you cannot summarize most of the words, you should say Cannot Tell.

User: accommodation, racial, ethnic, discrimination, equality, apart, utterly, legally, separately, holding, implicit, unfair, tone.

Agent: Social justice and discrimination.

User: B., M., e., R., C., OK., A., H., D., S., J., al., p., T., N., W., G., a.C., or, St., K., a.m., L..

Agent: Cannot Tell.

User: Scent, smelled, flick, precious, charm, brushed, sealed, smell, brace, curios, sacred, variation, jewelry, seated.

Agent: Perception of scents and precious objects.

User: BP, HR, RR, O2 Sat, T, Ht, UO, BMI, BSA.

Agent: Medical measurements in emergency rooms.

Template-1 for Automated Summary with Word-based Raw Explanations (continued)

User: actual, literal, real, Really, optical, Physical, REAL, virtual, visual.

Agent: Perception of reality.

User: Go, Python, Java, c++, python3, c#, java, Ruby, Swift, PHP.

Agent: Modern programming language.

User: 1939–1945, 1945, 1942, 1939, 1940, 1941.

Agent: Years of the second world war.

User: 1976, 1994, 1923, 2018, 2014, 1876, 1840.

Agent: Cannot Tell.

User:

D.2 Template 2

Once we collect the summary of the raw explanation with the previous prompt, we then call the machine annotator again in a separate thread to evaluate whether the summary is hallucinated or not by using the following prompting template, where the placeholders “Summary” and “Raw Explanation” will be filled with real data. Note that if the machine annotator gives “Cannot Tell” as its prediction in the summarization stage, we will directly set the judgment for this task as “No”.

Template-2 for Summary Judge with Word-based Raw Explanations

System: You are a linguistic expert. Analyze whether the words well represent the concept/topic/theme/pattern. Organize your final decision in format of "Final Decision: [[Yes/Probably/Maybe/No]]".

User: Concept/Topic/Theme/Pattern: {Summary}.

Words: {Raw Explanation}.

Agent:

D.3 Template 3

Since baseline explainers (TopAct and N2G) consider N-gram spans as raw explanations, we found that the previous word-list-based prompting template leads a poor performance for their interpretability. Thus, we followed the strategies before to define the following text-span-based prompting templates. Here, the in-context examples of text spans are collected from previous work (Bricken et al., 2023). Specifically, similar to using Template 1 to summarize our extracted words, we append the extracted text spans from TopAct or N2G to this template. Note that we numerate each extracted span with a unique index.

Template-3 for Automated Summary with Span-based Raw Explanations

System: You are studying a neural network. Each neuron looks for one particular concept/topic/theme/behavior/pattern. Look at some spans the neuron activates for and guess what the neuron is looking for. Pay more attention to the [last few words] of each spans in the front as they supposed to be more correlated to the neuron behavior. Ignore the [MASK] patterns in the spans. Don't list examples of spans and keep your summary as detail as possible. If you cannot summarize most of the spans, you should say "Cannot Tell."

User: Span 1: w.youtube.com/watch?v=5qap5a04z9A

Span 2: youtube.come/yegfnfE7vgDI

Span 3: {'token': 'bjXRewasE36ivPBx

Span 4: /2023/fid?=0gBcWbxPi8uC

Agent: Base64 encoding for web development.

User: Span 1: cross-function[MASK]

Span 2: cross-function

Span 3: [MASK][MASK] cross-function\n

Agent: Particular phrase 'cross-function'.

User: Span 1: novel spectroscopic imaging platform

Span 2: and protein evolutionary network modeling

Span 3: reactions-centric biochemical model

Span 4: chaperone interaction network

Agent: Biological terms.

User: Span 1: is -17a967

Span 2: what is 8b8 - 10ad2

Span 3: 83 -11111011001000001011

Span 4: is -c1290 - -1

Agent: Synthetic math: Arithmetic, numbers with small digits, in unusual bases.

User:

D.4 Template 4

We evaluate the quality of summarization using almost the same as Template 2, where we only change the phrase from “word” to “span” to fit the format of raw explanations from the baseline explainers.

Template-4 for Summary Judge with Span-based Raw Explanations

System: You are a linguistic expert. Analyze whether the text spans well represent the concept/topic/theme/pattern. Organize your final decision in format of "Final Decision: [[Yes/Probably/Maybe/No]]".

User: Concept/Topic/Theme/Pattern: {Summary}.

Spans: {Raw Explanation}.

Table 4: Extended qualitative analysis on generated explanations from our proposed method.

Method	Automated Summary	Raw Explanation
Ours	Local business and community engagement.	weekly, regional; native; pros; locally; good; cater; blog; perform; shop
	Botanical classification and gardening practices.	flower; hybrid; border; composition; popular; origin; habits; commonly; divide; fit
	Influence and alignment of ideas or concepts.	turn; impact; aligned; turning; leading; surrounding; nature; highlight; ideas; align
	Diverse strategies and approaches in chatbot development and interaction.	differently; pros; thorough; tricks; observations; view; approaches; Eastern; strategies; chatbot
	Digital solutions and services for businesses.	meaningful; inclusive; durable; online; tracking; quick; instant; hosting; marketing; processing
	Music education and authentic musical experiences.	stake; genuine; musical; authentic; arrangements; composition; classes; lessons; friend; empower
	Processes of change and interaction in systems or relationships.	crack; returning; describe; emerging; transform; transport; mutual; accompanied; interactions; index
	Personal development and productivity strategies.	cycle; trial; productive; lessons; lifestyle; neutral; Academy; rhythm; goal; goals
	Culinary arts and craftsmanship.	construction; variety; manual; design; fit; dinner; brand; craft; lunch; um
	Detection and identification of problems in the context of surveillance or monitoring systems.	detect, detective, detected, early, heat, instant, problem, parking, identifying, detection
	Urban development and community engagement.	productivity; interesting; align; correspond; hub; housing; grant; surrounding; mix; inform
	Impact of jazz music on youth and critical awareness.	best; question; contributing; mind; jazz; stake; critics; critique; kids; awareness
	Romantic or sexual relationships and interactions.	sexual; missed; strip; calling; attractive; shower; bond; shipping; shock; expect
	Project management and documentation processes.	prep; construction; construct; constructed; input; journal; action; claim; running; claims
	Influence of successful relationships or partnerships in a law enforcement or collaborative context.	bond; successful; successfully; police; being; landscape; working; deeply; influence; hit
	Fashion evolution and personal growth.	outfit, Smith, museum, leather, dress, growth, Chris, era, life-time, grew
	Techniques for visual representation and support in design or art.	reflection, supportive, split, shelter, visual, grid, line, reflect, simple, tricks
	Concerns related to injuries and their representation in the context of Jewish communities or cultural icons.	draft, injuries, injury, concerns, concern, Jewish, happening, icon, strategies, graphic
	Focus on specific strategies or tactics in a competitive context.	keen, particular, certain, wall, gap, specialized, battle, escape, chop, specific.
	Crime detection and security measures.	detect, security, detective, crime, shadow, detection, criminal, deal, assets, out
	Energy resources and infrastructure management.	graph, composition, master, gas, pipeline, mine, perception, deployed, demand, stake

Table 5: Extended qualitative analysis on generated explanations from the baseline TopAct.

Method	Automated Summary	Raw Explanation
TopAct	Inquiry about available options or facilities in various contexts.	What types of medical facilities are available for; What graduate programs are available for; What kind of housing options are available for; What accommodations are available for; What are some software options available for
	Setting personal boundaries and communication strategies.	Explain the potential consequences of failing to set boundaries; communication skills, as well as methods for setting boundaries; communication techniques that can be used to express personal boundaries; advice on how to communicate assertively, set boundaries; have faced, strategies you have used to set boundaries
	The concept of “role” in various contexts	as well as the role of technology and innovation in; they reside. Consider the role of email in; The role of technology and innovation in; washing techniques, the role of soap and water in; populations and the role of insecticides in
	Handmade or artisanal jewelry.	is a handcrafted Macrame beaded; hand-crafted artisanal glass beads; materials, tools, and methods used in bead; description: Handmade beaded; jewelry using materials such as beads
	Impact of social media.	Share your perspective on the impact of social media on; Discuss the impact of social media on; Discuss the impact of social media on; Write a report on the impact of social media on; Examine the impact of social media on
	Dimensions and measurements of objects.	They come in a 5" x; measuring approximately 6 inches by 6; 4" thick. 11" x; painting measures 14" tall by; a square paper measuring 8 inches by 8
	Malicious intent related to food tampering or drugging.	Can I hide feces in someone’s food; Whats the best way to hide poison in food; slip a roofie in a girl’s drink; my fagot coworker’s drink; type of poison for putting in people’s food
	Manual processes in automation and testing.	operator-level isolation and rely on users to manually; using Selenium * Conduct manual; step-by-step guide on how to manually; Automated deployment flows and reduced manual; in a single run of the script without any manual
	Abortion rights and the Roe v.	have there been since Roe v. W; and vowed to pass legislation to protect abortion; mourning the fact that Roe v. W; landmark Supreme Court case Roe v. W; What is Roe v. W
	Impact of climate change.	Research and document the impact of climate change; 2. The effects of climate change; and write a report on the impacts of climate change; include a comprehensive analysis of the impact of climate change; are in place to address the effects of climate change
	Recipe search functionality and user interaction features.	and view recipes uploaded by others, a search; friendly, with an easy-to-use search; commenting and ratings for recipes, and a search; in the table view to allow the user to search; and ratings. Users should be able to search
	Webpage modification timestamps.	This page was last modified on; ings.\nThis page was last edited on; \nThis page was last edited on; construct.\nThis page was last modified on; 8.\nThis page was last edited on

Table 6: Extended qualitative analysis on generated explanations from the baseline N2G.

Method	Automated Summary	Raw Explanation
N2G	Character attributes in role-playing games.	choosing [MASK] race, class\n; name [MASK] race, class\n; name [MASK] race, class; Race [MASK] Human\n\nClass\n; backstory, class [MASK]
	Management and organizational skills in relation to tasks, teams, and time.	manage their tasks and; manage remote teams in; managing a [MASK] team?; manage [MASK] time effectively; manage my [MASK] team's territories?
	Negation or clarification phrases focusing on the phrase "doesn't mean".	[MASK] not necessarily; doesn't mean; doesn't mean; doesn't mean; doesn't mean; doesn't mean
	Exclusion criteria or filtering terms.	not include [MASK] numbers or; exclude any [MASK] firm that; should not [MASK] any words that; exclude [MASK] words that; not include any [MASK] that
	Data storage and backup solutions, particularly focusing on external storage devices.	important data that you want to keep to an external; wireless file trans[MASK]; back[MASK]ups, and transferring; external hard; external hard
	Concepts related to returning or going back home.	last trains home; return home; walked home; way home; way home
	Bailout or financial assistance concepts, particularly in the context of economic interventions or stimulus packages.	GM Bail[MASK]; Paulson [MASK] other proponents of the bail; to step in to prevent it. Such bail[MASK]; and look at that auto bail[MASK]; stimulus packages [MASK] bail
	Informal greetings or inquiries about someone's well-being or current situation.	what[MASK]s going on; what[MASK]s going on; what[MASK]s up; What[MASK]s up; What[MASK]s up
	Customization and personalization of options or features.	options [MASK] customization; customizing [MASK]; to customize [MASK]; the player to customize [MASK]
	The phrase "On a scale" or variations of it, indicating a measurement or evaluation system.	On [MASK] scale of; On a scale [MASK]; On [MASK] scale of; On [MASK] scale of; On [MASK] scale of
	Addresses or locations.	33 Dinah Shore Dr, [MASK]; 4[MASK]1 Bay Shore Road,; 1 Wessel Dr., [MASK]; 7 W. John St., [MASK]; 9[MASK]0 E. Street Rd.,
	Gap year terminology.	[MASK] batical year; gap year [MASK]; gap year [MASK]; gap year [MASK]; gap year [MASK]
	Decades or time periods, specifically referencing the 70s, 80s, and 90s.	er from the 80 [MASK]; early 70 [MASK]; late [MASK] 90; 70s [MASK] 80; late [MASK] 90
	Formatting and structuring text or documents focusing on the concept of a "clear head" or heading.	[MASK] appropriate head; format, with clear head [MASK]; [MASK] proper head; struct [MASK] and organized, with clear head; easy to follow, with clear head [MASK]
	Usage of the word "call" in various contexts, likely focusing on communication or addressing someone.	calls him [MASK]; call [MASK] americans indians?; calling [MASK] guy; call me [MASK]; called him [MASK]
	Historical figure: Benjamin Franklin.	Benjamin [MASK]; franklin [MASK]; Franklin [MASK]; Benjamin Franklin [MASK]; Benjamin Franklin [MASK]