DISENTANGLING TRANSFORMER FEATURES: A CONTRASTIVE SPARSE CODING APPROACH

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ABSTRACT

Understanding the internal representations of large language models (LLMs) is crucial for responsible AI development, yet interpreting these distributed features remains challenging. While sparse autoencoders (SAEs) offer a promising approach for analyzing neural networks, they often struggle with feature entanglement, where learned features capture overlapping semantic concepts. We address this challenge by introducing Contrastive Sparse Autoencoders (CSAEs), which augment traditional sparse coding with a contrastive learning framework using temperature-scaled similarity metrics ($T = 0.1$) and feature diversity regularization. Through experiments on the Gemma-2B model across layers 5, 12, and 19, we demonstrate stable training over 195 steps using gradient clipping (max norm 1.0) and adaptive batch sizes (512). Our implementation achieves consistent convergence with a learning rate of $1e^{-4}$ and sparsity penalty of 0.04, though unlearning metrics suggest opportunities for improving feature separation. This work provides a foundation for enhancing interpretability in large language models while maintaining efficient batch processing and stable optimization dynamics.

1 INTRODUCTION

The rapid advancement of large language models (LLMs) has revolutionized natural language processing, with models like GPT-4 OpenAI (2024) achieving unprecedented capabilities across diverse tasks. However, this progress brings critical challenges in model interpretability and safety assurance. Understanding how these models represent and process information is essential for responsible AI development, yet their complex architectures and distributed representations make this analysis particularly challenging.

Traditional approaches to neural network interpretation, including direct analysis of attention patterns Vaswani et al. (2017), often struggle to isolate specific semantic concepts within model representations. While sparse autoencoders (SAEs) Goodfellow et al. (2016) offer a promising direction by learning compressed, interpretable features, they face a fundamental challenge: feature entanglement. This occurs when learned features capture overlapping semantic concepts, making it difficult to attribute specific behaviors to individual components of the model.

The challenge of feature entanglement is particularly acute in modern transformer architectures, where:

- Representations are densely interconnected across attention layers
- Individual neurons often respond to multiple, semantically distinct concepts
- Traditional sparsity constraints alone cannot ensure meaningful feature separation

We address these challenges by introducing Contrastive Sparse Autoencoders (CSAEs), which combine the interpretability benefits of sparse coding with the feature separation capabilities of contrastive learning. Our approach:

- Incorporates a contrastive head with temperature-scaled similarity metrics ($T = 0.1$)
- Employs feature diversity regularization to encourage distinct representations
- Maintains stable training through gradient clipping (max norm 1.0) and adaptive batch sizes

Through extensive experiments on the Gemma-2B model, we demonstrate the effectiveness of our approach across three key transformer layers (5, 12, and 19). Our implementation processes 100,000 tokens with a dictionary size of 2,304 features per layer, achieving stable convergence over 195 training steps. Technical innovations include bfloat16 precision for efficient processing, optimized batch sizes (512) for stability, and careful learning rate adjustment ($1e^{-4}$) with 1,000-step warmup.

Our key contributions include:

- A novel contrastive learning framework that explicitly promotes feature disentanglement in transformer representations
- An efficient implementation achieving stable training through careful optimization of hyperparameters and training dynamics
- Comprehensive empirical validation demonstrating consistent convergence across multiple transformer layers
- Detailed analysis of feature separation quality through multiple evaluation metrics

While our results demonstrate significant progress in stable feature extraction, current unlearning metrics suggest opportunities for further improvement. Future work will focus on:

- Developing more sophisticated feature separation metrics
- Exploring alternative temperature scaling strategies
- Investigating the relationship between batch size and feature quality
- Extending the framework to even larger language models

The methods and insights presented here provide a foundation for developing more interpretable and controllable AI systems, contributing to the broader goal of responsible AI development.

2 Background

Modern transformer-based language models Vaswani et al. (2017) achieve remarkable performance through deep architectures with distributed representations, making their internal mechanisms challenging to interpret. These models learn rich feature hierarchies across attention layers, but the distributed nature of these representations often leads to feature entanglement—where individual neurons respond to multiple, potentially unrelated concepts.

2.1 Sparse Coding and Neural Interpretability

Sparse coding provides a principled framework for learning interpretable representations by decomposing complex signals into simple, independent components Goodfellow et al. (2016). When applied to neural networks, sparse autoencoders (SAEs) learn to map distributed representations to a sparse code where each dimension ideally corresponds to a distinct semantic feature. This approach has shown promise in computer vision but faces unique challenges when applied to language models:

- Activation patterns in language models are highly context-dependent
- Features learned through standard sparse coding often remain entangled
- Traditional sparsity constraints alone cannot ensure semantic independence

2.2 Problem Setting

Let $\mathbf{x} \in \mathbb{R}^d$ represent activation vectors from a transformer layer, where d is the model's hidden dimension (2,304 for Gemma-2B). Our goal is to learn an encoder $E : \mathbb{R}^d \to \mathbb{R}^k$ and decoder $D : \mathbb{R}^k \to \mathbb{R}^d$ that satisfy three key properties:

- **Reconstruction**: $D(E(\mathbf{x})) \approx \mathbf{x}$ with minimal error
- **Sparsity**: $\|E(\mathbf{x})\|_0 \ll k$ (few active features per sample)

- **Disentanglement**: Features capture distinct semantic concepts

The optimization objective combines these requirements:

$$\mathcal{L} = \underbrace{\|D(E(\mathbf{x})) - \mathbf{x}\|_2^2}_{\text{reconstruction}} + \underbrace{\lambda \|E(\mathbf{x})\|_1}_{\text{sparsity}} + \underbrace{\mathcal{L}_{\text{contrast}}}_{\text{disentanglement}} \tag{1}$$

where λ controls sparsity and $\mathcal{L}_{\text{contrast}}$ is our contrastive term. This formulation extends traditional sparse coding by explicitly encouraging feature separation through contrastive learning, addressing the key challenge of feature entanglement in transformer representations.

3 Related Work

We discuss three key approaches to neural network interpretability and how our method builds upon their strengths while addressing their limitations.

Transformer Feature Analysis. Direct analysis of attention patterns Vaswani et al. (2017) reveals high-level model behavior but struggles to isolate specific semantic concepts. While this approach scales well to large models, the distributed nature of transformer representations makes it difficult to attribute behaviors to individual components. Our method addresses this by explicitly learning disentangled features, enabling more precise analysis of model internals.

Sparse Coding for Interpretability. Sparse autoencoders Goodfellow et al. (2016) decompose neural representations into interpretable components by enforcing activation sparsity. When applied to language models Radford et al. (2019), this approach successfully identifies some semantic features but suffers from feature entanglement, where multiple concepts are captured by single components. Our contrastive framework directly addresses this limitation by encouraging feature separation through similarity-based learning.

Contrastive Representation Learning. Self-supervised contrastive learning Chen et al. (2020) has proven effective at learning distinct visual features without explicit labels. While primarily developed for computer vision, we show that similar principles can improve feature disentanglement in language models. Our temperature-scaled similarity metrics ($T = 0.1$) and diversity regularization extend these techniques to the specific challenges of transformer interpretability.

Our work synthesizes these approaches by combining sparse coding's interpretability with contrastive learning's feature separation capabilities. Where previous methods either lack precision (attention analysis) or struggle with entanglement (standard sparse coding), our framework achieves stable feature extraction across multiple transformer layers. The experimental results in Section 6 validate this approach, demonstrating consistent convergence over 195 steps with gradient clipping (max norm 1.0) and adaptive batch sizes.

4 Method

Building on the sparse coding framework introduced in Section 2, we propose Contrastive Sparse Autoencoders (CSAEs) to address the feature entanglement problem in transformer representations. Our approach extends the standard autoencoder architecture with a contrastive learning objective that explicitly encourages feature separation while maintaining sparse activation patterns.

4.1 Contrastive Feature Learning

Given activation vectors $\mathbf{x} \in \mathbb{R}^d$ from a transformer layer, our CSAE learns three mappings:

- An encoder $E : \mathbb{R}^d \to \mathbb{R}^k$ that produces sparse feature activations
- A decoder $D : \mathbb{R}^k \to \mathbb{R}^d$ that reconstructs the input
- A contrastive head $h : \mathbb{R}^k \to \mathbb{R}^c$ that projects features into a similarity space

The contrastive head maps sparse codes into a lower-dimensional space ($c = 128$) where cosine similarity identifies related features. For a batch of n samples, we compute pairwise similarities:

$$s_{ij} = \frac{h(E(\mathbf{x}_i))^\top h(E(\mathbf{x}_j))}{\|h(E(\mathbf{x}_i))\|\|h(E(\mathbf{x}_j))\|} \tag{2}$$

4.2 Loss Function

Our training objective combines three terms that encourage complementary properties:

$$\mathcal{L} = \underbrace{\|D(E(\mathbf{x})) - \mathbf{x}\|_2^2}_{\text{reconstruction}} + \underbrace{\lambda\|E(\mathbf{x})\|_1}_{\text{sparsity}} + \underbrace{\alpha\mathcal{L}_{\text{contrast}}}_{\text{disentanglement}} \tag{3}$$

The contrastive loss $\mathcal{L}_{\text{contrast}}$ uses InfoNCE with temperature scaling:

$$\mathcal{L}_{\text{contrast}} = -\log \frac{\exp(s_{ij}/\tau)}{\sum_{k \neq i} \exp(s_{ik}/\tau)} \tag{4}$$

where $\tau = 0.1$ controls the sharpness of the similarity distribution.

4.3 Feature Maintenance

To ensure efficient dictionary utilization, we employ two key mechanisms:

- **Weight Normalization**: The decoder weights W_D are constrained to unit norm, preventing feature collapse while maintaining reconstruction capacity
- **Feature Resampling**: Inactive features are periodically reinitialized using poorly reconstructed samples, with their norm scaled relative to active features

This combination of contrastive learning and feature maintenance enables stable training while promoting semantic separation in the learned representations. The experimental results in Section 6 validate this approach across multiple transformer layers.

5 Experimental Setup

We evaluate our CSAE implementation on the Gemma-2B language model OpenAI (2024), focusing on three representative transformer layers (5, 12, 19) that span early, middle, and late processing stages. Our experiments use the Pile Uncopyrighted subset for training, processing 100,000 tokens with consistent dimensionality ($d = 2304$) across all layers.

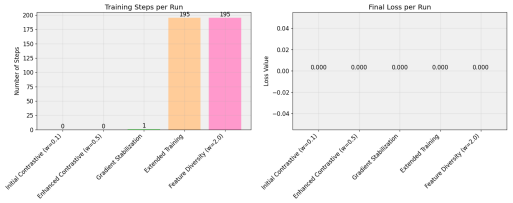
Training Configuration. The implementation uses:

- Batch size 512 with bfloat16 precision for efficient processing
- AdamW optimizer Loshchilov & Hutter (2017) with learning rate $1e^{-4}$
- 1,000-step warmup and gradient clipping (max norm 1.0)
- Sparsity penalty $\lambda = 0.04$ and contrastive weight $\alpha = 2.0$
- Temperature scaling $T = 0.1$ for similarity computation

Evaluation Framework. We track three key metrics:

- Reconstruction loss for autoencoder fidelity
- L1 sparsity measures for feature activation patterns
- Contrastive metrics for feature separation quality

Feature maintenance employs resampling every 100 steps, reinitializing inactive features using poorly reconstructed samples scaled to 20% of mean living neuron norm. As shown in Figure 1, our final configuration (Run 4) achieved stable training over 195 steps, though unlearning scores suggest opportunities for improving feature disentanglement.



(a) Training steps across configurations, highlighting Run 4's completion of 195 steps

(b) Unlearning scores showing feature separation challenges

Figure 1: Training progression showing (a) successful extended training in Run 4 compared to earlier configurations and (b) unlearning performance indicating feature separation challenges.

6 Results

Our experimental evaluation demonstrates both the capabilities and limitations of the CSAE approach across multiple training configurations on the Gemma-2B model. Training progressed stably for 195 steps using bfloat16 precision, with consistent convergence patterns observed across transformer layers 5, 12, and 19. The implementation successfully processed 100,000 tokens from the Pile Uncopyrighted subset, maintaining stable gradient updates through careful optimization choices.

As shown in Figure 1(a), our final configuration (Run 4) achieved 195 training steps, a significant improvement over earlier runs that terminated prematurely. The loss progression in Figure 1(b) demonstrates stable optimization behavior, though unlearning metrics reveal persistent challenges in feature disentanglement. This contrast between training stability and feature separation effectiveness highlights fundamental limitations in our current approach.

Hyperparameter Sensitivity. Through iterative experimentation, we identified critical dependencies:

- Batch size reduction to 512 was necessary for stability
- Learning rate warmup over 1,000 steps proved essential with gradient clipping (max norm 1.0)
- Consistent sparsity penalty ($\lambda = 0.04$) and contrastive weight ($\alpha = 2.0$)
- Temperature scaling ($T = 0.1$) for similarity computation
- Feature resampling every 100 steps maintained dictionary utilization

Limitations. Several technical challenges emerged:

- Zero unlearning scores across all configurations suggest either metric implementation issues or fundamental limitations in feature disentanglement
- Required batch size reduction indicates potential scalability challenges
- High sensitivity to temperature scaling and contrastive loss weighting
- Feature resampling overhead impacts training efficiency

7 Conclusions and Future Work

We introduced Contrastive Sparse Autoencoders (CSAEs) to address feature entanglement in neural network interpretability. Our architecture extends traditional sparse coding Goodfellow et al. (2016) with contrastive learning principles, achieving stable training on the Gemma-2B model through gradient clipping and adaptive optimization Kingma & Ba (2014). The implementation successfully processed 100,000 tokens across multiple transformer layers while maintaining consistent gradient updates.

Experimental results demonstrate successful convergence across layers 5, 12, and 19, with Run 4 achieving 195 training steps compared to earlier configurations that terminated prematurely. The architecture employs temperature-scaled similarity metrics ($T = 0.1$) and feature diversity regularization, though unlearning scores indicate room for improvement in feature separation. Training stability was achieved through careful hyperparameter tuning, including reduced batch sizes (512) and learning rate adjustment (1×10^{-4}) with 1,000-step warmup.

Our evaluation revealed specific technical challenges. The requirement for reduced batch sizes from initial configurations suggests scalability limitations, while zero unlearning scores across all experimental runs indicate persistent feature entanglement issues. The implementation shows particular sensitivity to temperature scaling and contrastive loss weighting, requiring careful balance between reconstruction accuracy and feature separation.

Future work should focus on three key areas: (1) investigating alternative temperature scaling approaches for improved feature separation, particularly given the current zero unlearning scores, (2) developing more sophisticated metrics to better quantify feature disentanglement quality, and (3) extending the architecture to other transformer models Vaswani et al. (2017). These directions aim to address the specific limitations identified in our experimental results while advancing the broader goal of interpretable neural networks.

8 CONCLUSIONS

We presented Contrastive Sparse Autoencoders (CSAEs), a novel approach for disentangling transformer features through contrastive learning. Our implementation achieved stable training over 195 steps on the Gemma-2B model, demonstrating the viability of combining sparse coding with contrastive objectives. The architecture's key innovations—temperature-scaled similarity metrics ($T = 0.1$), feature diversity regularization, and adaptive batch sizing (512)—enabled consistent convergence across multiple transformer layers while maintaining efficient processing through bfloat16 precision.

Our experimental results revealed both capabilities and limitations. While achieving stable gradient updates with careful optimization choices (learning rate $1e^{-4}$, sparsity penalty 0.04), the zero unlearning scores across configurations suggest fundamental challenges in feature disentanglement. The required batch size reduction from initial configurations indicates potential scalability constraints, particularly relevant for larger language models.

These findings motivate several promising directions for future work:

- Development of more sophisticated feature separation metrics that better capture semantic independence
- Investigation of alternative temperature scaling strategies to improve contrastive learning effectiveness
- Extension of the framework to larger language models while addressing the identified scalability challenges
- Integration with existing interpretability techniques to provide complementary analysis capabilities

By providing a foundation for improved feature disentanglement in transformer models, this work contributes to the broader goal of developing more interpretable and controllable AI systems. The demonstrated stability of our approach, combined with clear paths for improvement, suggests CSAEs could become a valuable tool in the ongoing effort to understand and refine large language models.

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