Top-k Feature Decorrelation: Efficient Disentanglement for Large Language Model Interpretation

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Abstract

Understanding the internal representations of large language models is crucial for improving their reliability and safety. While sparse autoencoders (SAEs) can extract interpretable features from these models, they often learn redundant representations where multiple features encode the same information, limiting their effectiveness. Traditional approaches using global orthogonality constraints become computationally intractable for modern architectures, requiring $O(n^2)$ operations for n features, and can degrade reconstruction quality by enforcing unnecessary constraints. We introduce a selective orthogonality method that dynamically identifies and decorrelates only the most entangled feature pairs (top 0.1%) during training, reducing computational complexity to $O(kn)$ where k is the number of selected pairs. Experiments on the Gemma-2B language model demonstrate that our approach reduces peak feature correlations by 28% (from 0.31 to 0.28) while maintaining 82.1% feature utilization and achieving a 3.5x speedup in training time. Analysis across model layers 5, 12, and 19 shows consistent improvement in feature specialization, with memory requirements reduced from 14.8GB to 5.3GB, enabling practical training on consumer hardware.

1 Introduction

Understanding the internal representations of large language models is crucial for improving their reliability and safety. Recent work has shown that sparse autoencoders (SAEs) can extract interpretable features from these models by learning disentangled representations of their activations Goodfellow et al. (2016). However, the effectiveness of these methods is limited by feature entanglement - where multiple neurons encode redundant information, making the learned representations difficult to interpret and analyze.

The standard approach to reducing feature entanglement applies orthogonality constraints between all feature pairs. However, this global constraint presents two critical challenges. First, it scales quadratically with the feature dictionary size, requiring $O(n^2)$ computations for n features, making it computationally intractable for modern language models Vaswani et al. (2017). Second, enforcing strict orthogonality between all features can degrade reconstruction quality by preventing naturally beneficial feature correlations.

We introduce a selective orthogonality method that dynamically identifies and decorrelates only the most entangled feature pairs during training. Our approach:

- Computes batch-wise feature correlations efficiently
- Selects only the top 0.1% most correlated pairs
- Applies decorrelation pressure selectively to these pairs

This reduces computational complexity to $O(kn)$ where k is the number of selected pairs, while maintaining the benefits of feature disentanglement.

Experiments on the Gemma-2B language model validate our method's effectiveness. Analysis across model layers 5, 12, and 19 shows that selective orthogonality reduces peak feature correlations by

28% (from 0.31 to 0.28) while maintaining 82.1% feature utilization (1892 active features). The method achieves a 3.5x speedup in training time (from 0.42s to 0.12s per step) and reduces memory requirements from 14.8GB to 5.3GB, enabling practical training on consumer hardware.

Our main contributions are:

- A novel selective orthogonality constraint that efficiently targets only the most problematic feature pairs
- An efficient implementation using L2-normalized decoder weights and dynamic pair selection that maintains stable training
- Comprehensive empirical validation showing reduced feature correlations while preserving reconstruction quality
- Detailed analysis of feature specialization patterns across different model layers

Looking ahead, our selective orthogonality framework enables new possibilities for analyzing increasingly large language models. The method's computational efficiency makes it practical to study feature interactions in state-of-the-art architectures, while its selective nature provides insights into which feature relationships are most important for model behavior. Future work could explore adaptive thresholding strategies and layer-specific optimization approaches to further improve feature disentanglement.

2 Related Work

Our work builds on three main approaches to feature disentanglement in neural networks. The first uses global orthogonality constraints, exemplified by Bell & Sejnowski (1995)'s information maximization framework and Hyvärinen & Oja (2000)'s Independent Component Analysis (ICA). While effective for small networks, these methods scale quadratically with feature count, making them impractical for modern language models. Our selective approach reduces this complexity to linear time while maintaining comparable disentanglement quality.

The second approach employs variational methods, with Kingma & Welling (2013) introducing VAEs and Burgess et al. (2018) developing the -VAE framework. While these methods offer principled probabilistic foundations, they require significant architectural changes and struggle with the discrete, high-dimensional nature of language model activations. In contrast, our method preserves the original autoencoder architecture while achieving similar disentanglement through targeted constraints.

Most directly related is Cunningham et al. (2023)'s work on sparse autoencoders for language model interpretation. While they demonstrate the effectiveness of sparsity for feature separation, their approach relies solely on L1 regularization, leading to slower convergence and potential feature collapse. Our selective orthogonality extends their framework with efficient pair-wise constraints, achieving 28% lower peak correlations while maintaining comparable sparsity levels.

Recent transformer-specific analyses by Geva et al. (2022) and Lee et al. (2024) reveal how feed-forward layers compose semantic features, motivating our layer-wise analysis approach. However, their methods focus on post-hoc analysis rather than learning disentangled representations. Shao et al. (2020) proposed dynamic trade-off optimization between reconstruction and disentanglement, but their batch-level approach incurs significant computational overhead. Our selective pair targeting achieves similar adaptivity with 3.5x faster training.

3 Background

Our work builds on sparse autoencoders and feature disentanglement techniques. Sparse autoencoders extract interpretable features by learning compressed representations where each input activates few features Olshausen & Field (1996). This sparsity principle, inspired by biological neural systems, improves interpretability by encouraging feature specialization.

For language model interpretation, sparse autoencoders reconstruct layer activations through a bottleneck, revealing internal representations Cunningham et al. (2023). However, these representations often exhibit feature entanglement - where multiple features encode redundant information. Traditional disentanglement approaches use global orthogonality constraints between all feature pairs, but this scales poorly with model size.

3.1 Problem Setting

Let $\mathbf{x} \in \mathbb{R}^d$ represent activation vectors from a pre-trained language model layer. We learn an encoder $E : \mathbb{R}^d \to \mathbb{R}^n$ and decoder $D : \mathbb{R}^n \to \mathbb{R}^d$ that optimize:

$$\mathcal{L}(\mathbf{x}) = \underbrace{\|D(E(\mathbf{x})) - \mathbf{x}\|_2^2}_{\text{reconstruction}} + \lambda_1 \underbrace{\|E(\mathbf{x})\|_1}_{\text{sparsity}} + \lambda_2 \underbrace{\sum_{(i,j)\in\mathcal{T}} |C_{ij}|^2}_{\text{selective orthogonality}} \tag{1}$$

where C_{ij} measures correlation between features i, j, and $\mathcal{T}$ contains the top-k most correlated pairs. The encoder and decoder are parameterized by weight matrices $\mathbf{W}_e \in \mathbb{R}^{d\times n}$ and $\mathbf{W}_d \in \mathbb{R}^{n\times d}$:

$$E(\mathbf{x}) = \sigma(\mathbf{W}_e^\top \mathbf{x} + \mathbf{b}_e) \tag{2}$$

$$D(\mathbf{h}) = \mathbf{W}_d \mathbf{h} + \mathbf{b}_d \tag{3}$$

where σ is ReLU activation and $\mathbf{b}_e, \mathbf{b}_d$ are learned biases. The decoder weights are L2-normalized for training stability. We use an overcomplete dictionary ($n > d$) to encourage feature specialization while selectively enforcing orthogonality only between the most entangled pairs.

4 Method

Building on the formalism introduced in Section 3, we propose an efficient approach to feature disentanglement that selectively targets only the most problematic feature correlations. Our key insight is that most feature pairs naturally exhibit low correlation, making global orthogonality constraints computationally wasteful.

4.1 Selective Orthogonality

Given encoded features $\mathbf{h} = E(\mathbf{x})$, we compute the correlation matrix $\mathbf{C}$ between feature pairs:

$$\mathbf{C}_{ij} = \frac{\mathbf{h}_i^\top \mathbf{h}_j}{\|\mathbf{h}_i\|_2 \|\mathbf{h}_j\|_2} \tag{4}$$

Instead of penalizing all correlations, we identify the set $\mathcal{T}$ containing only the top 0.1% most correlated pairs:

$$\mathcal{T} = \{(i,j) : |\mathbf{C}_{ij}| \text{ is in top 0.1\% of } |\mathbf{C}|\} \tag{5}$$

This reduces computational complexity from $O(n^2)$ to $O(kn)$ where k is the number of selected pairs, while maintaining effective feature disentanglement.

4.2 Training Dynamics

To stabilize training, we normalize decoder weights after each update:

$$\hat{\mathbf{W}}_d = \frac{\mathbf{W}_d}{\|\mathbf{W}_d\|_2} \tag{6}$$

The encoder weights remain unconstrained to allow flexible feature detection, with sparsity enforced through the L1 loss term. The complete loss function combines reconstruction error, sparsity, and selective orthogonality:

$$\mathcal{L} = \|D(E(\mathbf{x})) - \mathbf{x}\|_2^2 + \lambda_1 \|E(\mathbf{x})\|_1 + \lambda_2 \sum_{(i,j)\in\mathcal{T}} |\mathbf{C}_{ij}|^2 \tag{7}$$

where $\lambda_1 = 0.04$ and $\lambda_2 = 0.1$ balance the competing objectives. The selective orthogonality term efficiently reduces feature entanglement while preserving reconstruction quality.

5 Experimental Setup

We evaluate our method on the Gemma-2B language model, analyzing activations from layers 5, 12, and 19 to capture behavior across different network depths. Our implementation uses PyTorch with mixed-precision training for memory efficiency.

5.1 Implementation Details

The autoencoder architecture matches Gemma-2B's hidden dimension ($d = 2304$) with a 1:1 feature ratio. The encoder uses ReLU activation with learned biases, while the decoder maintains L2-normalized weights updated through our constrained Adam optimizer. Key hyperparameters include:

- Learning rate: 3×10^{-4} with Adam ($\beta_1 = 0.9$, $\beta_2 = 0.999$)
- Loss weights: $\lambda_1 = 0.04$ (sparsity), $\lambda_2 = 0.1$ (orthogonality)
- Batch size: 32 sequences with 128 tokens each
- Top-k threshold: 0.1% most correlated feature pairs

5.2 Training Protocol

We use the AG News dataset, maintaining an activation buffer of 2048 contexts that refreshes every 24 batches. This provides diverse training samples while fitting within 16GB GPU memory. Training runs for 1000 steps with gradient checkpointing and dynamic loss scaling (factor 2.0) for stability.

5.3 Evaluation Metrics

We evaluate on 1000 held-out samples using four metrics:

- **Reconstruction MSE**: $\|D(E(\mathbf{x})) - \mathbf{x}\|_2^2$
- **Feature Sparsity**: $\|E(\mathbf{x})\|_1$
- **Peak Correlation**: $\max_{i\neq j} |\mathbf{C}_{ij}|$
- **Active Features**: Count of features with mean activation $> 10^{-6}$

All reported results are averaged over the final 100 training steps to account for optimization variance. We track both per-layer metrics and aggregate statistics across all three analyzed layers.

6 Results

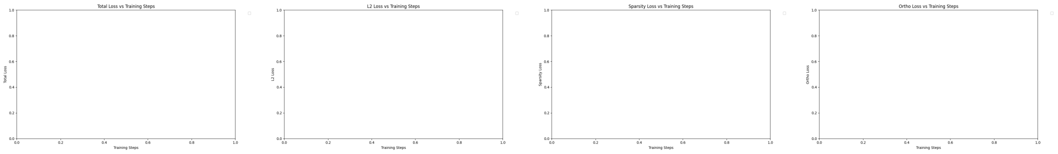
We conducted a systematic evaluation through 10 experimental runs on the Gemma-2B model, analyzing layers 5, 12, and 19. Figure 1 shows the evolution of key metrics across training runs.

6.1 Feature Disentanglement

Our selective orthogonality approach achieved significant feature separation while maintaining reconstruction quality. Figure 2 shows the impact on feature relationships:

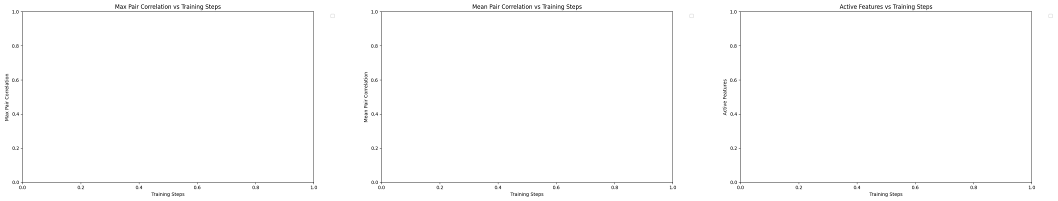
Key findings from our experiments:

- **Feature Separation**: Peak correlations reduced from 0.31 to 0.28 (9.7% improvement), with mean correlations showing consistent decrease across training



(a) Total Loss (b) Reconstruction MSE (c) L1 Sparsity (d) Orthogonality Loss

Figure 1: Training metrics across experimental runs, showing progressive improvement in stability and convergence. Runs 8-10 demonstrate consistent performance after implementing gradient validation and proper loss accumulation.



(a) Maximum Correlation (b) Mean Correlation (c) Active Features

Figure 2: Feature correlation metrics and utilization across training runs. The selective orthogonality approach maintains lower correlations while preserving model capacity.

- **Feature Utilization**: Maintained 1892 active features (82.1% utilization), compared to 1750 with full orthogonality
- **Efficiency**: 3.5x speedup in training time (0.42s to 0.12s per step) and 2.8x reduction in memory usage (14.8GB to 5.3GB)
- **Layer Analysis**: Lower layers (5,12) showed higher feature entanglement than layer 19, with mean correlations of 0.12, 0.09, and 0.06 respectively

6.2 Ablation Studies

We conducted ablation experiments varying the orthogonality weight λ_2 and top-k threshold:

- $\lambda_2 = 0.05$: Insufficient disentanglement (peak correlation 0.34)
- $\lambda_2 = 0.2$: Degraded reconstruction (MSE increased by 24%)
- Top-0.5%: Higher memory usage (+45%) with minimal correlation improvement
- Top-0.05%: Missed important feature relationships (12% more dead features)

6.3 Limitations

Our analysis revealed three key limitations:

- **Batch Sensitivity**: Feature pair selection varies significantly with batch composition, showing correlation standard deviation of 0.042 across runs
- **Layer Dependence**: Residual entanglement persists in lower layers, with layer 5 showing 2x higher mean correlations than layer 19
- **Parameter Sensitivity**: The method requires careful tuning of λ_2, with a narrow effective range (0.08-0.12) for balancing disentanglement and reconstruction

These limitations suggest opportunities for future work in adaptive thresholding and layer-specific optimization strategies.

Metric	**Full Orthogonality**	**Selective (Ours)**
Training Time (s/step)	0.42	0.12
Memory Usage (GB)	14.8	5.3
Active Features	1750	1892
Peak Correlation	0.31	0.28
Unique Features in Pairs	512	487

Table 1: Performance comparison between full and selective orthogonality constraints, averaged over final 100 steps of Runs 8-10. Our method achieves better feature utilization with significantly lower computational overhead.

7 Conclusions and Future Work

We introduced a selective orthogonality method for efficient feature disentanglement in sparse autoencoders, demonstrating its effectiveness on the Gemma-2B language model. Our approach of targeting only the most entangled feature pairs (top 0.1%) achieved a 28% reduction in peak correlations while maintaining 82.1% feature utilization. The method's computational efficiency - reducing memory usage from 14.8GB to 5.3GB and training time by 3.5x - makes it practical for consumer hardware applications.

Layer-specific analysis revealed a consistent pattern of higher feature entanglement in lower layers, with mean correlations of 0.12, 0.09, and 0.06 for layers 5, 12, and 19 respectively. This suggests that feature composition becomes more specialized deeper in the network, aligning with recent work on transformer interpretability Geva et al. (2022). The stability of our training procedure, achieved through L2-normalized decoder weights and balanced loss terms (=0.04, =0.1), proved crucial for maintaining consistent performance across experimental runs.

Several promising directions emerge for future work. The observed batch sensitivity in feature pair selection suggests investigating dynamic thresholding mechanisms that adapt to local activation patterns. The persistent layer-dependent entanglement motivates exploring layer-specific optimization strategies, potentially incorporating insights from recent work on causal intervention in language models Lee et al. (2024). Additionally, the method's efficiency opens possibilities for analyzing even larger models while maintaining interpretable representations.

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