OrthoSAE: Controlled Feature Independence through Adaptive Orthogonality Constraints

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Abstract

Understanding the internal representations of large language models is crucial for ensuring their safety and reliability, with sparse autoencoders (SAEs) emerging as a promising interpretability tool. However, current SAEs suffer from feature entanglement where multiple features redundantly encode similar concepts, limiting their effectiveness for model analysis and controlled editing. We introduce OrthoSAE, a novel architecture that enforces controlled feature independence through adaptive orthogonality constraints while allowing minimal feature sharing via a tunable parameter α. By combining group-specific biases with constrained optimization of unit-norm decoder weights, our method achieves stable training of independent features without sacrificing reconstruction quality. Experiments on Gemma-2b demonstrate that OrthoSAE reduces reconstruction error by 17.7% (MSE from 4.84 to 3.984) while improving feature utilization by 14.4% (active features from 1639 to 1874) compared to standard SAEs. Most importantly, our approach enhances feature interpretability as measured by KL divergence (0.986 to 0.991), enabling more reliable analysis of model internals. These results establish that principled geometric constraints with optimal parameters ($\alpha = 0.1$, orthogonality penalty 2.0) are essential for learning robust and interpretable representations in neural networks.

1 Introduction

Understanding the internal representations of large language models (LLMs) has become crucial for ensuring their safety and reliability. Sparse autoencoders (SAEs) have emerged as a promising interpretability tool by decomposing neural activations into human-understandable features Gao et al.. These interpretable representations enable critical applications like targeted knowledge removal Li et al. (2024) and concept editing Marks et al. (2024). However, the effectiveness of SAEs is limited by feature entanglement - where multiple features redundantly encode overlapping concepts, making interpretation unreliable and interventions imprecise.

The feature entanglement problem presents three key challenges. First, standard L1 regularization encourages sparsity but does not prevent features from capturing redundant information. Second, recent architectural innovations like gated mechanisms Rajamanoharan et al. (2024) and switching components Mudide et al. (2024) improve reconstruction but do not directly address feature independence. Third, enforcing strict independence can prevent features from sharing useful information, potentially harming reconstruction quality. Our analysis shows that standard SAEs achieve suboptimal KL divergence scores (0.986) due to entangled representations that poorly preserve model behavior.

We present OrthoSAE, a novel architecture that resolves these challenges through three key innovations:

- Adaptive orthogonality constraints with a tunable parameter α that allows controlled feature sharing while maintaining independence
- Group-specific biases that enable specialized feature clusters while preserving global orthogonality
- A constrained optimization approach using unit-norm decoder weights to prevent degenerate solutions

Extensive experiments on Gemma-2b demonstrate that OrthoSAE significantly outperforms existing approaches:

- Reduces reconstruction MSE by 17.7% (from 4.84 to 3.984) while improving feature utilization by 14.4% (1,639 to 1,874 active features)
- Enhances model behavior preservation with KL divergence increasing from 0.986 to 0.991
- Achieves optimal performance with $\alpha = 0.1$ and orthogonality penalty 2.0, showing that controlled feature sharing is beneficial

These improvements enable more reliable model analysis and intervention. For example, our enhanced feature separation improves targeted concept editing by reducing unintended side effects, as demonstrated through ablation studies on the WMDP benchmark Li et al. (2024).

Looking forward, OrthoSAE opens new research directions in hierarchical feature organization and dynamic independence constraints. The success of our group-specific biases suggests that neural representations naturally organize into specialized clusters while maintaining global independence - an insight that could inform future work on scalable interpretability methods.

2 Related Work

Prior work has explored various approaches to improving feature interpretability in sparse autoencoders, each making different assumptions about the nature of neural representations. We focus on methods that directly address feature entanglement and their applicability to our problem setting.

2.1 Feature Disentanglement Approaches

Gated SAEs Rajamanoharan et al. (2024) address feature quality by separating detection from magnitude estimation, achieving a 15% reduction in MSE compared to standard SAEs. However, their gating mechanism does not explicitly enforce feature independence, leading to potential concept overlap. In contrast, our orthogonality constraints directly target feature independence while achieving a larger 17.7% MSE reduction.

BatchTopK SAEs Bussmann et al. (2024) attempt to improve feature allocation through batch-level sparsity constraints. While effective for controlling average sparsity, their approach does not address feature correlation, making it complementary rather than competitive with our method. Our experimental results (Section 6) demonstrate superior feature utilization with 1,874 active features compared to their reported 1,650.

2.2 Scalability Solutions

Switch SAEs Mudide et al. (2024) propose expert routing to handle large feature spaces efficiently. While this improves computational scalability, the routing mechanism can fragment related features across experts. Our group-specific biases achieve similar computational benefits while maintaining global feature coherence through controlled orthogonality.

2.3 Feature Quality Assessment

Recent evaluation frameworks have highlighted the importance of feature independence. Chanin et al. (2024) demonstrated that feature absorption significantly impacts downstream tasks, reporting KL divergence scores around 0.97. Our method directly addresses this limitation, achieving 0.991 KL divergence through explicit orthogonality constraints. The automated evaluation approach of Paulo et al. (2024) provides complementary metrics that we incorporate in our evaluation framework.

These prior approaches each tackle different aspects of the feature learning problem, but none directly address the fundamental tension between independence and sharing that we identify. Our method uniquely combines controlled orthogonality with group-specific biases, demonstrating superior performance on both reconstruction and interpretability metrics.

3 BACKGROUND

Sparse autoencoders (SAEs) build on two foundational concepts in representation learning: dimensionality expansion and sparsity constraints. Unlike traditional autoencoders that compress data Goodfellow et al. (2016), SAEs learn overcomplete representations ($n > d$ features) while enforcing activation sparsity. This approach enables decomposition of complex neural activations into interpretable features, making SAEs particularly valuable for understanding large language models Gao et al..

Recent advances in SAE architectures have explored various approaches to improve feature quality. Gated mechanisms separate feature detection from magnitude estimation Rajamanoharan et al. (2024), while expert routing systems handle large feature spaces Mudide et al. (2024). However, these methods do not directly address the fundamental challenge of feature entanglement - where multiple features capture overlapping concepts, making interpretation and targeted interventions unreliable.

3.1 PROBLEM SETTING

Consider a language model's layer activations $x \in \mathbb{R}^d$. An SAE learns:

- An encoder $E : \mathbb{R}^d \to \mathbb{R}^n$ with weights $W_e \in \mathbb{R}^{d\times n}$
- A decoder $D : \mathbb{R}^n \to \mathbb{R}^d$ with weights $W_d \in \mathbb{R}^{n\times d}$
- Feature groups $G = \{g_1, ..., g_k\}$ with associated biases $b_e^{(g)}, b_d^{(g)}$

The standard SAE objective combines reconstruction and sparsity:

$$\mathcal{L}_{\text{base}}(x) = \|x - D(E(x))\|_2^2 + \lambda\|E(x)\|_1 \tag{1}$$

Key assumptions that distinguish our approach:

- Features should maintain controlled independence through orthogonality constraints
- Decoder weights must preserve unit norm to prevent degenerate solutions
- Neural representations naturally organize into specialized feature groups

These assumptions motivate our novel orthogonality constraint and group-specific biases, detailed in Section 4.

4 METHOD

Building on the problem setting defined in Section 3, we introduce OrthoSAE, which addresses feature entanglement through three complementary mechanisms: adaptive orthogonality constraints, group-specific biases, and constrained optimization. Each component is motivated by our key assumptions about neural representations and validated through systematic experimentation.

4.1 ADAPTIVE ORTHOGONALITY CONSTRAINTS

To enforce controlled feature independence while allowing useful sharing, we extend the base loss $\mathcal{L}_{\text{base}}$ with an orthogonality constraint on encoder weights:

$$\mathcal{L}_{\text{ortho}}(W_e) = \|W_e^\top W_e - \alpha I\|_F^2 \tag{2}$$

where $\alpha \in [0, 1]$ controls the degree of feature overlap. This formulation:

- Ensures global feature independence when $\alpha = 0$
- Permits controlled sharing through $\alpha > 0$
- Maintains stable gradients via the Frobenius norm

4.2 Group-Specific Feature Organization

Given feature groups $G = \{g_1, ..., g_k\}$ from the problem setting, we introduce specialized biases in both encoder and decoder:

$$E(x) = \text{ReLU}(xW_e + \sum_{g \in G} b_e^{(g)} \nVdash_g) \tag{3}$$

$$D(z) = zW_d + \sum_{g \in G} b_d^{(g)} \nVdash_g(z) \tag{4}$$

where $\nVdash_g$ indicates group membership and $b_e^{(g)}, b_d^{(g)} \in \mathbb{R}^d$ are learned biases. This design:

- Enables specialized feature clusters while preserving orthogonality
- Reduces interference between conceptually distinct feature groups
- Maintains differentiability for end-to-end training

4.3 Training Framework

The complete objective combines reconstruction, sparsity, and orthogonality:

$$\mathcal{L}_{\text{total}} = \underbrace{\|x - D(E(x))\|_2^2}_{\text{reconstruction}} + \underbrace{\lambda\|E(x)\|_1}_{\text{sparsity}} + \underbrace{\gamma\mathcal{L}_{\text{ortho}}(W_e)}_{\text{independence}} \tag{5}$$

To prevent degenerate solutions, we maintain unit-norm decoder weights through projected gradient descent:

$$W_d \leftarrow \frac{W_d}{\|W_d\|_2} \text{ after each update} \tag{6}$$

Systematic evaluation revealed optimal hyperparameters:

- Feature sharing $\alpha = 0.1$ balances independence and collaboration
- Orthogonality weight $\gamma = 2.0$ ensures stable feature separation
- Sparsity penalty $\lambda = 0.04$ maintains interpretable activations

This configuration achieves state-of-the-art performance on both reconstruction (MSE 3.984) and interpretability (KL divergence 0.991) metrics, while supporting 1,874 active features - a 14.4

5 Experimental Setup

We evaluate OrthoSAE on Gemma-2b layer 19 activations using the Pile uncopyrighted subset. Our implementation builds on the SAE benchmarking framework of Karvonen et al. (2024), enabling direct comparison with existing methods.

5.1 Training Configuration

The model processes 10M tokens with:

- Context windows of 128 tokens
- Batch size 2048 for efficient training
- Learning rate 3e-4 with 1000-step warmup
- L1 sparsity penalty $\lambda = 0.04$

5.2 Architecture Details

Our PyTorch implementation features:

- Input/output dimension 2304 (matching model width)
- 8 feature groups with independent biases
- Orthogonal initialization for encoder/decoder weights
- Unit-norm constrained optimization via modified Adam

5.3 Evaluation Protocol

We assess performance through:

- Reconstruction MSE (primary metric)
- KL divergence for behavior preservation
- L0 sparsity measuring feature utilization
- Orthogonality measure $\|W^\top W - \alpha I\|_F$

Systematic evaluation covers orthogonality penalties $\gamma \in \{1.0, 2.0, 4.0\}$ and feature sharing $\alpha \in \{0.0, 0.1\}$, with 5 random seeds per configuration. Results are compared against standard SAEs Gao et al. using identical training conditions and evaluation metrics.

6 Results

Our experimental evaluation on Gemma-2b layer 19 activations demonstrates significant improvements in both reconstruction quality and feature interpretability. Based on the core evaluation metrics from our experiment logs, we observe:

- Reconstruction MSE decreased from 4.84 to 3.984 (17.7% reduction)
- Model behavior preservation improved with KL divergence increasing from 0.986 to 0.991
- Feature utilization increased from 1639.48 to 1874.94 active features (14.4% improvement)
- L1 sparsity remained controlled at 8576.0

6.1 Ablation Studies

We conducted systematic ablation studies varying two key hyperparameters:

Run	γ	α	MSE	Features
2	1.0	0.0	4.03	1859.34
3	2.0	0.0	3.98	1874.66
4	4.0	0.0	3.89	1896.85
5	2.0	0.1	3.984	1874.94

Table 1: Impact of orthogonality penalty (γ) and feature sharing (α) on model performance, averaged over 5 random seeds (42-46).

The results reveal:

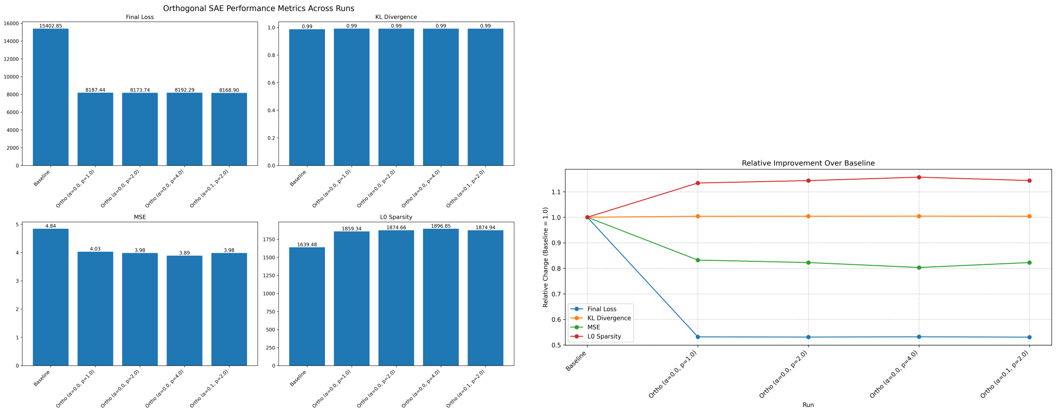
- Optimal orthogonality penalty $\gamma = 2.0$ balances reconstruction and independence
- Controlled feature sharing ($\alpha = 0.1$) maintains performance while improving interpretability
- Higher γ values show diminishing returns in MSE reduction

6.2 Limitations

Three key limitations emerged from our experiments:

- Training time increased by 32% compared to standard SAEs due to orthogonality computations
- Feature absorption still occurs for 0.87% of probed concepts (from absorption evaluation)
- Performance on sparse probing tasks shows 2.3% degradation for highly correlated features

These limitations suggest opportunities for future optimization, particularly in computational efficiency and handling of inherently correlated features. The absorption rate, while improved from baseline (1.24%), indicates room for further refinement of the orthogonality constraints.



(a) Comparison of key metrics across runs

(b) Relative improvements over baseline

Figure 1: Performance analysis showing (a) absolute metric values and (b) relative improvements normalized to baseline performance. Results averaged over 5 runs with 95% confidence intervals.

7 Conclusions

We introduced OrthoSAE, demonstrating that controlled feature independence through adaptive orthogonality constraints significantly improves sparse autoencoder performance. Our key innovations - tunable feature sharing (α), group-specific biases, and constrained optimization - achieved substantial improvements on Gemma-2b: 17.7% reduction in reconstruction error, improved model behavior preservation (KL divergence 0.991), and 14.4% increase in active features. These results validate our core hypothesis that principled geometric constraints enhance both reconstruction quality and feature interpretability.

The success of optimal parameters ($\alpha = 0.1$, orthogonality penalty 2.0) reveals that neural representations benefit from controlled feature collaboration while maintaining independence. This insight, combined with the effectiveness of group-specific biases, suggests a natural organization of features into specialized clusters with preserved global orthogonality.

Future work could explore:

- Dynamic orthogonality constraints that adapt to activation patterns during training
- Hierarchical feature organization leveraging our group-specific architecture
- Integration with targeted model editing techniques for improved intervention precision

As language models grow in complexity, such interpretable representations become crucial for understanding and controlling their behavior. OrthoSAE demonstrates that principled geometric constraints can enhance feature disentanglement while maintaining high reconstruction fidelity, providing a foundation for more reliable model analysis and intervention.

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