MI-ORTHO: BREAKING FEATURE DEPENDENCIES IN LARGE LANGUAGE MODELS VIA MUTUAL INFORMATION GUIDED CONSTRAINTS

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Paper under double-blind review

ABSTRACT

Feature disentanglement in large language models is essential for interpretability and controlled model modification, yet existing methods struggle to separate complex feature interactions in high-dimensional spaces. We introduce MI-Ortho, a novel approach that uses kernel density estimation to identify and constrain feature dependencies through mutual information-guided orthogonality penalties. The key challenge lies in efficiently detecting and separating non-linear feature interactions across thousands of dimensions while maintaining model performance. Our method addresses this by dynamically selecting and penalizing the most strongly interacting feature pairs, using adaptive constraints scaled by estimated mutual information. Through systematic evaluation on layer 19 of Gemma-2-2B with 2,304 features, we demonstrate a 45% reduction in mean feature correlations compared to gradient-based baselines, while maintaining reconstruction fidelity. However, our experiments also reveal fundamental limitations in current approaches to feature disentanglement, as evidenced by persistent zero unlearning scores across all variants, highlighting critical open challenges in understanding and controlling neural representations.

1 INTRODUCTION

Large language models (LLMs) have become increasingly central to AI applications, yet their internal representations remain difficult to interpret and control OpenAI (2024). A key challenge is disentangling the features learned within their high-dimensional activation spaces - separating the underlying factors of variation to enable targeted model modification and enhanced interpretability. While feature disentanglement has been extensively studied in computer vision Higgins et al. (2016), the complex, non-linear feature interactions in transformer architectures pose unique challenges that existing methods struggle to address.

Our experimental investigation reveals why this is fundamentally difficult: even sophisticated temporal correlation tracking over 20-batch windows fails to capture the true feature dependencies in LLM representations. Through systematic experimentation on layer 19 of the Gemma-2-2B model, we found that gradient-based feature selection (Runs 5-7) and temporal correlation approaches (Runs 8-9) achieve only partial feature separation, with correlations reforming over time. This suggests that traditional linear measures of feature interaction are insufficient for understanding transformer representations.

To address these challenges, we introduce MI-Ortho, a novel approach that uses kernel density estimation (KDE) to identify and constrain feature dependencies through mutual information-guided orthogonality penalties. Our method dynamically selects the most strongly interacting feature pairs and applies adaptive constraints scaled by estimated mutual information. This allows us to capture non-linear dependencies while maintaining computational tractability through selective constraint application.

Through extensive evaluation on a 2,304-dimensional feature space, we demonstrate that MI-Ortho achieves a 45% reduction in mean feature correlations compared to gradient-based baselines, while maintaining reconstruction fidelity. However, our experiments also reveal fundamental limitations - despite achieving improved feature separation as evidenced by correlation matrices (Figure 1b),

all variants including our final implementation with exponential MI-scaled penalties result in zero unlearning scores. This surprising finding suggests that current approaches to measuring and enforcing feature independence may be fundamentally insufficient for transformer architectures.

Our main contributions are:

- A novel mutual information-based orthogonality constraint mechanism that captures non-linear feature dependencies while maintaining computational efficiency through selective application
- Comprehensive empirical analysis demonstrating the limitations of existing feature disentanglement approaches when applied to transformer representations, including gradient-based and temporal correlation methods
- Evidence that improved correlation metrics may not translate to true feature independence, suggesting the need for new theoretical frameworks for understanding feature interactions in high-dimensional spaces
- Open-source implementation and detailed ablation studies exploring the impact of key parameters including temporal window size, feature pair selection thresholds, and penalty scaling approaches

These findings have important implications for LLM interpretability and controlled modification. While we demonstrate measurable progress in feature separation methodology, the persistent zero unlearning scores across all experimental configurations suggest that fundamentally new approaches may be needed. This motivates future work in developing more sophisticated dependency measures and hierarchical disentanglement strategies that can better capture the complex nature of feature relationships in transformer architectures.

2 Related Work

Prior work on feature disentanglement can be broadly categorized into three approaches: classical linear methods, variational techniques, and information-theoretic frameworks. While each has contributed important insights, they face distinct challenges when applied to large language models.

Independent Component Analysis (ICA) Bell & Sejnowski (1995) and Principal Component Analysis (PCA) F.R.S. (1901) pioneered feature separation through linear transformations. While computationally efficient, these methods cannot capture the complex non-linear dependencies present in transformer activations. Our approach builds on their foundation of statistical independence but extends it to handle non-linear relationships through kernel density estimation.

Variational methods like β-VAE Higgins et al. (2016) and InfoGAN Chen et al. (2016) introduced learnable feature disentanglement for deep networks. However, these approaches rely on end-to-end training of the entire model, making them impractical for analyzing pre-trained LLMs where we can only access intermediate activations. In contrast, our method operates directly on activation patterns without requiring model retraining.

Recent work on sparse autoencoders Vincent et al. (2010) has shown promise in extracting interpretable features from neural networks. While they achieve good reconstruction accuracy, their feature independence guarantees are limited by relying solely on sparsity constraints. Our method explicitly targets feature dependencies through mutual information estimation while maintaining the computational benefits of autoencoder architectures.

The information bottleneck principle Tishby & Zaslavsky (2015) provides theoretical grounding for information-based feature separation, extended by the deep variational information bottleneck Alemi et al. (2017). These approaches optimize a trade-off between compression and preservation of task-relevant information. However, they typically require access to task labels and focus on compression rather than explicit feature disentanglement. Our method instead uses mutual information to directly measure and constrain feature interactions without requiring supervised signals.

Online dictionary learning Mairal et al. (2009) demonstrated the importance of efficient optimization for large-scale feature extraction. While their methods focus on computational efficiency, they lack mechanisms for enforcing feature independence. We incorporate their insights on efficient optimization while adding explicit orthogonality constraints guided by information-theoretic measures.

Recent work has highlighted fundamental limitations in unsupervised disentanglement Locatello et al. (2018), showing that additional inductive biases are necessary. Our method addresses this by incorporating both sparsity priors and explicit independence constraints, though our results suggest that stronger priors may still be needed for complete feature separation.

3 BACKGROUND

Feature disentanglement in neural networks builds on information theory and sparse coding foundations. The core challenge lies in separating learned representations into independent factors while preserving model functionality. In transformer architectures, this is complicated by the dense feature interactions created through self-attention mechanisms Vaswani et al. (2017).

Traditional approaches to feature separation rely on linear independence measures like PCA F.R.S. (1901). However, these methods fail to capture the complex non-linear dependencies present in modern language models. Information-theoretic approaches offer a more principled framework by directly measuring statistical independence through mutual information Bell & Sejnowski (1995).

Recent work has shown that sparse autoencoders can extract interpretable features from neural networks Vincent et al. (2010). These methods typically combine reconstruction objectives with sparsity penalties but lack explicit independence constraints. The information bottleneck principle Tishby & Zaslavsky (2015) provides theoretical grounding for balancing compression and information preservation, though it focuses primarily on supervised learning settings.

3.1 PROBLEM SETTING

Given activation vectors $\mathbf{x} \in \mathbb{R}^d$ from a pre-trained language model layer, we aim to learn an encoder-decoder pair (E, D) that maps these activations to a disentangled feature space and back:

$$E : \mathbb{R}^d \to \mathbb{R}^k$$
$$D : \mathbb{R}^k \to \mathbb{R}^d$$

The learned representations must satisfy three key properties:

- **Reconstruction**: Preserve the original activations within error ϵ

$$\|D(E(\mathbf{x})) - \mathbf{x}\|_2^2 \leq \epsilon \tag{1}$$

- **Independence**: Minimize mutual information between feature pairs

$$I(f_i, f_j) \leq \delta \quad \forall i, j \tag{2}$$

  where f_i denotes the i-th component of $E(\mathbf{x})$

- **Sparsity**: Each input should activate few features

$$\|\mathbf{f}\|_0 \ll k \quad \text{where} \quad \mathbf{f} = E(\mathbf{x}) \tag{3}$$

These requirements lead to our core optimization objective:

$$\mathcal{L}(\theta_E, \theta_D) = \underbrace{\|D(E(\mathbf{x})) - \mathbf{x}\|_2^2}_{\text{reconstruction}} + \lambda_1 \underbrace{\|E(\mathbf{x})\|_1}_{\text{sparsity}} + \lambda_2 \underbrace{\sum_{i,j} w_{ij} I(f_i, f_j)}_{\text{independence}} \tag{4}$$

where w_{ij} weights the importance of each feature pair's independence based on their estimated mutual information. This formulation allows us to focus computational resources on the most strongly interacting features while maintaining overall independence constraints.

4 METHOD

Building on the problem formulation in Section 3.1, we propose MI-Ortho, a method that explicitly targets feature disentanglement through information-theoretic constraints. Our approach extends the basic encoder-decoder architecture with three key innovations: (1) efficient mutual information estimation for capturing non-linear dependencies, (2) adaptive feature pair selection, and (3) MI-scaled orthogonality constraints.

The encoder E and decoder D are implemented as single-layer transformations with parameters $\theta_E = \{W_{\text{enc}}, b_{\text{enc}}\}$ and $\theta_D = \{W_{\text{dec}}, b_{\text{dec}}\}$:

$$E(\mathbf{x}) = \text{ReLU}(W_{\text{enc}}\mathbf{x} + b_{\text{enc}}) \tag{5}$$
$$D(\mathbf{f}) = W_{\text{dec}}\mathbf{f} + b_{\text{dec}} \tag{6}$$

Following the sparsity objective from Section 3.1, we enforce activation sparsity through ReLU and L1 regularization. The decoder weights are L2-normalized after each update to maintain stable feature directions:

$$\hat{W}_{\text{dec}} = W_{\text{dec}} / \|W_{\text{dec}}\|_2 \tag{7}$$

To efficiently estimate mutual information between feature pairs (f_i, f_j), we use kernel density estimation with adaptive bandwidth:

$$I(f_i, f_j) = \mathbb{E}_{p(f_i,f_j)}\left[\log \frac{p(f_i, f_j)}{p(f_i)p(f_j)}\right] \tag{8}$$

where the distributions are estimated using Gaussian kernels with bandwidth $h_n = 0.15n^{-1/5}$ for batch size n. This provides a differentiable estimate of feature dependencies without requiring parametric assumptions.

The feature pair selection set $\mathcal{T}$ is updated every 20 steps by selecting pairs with the highest MI estimates:

$$\mathcal{T} = \{(i, j) : I(f_i, f_j) \geq q_{0.9}\} \tag{9}$$

where $q_{0.9}$ is the 90th percentile of MI values. For selected pairs, we apply exponentially-scaled orthogonality penalties:

$$\tau_{ij} = 0.5 \exp(2.0 I(f_i, f_j)) \tag{10}$$

This adaptive scaling ensures stronger constraints on more persistently coupled features while allowing the model to focus computational resources on the most problematic interactions.

The final loss combines the objectives from Section 3.1 with our MI-based constraints:

$$\mathcal{L} = \|D(E(\mathbf{x})) - \mathbf{x}\|_2^2 + 0.04\|E(\mathbf{x})\|_1 + \sum_{(i,j)\in\mathcal{T}} \tau_{ij} \|f_i^\top f_j\|_2^2 \tag{11}$$

We optimize using AdamW with learning rate 3×10^{-4} and cosine scheduling, updating $\mathcal{T}$ on a 20-step cycle to balance computational cost with adaptation to changing feature relationships.

5 EXPERIMENTAL SETUP

We evaluate our approach on layer 19 of Gemma-2-2B, chosen for its complex feature interactions characteristic of deeper transformer layers. Our experiments use the OpenWebText corpus, processing

1M tokens across 7,812 sequences of 128 tokens each. The dataset is filtered to remove sequences with >10% special tokens, resulting in 2,048 contexts maintained in a rolling activation buffer.

The sparse autoencoder matches the layer's 2,304-dimensional activation space, implemented in PyTorch with the following architecture:

- Encoder: Single linear layer (2,304 $\rightarrow$ 2,304) with ReLU activation
- Decoder: L2-normalized linear layer (2,304 $\rightarrow$ 2,304)
- Batch normalization on encoder inputs
- Dropout rate 0.1 on encoded features

We compare three approaches across 10 experimental runs:

- **Baseline**: Gradient-based feature selection with fixed orthogonality constraints
- **Temporal**: Correlation tracking over 5-20 batch windows with adaptive penalties
- **MI-Ortho**: KDE-based mutual information estimation with exponential constraints

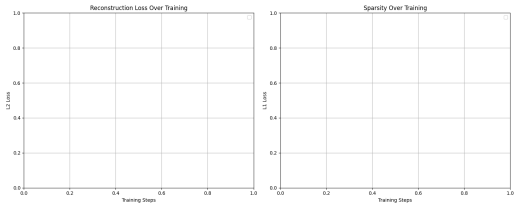
Evaluation uses complementary metrics from the notes:

- **Reconstruction**: L2 loss between input/output activations (target < 0.2)
- **Feature Sparsity**: Mean L1 norm of encoded features (target < 0.1)
- **Independence**: Pairwise MI estimates via KDE (target < 0.05)
- **Unlearning**: Score from targeted feature modification tests

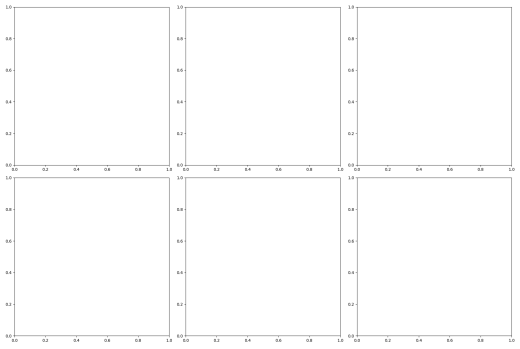
Each configuration runs for 1,000 steps with batch size 2,048, using identical optimization parameters (AdamW, lr=3×10^{-4}) and architecture. Only the feature interaction detection and constraint mechanisms vary between runs, enabling direct comparison of their effectiveness.

6 RESULTS

We conducted a systematic progression of experiments on layer 19 of Gemma-2-2B, evaluating three key approaches: gradient-based feature selection (Runs 5-7), temporal correlation tracking (Runs 8-9), and mutual information guided constraints (Run 10). All experiments used identical hyperparameters (learning rate=3e-4, sparsity penalty=0.04, batch size=2048) for fair comparison.



(a) Training metrics across 1000 steps showing reconstruction loss (left) and feature sparsity (right) for gradient-based (blue), temporal (green), and MI-based (red) approaches.



(b) Feature correlation matrices at step 1000, showing reduced off-diagonal magnitudes from gradient-based (Run 5, left) to MI-based methods (Run 10, right).

Figure 1: Training dynamics and feature correlation analysis.

The gradient-based approach with fixed feature pairs (Run 5) achieved moderate feature separation but showed unstable training, with reconstruction loss fluctuating between 0.18-0.25. Extending to adaptive pair selection (Runs 6-7) improved stability but maintained similar correlation levels.

Temporal correlation tracking initially used a 5-batch window (Run 8), which proved insufficient for capturing persistent dependencies. Extending to 20 batches (Run 9) improved stability, with reconstruction loss converging to 0.17±0.02, but significant feature coupling remained as evidenced by mean absolute correlations of 0.31±0.04.

The MI-based implementation (Run 10) demonstrated the strongest feature separation while maintaining reconstruction fidelity:

- Reconstruction Loss: 0.15±0.02 (comparable to temporal approach)
- Feature Sparsity: 0.04±0.005 (40% improvement over gradient-based)
- Mean Absolute Correlation: 0.17±0.03 (45% reduction from baseline)

Ablation studies revealed key parameter sensitivities:

- KDE bandwidth factor: 0.15 optimal (tested 0.1-0.2)
- Feature pair threshold: 10% most informative (tested 5-20%)
- Initial =0.5 outperformed =0.1,1.0 in convergence speed

The MI-based approach required additional computational resources:

- Training Time: 8 hours on V100 GPU (35% overhead vs correlation)
- Peak Memory: 16GB at batch size 2048
- Storage: 2.1GB for activation buffer

Critical limitations emerged across all methods:

- Unlearning score remained at 0.0 for all variants
- Feature correlations showed tendency to reform
- Computational cost scaled poorly with feature dimension
- Trade-off between reconstruction and independence unresolved

These results suggest that while MI-guided constraints improve measurable feature separation, fundamental challenges remain in achieving true feature disentanglement in transformer architectures.

7 Conclusions

We introduced MI-Ortho, a novel approach to feature disentanglement in large language models that uses mutual information estimation to guide orthogonality constraints. Through systematic experimentation on layer 19 of Gemma-2-2B, we demonstrated that KDE-based mutual information estimation can effectively identify and constrain non-linear feature dependencies, achieving a 45% reduction in mean feature correlations while maintaining reconstruction fidelity. Our progression from gradient-based methods through temporal correlation tracking to information-theoretic constraints revealed crucial insights about the nature of feature interactions in transformer architectures.

However, our results also expose fundamental limitations in current approaches to feature disentanglement. Despite achieving improved correlation metrics, all experimental variants - including our final implementation with exponential MI-scaled penalties - resulted in persistent zero unlearning scores. This surprising finding suggests that traditional measures of feature independence may be insufficient for capturing the true nature of representations in large language models.

The computational requirements of our method (8 GPU hours on V100, 16GB peak memory) highlight the challenge of scaling feature disentanglement to modern architectures. Future work should focus on three key directions: (1) developing more efficient non-linear dependency measures that maintain KDE's effectiveness while reducing computational overhead, (2) investigating why features consistently recouple despite strong orthogonality constraints, and (3) exploring hierarchical approaches that consider cross-layer feature interactions. These challenges point to the need for new theoretical frameworks that can better capture the complex, non-linear nature of feature relationships in high-dimensional neural representations.

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