

# 000 001 002 003 004 005 MIRAGES OF MISALIGNMENT: HOW SUPERPOSITION 006 DISTORTS NEURAL REPRESENTATION GEOMETRY 007 008 009

010 **Anonymous authors**  
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## ABSTRACT

032 Neural networks trained on the same tasks achieve similar performance, but this is  
033 not always reflected in their measured representational alignment. We propose that  
034 this discrepancy arises from superposition or mixed selectivity, where individual  
035 neurons represent mixtures of features. Consequently, two networks representing  
036 an identical set of features can appear dissimilar if their neurons mix those fea-  
037 tures differently. This may explain why higher-dimensional networks, which are  
038 less prone to compressing mixtures of features, often show better alignment than  
039 smaller models with greater behavioral similarity. We formalize this through an  
040 analytic theory predicting apparent misalignment for common linear metrics like  
041 Representational Similarity Analysis (RSA) and Linear Regression, validating it  
042 from random projections to real neural networks. Using sparse autoencoders and  
043 K-Means to extract disentangled features while controlling for dimensionality, we  
044 find that feature-based alignment reveals higher similarity, particularly for early  
045 and lower-dimensional regions. **Some comparisons show decreased alignment**  
046 **with disentanglement, and RSA and Linear Regression often disagree in these**  
047 **cases. Simulations predict that higher RSA relative to Linear Regression in neu-**  
048 **ral space indicates shared inductive biases—a pattern confirmed in real data. Our**  
049 **results demonstrate that superposition and dimensionality interactions obscure the**  
050 **true alignment of lower-dimensional systems, while feature-based alignment al-**  
051 **lows us to more directly interrogate performance-relevant sources of misalign-**  
052 **ment, with important implications for model selection.**

## 1 INTRODUCTION

032 The development of deep neural networks capable of human-level performance on tasks such as  
033 object recognition and natural language has prompted a fundamental question: do different neural  
034 systems converge to similar representations (Rumelhart et al., 1986; Goldstein et al., 2022; Peterson  
035 et al., 2018; Sucholutsky et al., 2023; Huh et al., 2024; Reizinger et al., 2024)? Answering this  
036 requires comparing representations across models with varied architectures, training data, and ob-  
037 jectives, a challenge central to ideas like the platonic representation hypothesis (Huh et al., 2024;  
038 Reizinger et al., 2025). To measure these similarities, researchers turn to alignment metrics such as  
039 Representational Similarity Analysis (RSA) (Kriegeskorte & Wei, 2021) which abstract away from  
040 individual neurons to compare the geometry of population-level activity. Alternatively, Linear Re-  
041 gression is also used which learns a linear map to predict one network’s activity from another. Both  
042 metrics have become powerful alignment tools, yielding remarkable insights into shared structure  
043 (Yamins et al., 2014; Khaligh-Razavi & Kriegeskorte, 2014; Cadena et al., 2019; Khosla et al., 2021;  
044 Schrimpf et al., 2021; Conwell et al., 2024; Prince et al., 2024). However, the neural networks with  
045 highest alignment scores are not always the most behaviorally (e.g., task performance) or mech-  
046 anistically (e.g., sharing computational strategies) similar, leading to low performance-alignment  
047 correspondence (Schaeffer et al., 2024). This prompts the question: do behaviorally-similar models  
048 truly arrive at distinct representational solutions, or do confounding factors obscure the true repre-  
049 sentational similarities captured by standard metrics?

050 We propose the performance-alignment gap arises from *superposition* (or *mixed selectivity*), where  
051 individual neurons represent mixtures of multiple independent features (Smolensky, 1990; Elhage  
052 et al., 2022; Klindt et al., 2025). In this regime, neural networks can *linearly* represent more features  
053 than they have neurons by distributing features across overlapping neural codes. Consequently,

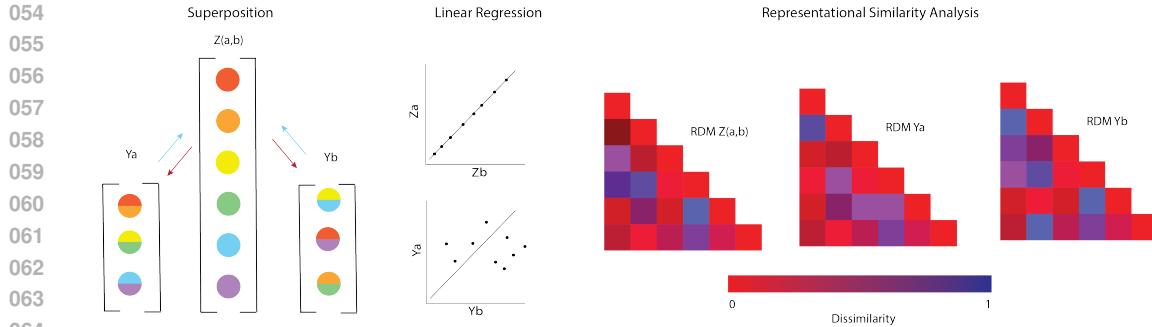


Figure 1: **Illustration of Core Idea.** **Superposition:** Two neural networks share an identical set of latent features ( $Z_a = Z_b$ ), but compress them (red arrows) in different ways  $Y_a \neq Y_b$ . Thus, computing alignment over the raw neural activations of network A ( $Y_a$ ) and B ( $Y_b$ ) leads to low representational similarity of these networks. We propose using sparse dictionary learning to recover (blue arrows) the shared features of networks from their raw activations prior to using alignment metrics (Donoho, 2006). **Linear regression:** Assuming perfect latent recovery, the maximum pairwise correlation between latent activations is 1.0, and will be greater than the correlation between raw neural activations. **Representational similarity analysis:** Rather than directly correlating neural (or latent) activation, RSA first computes pairwise (dis)similarity matrices of neural responses to features. Depicted are representational similarity matrices (or their dissimilarity counterparts), which are correlated to produce an alignment score. As with linear regression, the RSA score for perfectly recovered latents is 1.0, and greater than the RSA score over neural activations.

two networks could learn the *exact same* set of underlying features, yet appear dissimilar under linear metrics like RSA and Linear Regression if they mix those features differently across neurons. While different feature arrangements may reflect genuine differences in how networks organize – and therefore act on – information, this phenomenon creates an unfair comparison problem: higher-dimensional models achieve higher alignment scores simply because they can represent features with less superposition (i.e., closer to one feature per neuron), making them inherently more linearly decodable (Elmoznino & Bonner, 2024). This dimensional advantage occurs even when comparing to lower-dimensional models with greater behavioral similarity to a target network.

We propose *feature-based alignment* to address these confounds and explore more performance-relevant sources of representational (mis)alignment. The key insight is that if superposition causes networks with identical features to appear misaligned, then *disentangling* those features should reveal their true similarity. Our approach has two steps: (1) extract disentangled features from each network’s activations, and (2) compare networks using standard alignment metrics (RSA, Linear Regression) applied to these disentangled feature representations rather than raw neural activations. We fix the dimensionality of the disentangled space to be identical across all models, alleviating the dimensional advantage that confounds standard comparisons. For deep neural networks, we disentangle features using sparse autoencoders (SAEs) (Ng et al., 2011; Cunningham et al., 2023; Rao et al., 2024; Lan et al., 2024), a form of sparse dictionary learning (Olshausen & Field, 1997) that learns an overcomplete basis for neural activations. SAEs aim to represent each input as a sparse combination of interpretable features (Bricken et al., 2023), effectively reversing the feature mixing that occurs in superposition. For biological neural data (fMRI), where meaningful sparse features are more difficult to extract, we use K-means clustering on the mixed-selective neural responses instead.

In this work, we develop an analytic theory that quantifies how feature mixtures in superposition lead to misalignment under RSA and Linear Regression, and validate it across settings of increasing complexity. Applying feature-based alignment to real neural networks, we find that disentanglement often increases alignment between systems, but also observe cases where relative alignment between networks changes—with some networks becoming less similar in the latent space. Through simulations and analysis of feature representations, we identify that alignment increases with shared feature arrangements and feature weights. This is consistent with recent work showing elevated alignment with increased overlap in training data (which influences feature arrangements) and shared training

108 objectives (which influence feature weights and inductive biases) Li et al. (2025). Together, our re-  
 109 sults demonstrate that feature-based alignment facilitates fair comparisons and allows us to more  
 110 directly observe the factors (i.e., feature arrangements and biases) that truly differentiate neural sys-  
 111 tems.

112

## 113 2 THEORY

114

115 Let  $z \in \mathbb{R}^n$  be *latent variables* and  $y \in \mathbb{R}^m$  be neural *representations*, which are functions of these  
 116 latent variables, i.e.,  $y = f(z)$ .

117

118 **Definition 2.1 (Superposition).** *We say that a representation  $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$  is in superposition if it*  
 119 *is a linear map and a low-dimensional projection, i.e.,  $m < n$ .*

120

### 121 2.1 ASSUMPTIONS

122 Throughout our analysis, we make the following assumptions:

123

- 124 **Linearity:** The neural representations are in superposition and are thus linear, described  
 125 by a matrix  $A \in \mathbb{R}^{m \times n}$ :

126

$$y = Az \quad (1)$$

127

128 The condition  $m < n$  implies that the columns of  $A$  are not all orthogonal, aligning with  
 129 the common assumption of having fewer neurons than latent variables.

130

- 131 **Sparsity of Latent Variables:** The latent variables are sparse, e.g.,  $\|z\|_0 \leq K$  for some  
 132  $K \ll n$ .

133

- 134 **Restricted Isometry Property (RIP):** The matrix  $A$  satisfies the RIP, which allows for the  
 135 theoretical possibility of recovering  $z$  from observations of  $y$  via compressed sensing.

136

- 137 **Distribution of Latent Variables:** For a dataset of  $d$  inputs, the latent vectors  $z_1, \dots, z_d$   
 138 are treated as independent and identically distributed (i.i.d.) random variables satisfying:

139

- 140 • Zero mean:  $\mathbb{E}[z_i] = \mathbf{0}$  for all  $i$ .
- 141 • White distribution (Identity covariance):  $\mathbb{E}[z_i z_i^\top] = I_n$  for all  $i$ .

142

143 If these assumptions do not fully hold, we incur an irreducible reconstruction error when retrieving  
 144 the sparse codes. This error would lower the ceiling of RSA alignment, correctly reflecting that if  
 145 two features cannot be separated in one system, it should count as a representational misalignment.

146

### 147 2.2 REPRESENTATIONAL SIMILARITY MATRIX (RSM)

148

149 For a dataset of neural responses  $Y = (y_1, \dots, y_d)$ , the *representational similarity matrix* (RSM) is  
 150 defined as:

151

$$M(Y)_{i,j} = \langle y_i, y_j \rangle \quad \forall i, j \in \{1, \dots, d\}. \quad (2)$$

152

153 Given the linearity assumption equation 1, we can rewrite the RSM in terms of the latent variables:

154

$$M(Y)_{i,j} = \langle y_i, y_j \rangle = \langle Az_i, Az_j \rangle = z_i^\top A^\top A z_j \quad (3)$$

155

156 This shows that the similarity between latent variables  $z_i, z_j$  is measured by a semi-inner product  
 157  $\langle \cdot, \cdot \rangle_G$  induced by the positive semi-definite Gram matrix  $G := A^\top A$ .

158

## 159 3 ALIGNMENT UNDER SUPERPOSITION

160

161 Consider two neural representations in superposition, with matrices  $A_a, A_b$ , generating responses  
 162  $Y_a = (A_a z_1, \dots, A_a z_d)$  and  $Y_b = (A_b z_1, \dots, A_b z_d)$  to the same set of latent variables  $Z =$   
 163  $(z_1, \dots, z_d)$ . While the underlying latent variables are identical, the observed neural representations  
 164  $Y_a$  and  $Y_b$  may differ. We now analyze how standard alignment metrics behave in this scenario.

165

166 The key insight of our work is that while these two neural representations  $Y_a, Y_b$  originate from the  
 167 same latent variables, any direct linear measure of alignment will be confounded by the differing  
 168 projection matrices.

162 3.1 REPRESENTATIONAL SIMILARITY ANALYSIS (RSA)  
163164 The RSA metric is the Pearson correlation between the vectorized upper-triangular elements of two  
165 RSMs,  $\vec{m}_a$  and  $\vec{m}_b$ .

166 
$$\rho(Y_a, Y_b) = \frac{\text{Cov}(\vec{m}_a, \vec{m}_b)}{\sqrt{\text{Var}(\vec{m}_a)\text{Var}(\vec{m}_b)}} \quad (4)$$
  
167

168 Under the assumptions outlined previously, we arrive at the following result in the limit of large  
169 datasets.170 **Theorem 3.1** (Asymptotic RSA Alignment). *The RSA correlation between two representations  $Y_a$   
171 and  $Y_b$  in superposition is approximately the cosine similarity between their respective Gram matri-  
172 ces,  $G_a = A_a^\top A_a$  and  $G_b = A_b^\top A_b$ .*  
173

174 
$$\rho(Y_a, Y_b) \approx \frac{\text{Tr}(G_a G_b)}{\sqrt{\text{Tr}(G_a^2)\text{Tr}(G_b^2)}} = \frac{\langle G_a, G_b \rangle_F}{\|G_a\|_F \|G_b\|_F} \quad (5)$$
  
175  
176

177 where  $\langle \cdot, \cdot \rangle_F$  and  $\| \cdot \|_F$  are the Frobenius inner product and norm, respectively.  
178179 This result shows that RSA is fundamentally sensitive to the similarity of the metric tensors induced  
180 by the representations on the latent space.181 3.2 LINEAR REGRESSION  
182183 Alternatively, we can measure alignment by determining how well one representation can be linearly  
184 predicted from the other using a multivariate linear model  $Y_b = WY_a + E$ . The Ordinary Least  
185 Squares (OLS) estimator  $\hat{W}$  minimizes the squared Frobenius norm of the residuals,  $\|Y_b - WY_a\|_F^2$ .  
186187 **Theorem 3.2** (Asymptotic Linear Regression). *In the asymptotic limit and under the stated assump-  
188 tions, the OLS estimator  $\hat{W}$  and the resulting model performance are given by:*189 1. **Optimal Weights:** The weight matrix  $\hat{W}$  converges to:  
190

191 
$$\hat{W} \approx A_b A_a^\top (A_a A_a^\top)^{-1} \quad (6)$$
  
192

193 2. **Mean-Squared Error (MSE):**

194 
$$\text{MSE}(Y_b|Y_a) \approx \frac{1}{m_b} \|A_b - \hat{W} A_a\|_F^2 \quad (7)$$
  
195  
196

197 3. **Explained Variance ( $R^2$ ):**

198 
$$R^2 = 1 - \frac{\text{Tr}((A_b - \hat{W} A_a)^\top (A_b - \hat{W} A_a))}{\text{Tr}(A_b^\top A_b)} \quad (8)$$
  
199

200 4. **Pearson Correlation** ( $\rho(\hat{Y}_b, Y_b)_{ij}$ ):  
201

202 
$$\rho(\hat{Y}_b, Y_b)_{ij} = \frac{(\hat{W} A_a A_b^\top)_{ij}}{\sqrt{(\hat{W} A_a A_b^\top)_{ii} (A_b A_b^\top)_{jj}}} \quad (9)$$
  
203  
204

211 4 SUPERPOSITION’S IMPACT ON ALIGNMENT IN REAL NETWORKS  
212213 4.1 EXPERIMENTAL SETUP  
214215 After verifying that idiosyncratic superposition arrangements are sufficient to reduce alignment (Fig  
7), we now test whether superposition disentanglement changes alignment in real neural networks.

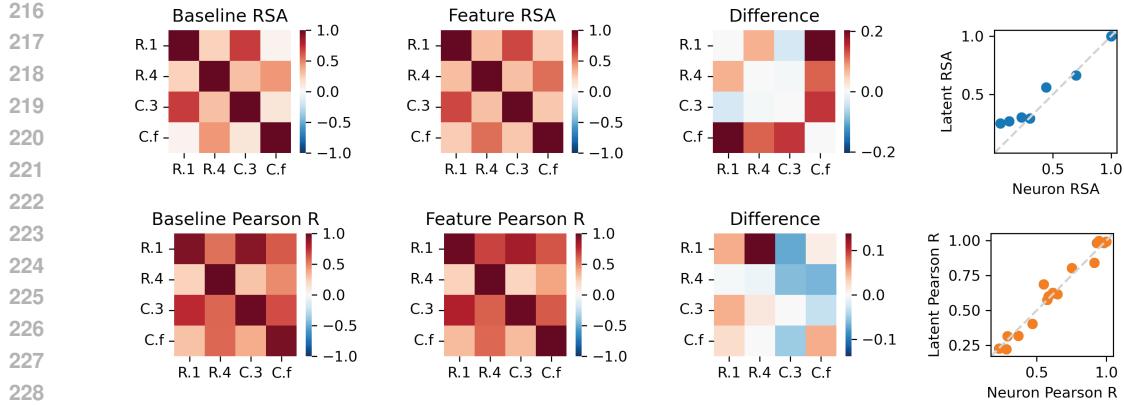


Figure 2: **Model-Model Comparison for SAE latents.** **Top Plots:** Heatmaps: Neuron based RSA (left), latent based RSA (middle), and difference (right). Scatterplot: Neuron versus latent based RSA. **Bottom Plots:** Same as top row, but for Linear Regression. On the scatterplot, blue datapoints indicate the X axis was used as the source for Linear Regression mapping, and orange points indicate the Y axis was used as the source for Linear Regression mapping.

We measure model-model (Fig. 2), model-brain (Fig. 3), and brain-brain (Fig. 4) alignment using RSA and Linear Regression. To begin, we measure alignment on raw neural activations to obtain a baseline. Next, we train SAEs and K-Means on models and brains to recover latent features and use them in place of neurons for computing alignment. For RSA, we replace the neurons of both systems with latents, whereas with Linear Regression, only the source neurons are replaced with latents. This is done to keep the targets the same as in the base comparison (i.e., predicting neurons). It is technically sound because Linear Regression is capable of remixing the source latents back into the target’s superposition arrangement. Finally, we report the difference between alignment over latent activations and alignment over raw neural activations to quantify the relative increase in alignment provided by disentangling features from superposition.

## 4.2 DATA

We obtained neural activations from both biological and artificial neural networks. Biological data is from the publicly available Natural Scenes Dataset (NSD) (Allen et al., 2022), which uses fMRI to record human neural responses to subsets of the COCO natural images dataset (Lin et al., 2014). We use data from six brain areas along the visual processing hierarchy: early to mid-level visual cortex (V1v, V2v, V3v, hV4), the occipital face area (OFA) and the fusiform face area 1 (FFA-1). All activations were preprocessed (the result of Step 5 described in (Allen et al., 2022)) neural responses from NSD Subject 1 in response to 10,000 unique COCO images. Each neural response was averaged over 3 image presentations and z-scored.

Model activations are from the early and penultimate layers of ResNet-50 (layer 1 and layer4.2) (He et al., 2016) and CLIP-ViT-B/32 (layer 3 and feature layers) (Radford et al., 2021). Both models are trained on ImageNet classification (Deng et al., 2009), with activations from the same 10,000 images viewed by Subject 1 of the NSD for consistency.

## 4.3 SAE TRAINING

We train sparse autoencoders with an L1 sparsity penalty (L1-SAEs) to learn disentangled latent features ( $z$ ). The SAE has an encoder and a decoder. Encoding is given by:

$$z = \text{ReLU}(W_{\text{enc}}x + b_{\text{enc}})$$

where  $x$  represents the raw neural activations, and learned parameters  $W_{\text{enc}}$  and  $b_{\text{enc}}$  are the encoder weights and bias respectively. Decoding is given by:

$$\hat{x} = W_{\text{dec}}z + b_{\text{dec}}$$

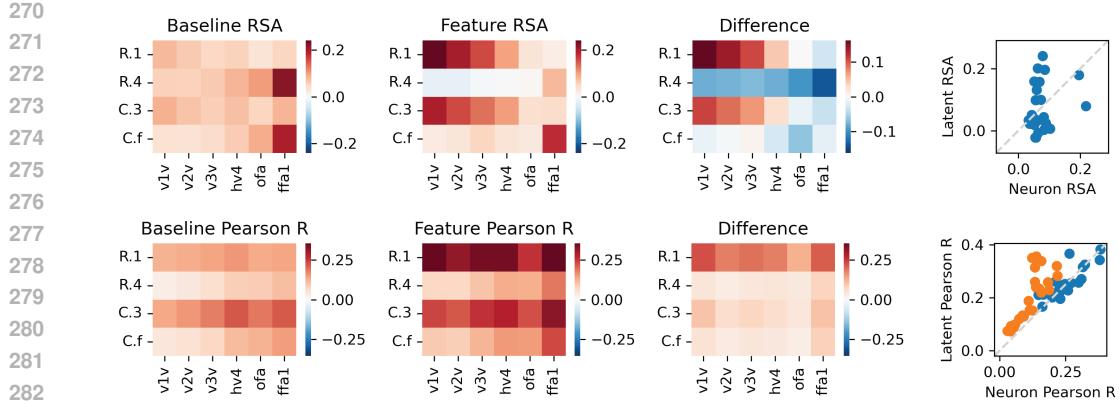


Figure 3: **Model-Brain Comparison for K-Means latents.** **Top Plots:** Heatmaps: Neuron based RSA (left), latent based RSA (middle), and difference (right). Scatterplot: Neuron versus latent based RSA. **Bottom Plots:** Same as top row, but for Linear Regression. On the scatterplot, blue datapoints indicate the X axis was used as the source for Linear Regression mapping, and orange points indicate the Y axis was used as the source for Linear Regression mapping.

where  $\hat{x}$  are reconstructed neural activations, and learned parameters  $W_{\text{dec}}$  and  $b_{\text{dec}}$  are the decoder weights and bias respectively. The model is trained using a combined loss function, which is the sum of a reconstruction loss

$$\mathcal{L}_{\text{reconstruction}} = \frac{1}{d \cdot M} \sum_{i=1}^d (x_i - \hat{x}_i)^2$$

and sparsity loss

$$\mathcal{L}_{\text{sparsity}} = \frac{\lambda}{d \cdot N} \sum_{i=1}^d \sum_{j=1}^N |(W_{\text{dec}})_{:,j}| \cdot |z_i^j|$$

which is the L1 norm of latent activations scaled by the decoder norm (to avoid collapse with vanishing latents and exploding decoder norms) and weighted by the hyperparameter  $\lambda$ . We varied  $\lambda$  from  $10^{-3}$  to 20 and set the number of latent dimensions to 2048 for all neural networks.

We train SAEs on activations of all models and brains to the the 10,000 Natural Scenes Dataset (NSD) images shown to Subject 1 in the Allen et al. (2022) study. A total of 100 SAEs are trained on each set of neural responses. We choose the best SAE using an unsupervised metric described in section 4.5

#### 4.4 K-MEANS LATENT TRANSFORMATION

We perform K-means clustering over columns (images) on the original ( $M \times I$ ) neural datasets, where  $M$  is the number of neurons and  $I$  is the number of images. In the resulting feature space of  $N$  clusters, each cluster represents a visual feature (i.e., cat images), each datapoint is an  $(M, 1)$  vector containing all single-neuron responses to one image, and each centroid can be thought of as representing the canonical population response associated with a particular visual feature. We transform each original datapoint  $(M, 1)$  into a population response vector  $(N, 1)$  by computing the negative Euclidean distance between the datapoint and  $N$  cluster centers. This results in a population response dataset  $(N \times I)$ , which represents the distance of each population vector from the canonical response to a given feature. We train 50 randomly initialized K-means seeds per neural network comparison, choosing the best model with an unsupervised metric outlined in section 4.5.

#### 4.5 MODEL SELECTION AND VALIDATION

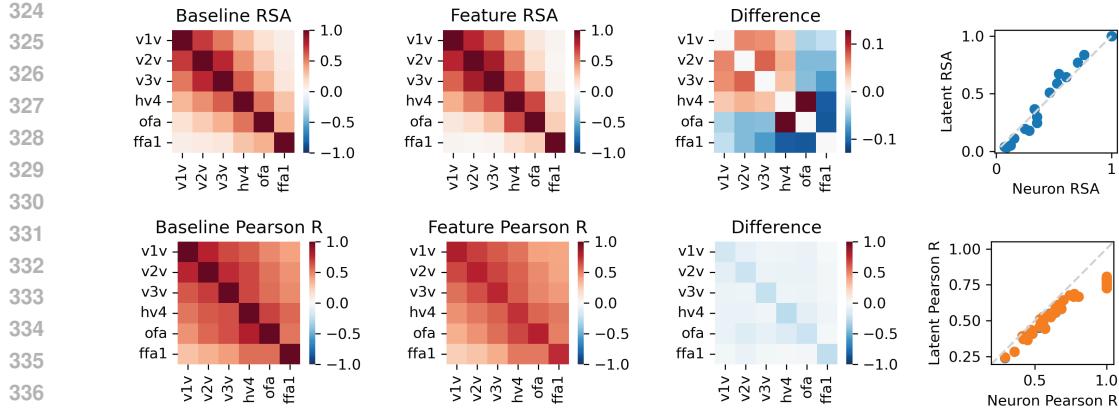


Figure 4: **(Within-Subject) Brain-Brain Comparison for K-Means latents.** **Top Plots:** Heatmaps: Neuron based RSA (left), latent based RSA (middle), and difference (right). Scatterplot: Neuron versus latent based RSA. **Bottom Plots:** Same as top row, but for Linear Regression. On the scatterplot, blue datapoints indicate the X axis was used as the source for Linear Regression mapping, and orange points indicate the Y axis was used as the source for Linear Regression mapping.

For both SAEs and K-Means, we report alignment results using the most disentangled model, identified via a variant of the Unsupervised Disentanglement Ranking (UDR) metric (Higgins et al., 2021). Briefly, we train multiple models (100 for SAEs, 50 for K-Means) and compute an RSA-based similarity matrix across all models. The model with the highest average pairwise similarity to all others receives the highest UDR score and is considered most disentangled, as it represents the most consistent solution across the optimization landscape. Validating this approach, we find that UDR scores correlate with alignment performance: models with higher UDR achieve higher cross-system alignment (Figure 8).

To verify that UDR-selected models produce visually interpretable features consistent with observed alignment changes, we employed an automated interpretability metric derived from human psychophysics. This metric quantifies feature interpretability through an odd-one-out task, analogous to word intrusion tasks used to evaluate topic models Chang et al. (2009), but adapted for the visual modality. We identify the top K preferred images (or maximally exciting images; MEIs) for each neuron or latent and compute their average pairwise similarity to establish a top K image similarity threshold. We then compute the average similarity between each remaining image in the dataset and these top K images. The feature or neuron receives one point for each image whose average similarity falls below the top K threshold, indicating the algorithm correctly identified it as an 'odd one out' or dissimilar to the feature's preferred stimuli. Higher odd-one-out scores indicate more interpretable features with consistent selectivity. We visualize the preferred images of the most interpretable features for a subset of comparisons in the Appendix.

## 4.6 RESULTS

**Model to Model.** Alignment results between models are presented in Figure 2. **RSA:** Both neural and feature space showed the highest similarity between more analogous model layers. Feature-based alignment yielded overall higher scores. Notably, ResNet-50 layer 1 showed a shift in its alignment profile, with the highest alignment increase with the CLIP feature layer, followed by ResNet50-layer 4 and decreased alignment with earlier CLIP layer 3. Figure 9 visualizes the preferred images for neurons versus latents, confirming greater correspondence in preferred features between the CLIP feature layer and ResNet-50 layer 1 in latent space compared to neural space.

**Linear Regression:** As with RSA, early model layers are most related. Unlike RSA, late model layers showed less selective similarity profiles, and feature-based alignment did not produce a pronounced overall increase in alignment scores. Where alignment increased in RSA, it sometimes decreased with Linear Regression (e.g., CLIP feature layer's comparisons to both ResNet50 layer3 and CLIP layer 3), and this was enough to invert similarity profiles in feature space for Linear Re-

378 gression relative to RSA (e.g., for the CLIP feature layer). The opposite was also true: ResNet-50  
 379 layer 1 and CLIP layer 3 become more similar with feature-based Linear Regression, and less similar  
 380 with feature-based RSA. We explore the sources metric disagreement in Section 5.  
 381

382 **Model to Brain.** Alignment results for model-to-brain comparisons are presented in Figure 3.  
 383 **RSA:** In neural space, early model layers roughly aligned more strongly with early visual cortex  
 384 (V1-V3) while later layers aligned with late visual cortex (V4-FFA-1). Feature-based alignment  
 385 strengthened this hierarchical bias for early layers/regions and decreased it for later layers/regions.  
 386 **Linear Regression:** In neural space, early model layers showed broader alignment across visual  
 387 cortex, with a subtle hierarchical alignment observed for later model layers. Feature-based align-  
 388 ment produced different effects than RSA. Early layers, particularly ResNet-50 layer 1, became  
 389 more strongly aligned to all visual cortical regions. Late layers showed modest increases in align-  
 390 ment—contrasting with the decreases observed using RSA. We address potential causes of the dif-  
 391 ferences between Linear Regression and RSA in Section 5.  
 392

393 **Brain to Brain.** Alignment results for brain-to-brain comparisons are presented in Figure 4.  
 394 **RSA:** Both neural and feature space exhibited hierarchically organized alignment, with neighbor-  
 395 ing visual regions showing greater similarity. **Feature-based alignment strengthened this pattern for**  
 396 **early visual areas but weakened it for higher-order regions.** Notably, hV4—a mid-level visual re-  
 397 gion—shifted its alignment profile in feature space: while most similar to V3v in neural space, it  
 398 became most similar to OFA (a face-selective area) in feature space. Figure 10 visualizes the pre-  
 399 **ferred images for neurons versus latents in V3v, hV4, and OFA, demonstrating greater overlap in**  
 400 **preferred features between hV4 and OFA in the latent space compared to the neural space.** This shift  
 401 in relative alignment demonstrates how feature-based methods can reveal functional relationships  
 402 obscured by neural-level comparisons. We hypothesize this shift arises because disentanglement re-  
 403 duces the geometric effects of OFA’s strong bias towards facial features, allowing shared mid-level  
 404 representations to emerge. We explore this mechanism in Section 5. **Linear Regression:** Neural  
 405 space showed weaker hierarchical organization than RSA, though neighboring regions still exhib-  
 406 ited some preferential alignment. In contrast to RSA, feature-based alignment uniformly decreased  
 407 similarity scores across all region pairs, suggesting that Linear Regression is differentially sensitive  
 408 to disentanglement. We elaborate on how bias may also contribute to RSA - Linear Regression  
 409 disagreement in Section 5.  
 410  
 411

## 412 5 INVESTIGATING SOURCES OF REPRESENTATIONAL ALIGNMENT

413  
 414 In the previous section, we observed several intriguing trends in neural alignment. First, early and  
 415 lower-dimensional model layers and brain regions exhibited increased alignment in feature space  
 416 for both RSA and Linear Regression, consistent with our initial hypothesis about superposition ar-  
 417 rangements obscuring their true similarity. Second, higher-order brain regions with similar intrinsic  
 418 dimensionality to lower-level areas often exhibited decreases in alignment. In several of these cases,  
 419 RSA and Linear Regression even disagreed, causing changes in selectivity profiles for regions mea-  
 420 sured with one metric but not the other. These last two findings prompt us to investigate whether  
 421 (un)known inductive biases (e.g., shared face selectivity), particularly of higher-order regions, con-  
 422 tributes to relatively high alignment in the neural space that is reduced in feature space.  
 423

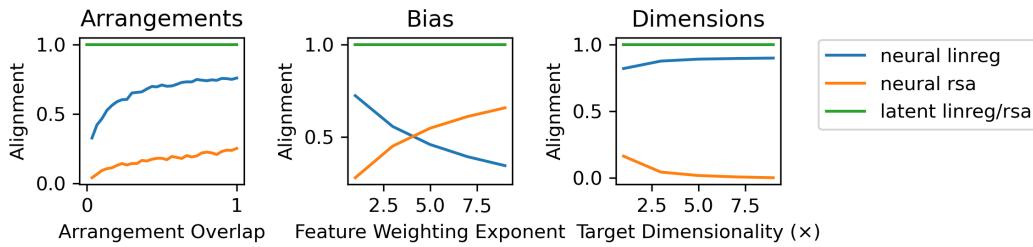
### 424 5.1 EXPERIMENTAL SETUP FOR SIMULATION STUDIES

425 For all simulation studies, we produce two random linear projections from a shared set of features.  
 426 Specifically, we generate a single feature set  $Z$  of  $d \times N$  dimensional features (i.e.  $Z \in \mathbb{R}^{d \times N}$ ),  
 427 which are random uniform values between 0 and 1, i.e.,  $Z_{i,j} \sim \mathcal{U}(0, 1)$ . To simulate the sparsity  
 428 condition, we then zero mask all but the top  $K$  activating latent variables within each generated  
 429 sample (i.e. individual row in  $Z$ ). Next, we generate two projection matrices, each  $N \times M$  di-  
 430 mensional, with elements drawn from a standard normal distribution, i.e.,  $A_0, A_1 \in \mathbb{R}^{N \times M}$  where  
 431  $A_{i,j} \sim \mathcal{N}(0, 1)$ . These matrices are used to produce two random linear projections of a shared set  
 432 of features. We perform Linear Regression and RSA on the resulting simulated neural activations.

432 In Experiment 1, we simulate the impact of shared feature arrangements by progressively constraining  
 433 the projection matrices  $A_0$  and  $A_1$  such that features maintain similar projection patterns across  
 434 systems. This is achieved by generating a random feature correlation matrix and multiplying it  
 435 with an increasing number of columns in  $A_0$  and  $A_1$ . In Experiment 2, we simulate the impact  
 436 of shared biases by multiplying the columns of projection matrices  $A_0$  and  $A_1$  with progressively  
 437 larger weights from a feature importance matrix. This matrix follows an exponential decay function  
 438 that assigns the highest weights to the initial features. In Experiment 3, we simulate the impact of  
 439 dimensionality on one of the networks by increasing its dimensionality through a scalar multiplier.  
 440

## 441 5.2 SIMULATION STUDY RESULTS

442 Experiment 1 reveals that overlapping feature arrangements increase alignment similarly for both  
 443 RSA and Linear Regression, consistent with shared training statistics benefiting both metrics. Ex-  
 444 periment 2 shows a strong dissociation: shared feature bias decreases Linear Regression alignment  
 445 but increases RSA alignment, with RSA yielding higher absolute scores when bias is sufficiently  
 446 strong. This mirrors the metric dissociations we observed in real neural data for multiple compar-  
 447 isons involving FFA-1, a region known to exhibit bias towards faces. Experiment 3 demonstrates  
 448 that the RSA-Linear Regression gap is amplified by high dimensionality, confirming that dimen-  
 449 sional mismatches disproportionately inflate Linear Regression scores.  
 450



460 **Figure 5: Sources of (mis) alignment in neural space** **Left:** Simulation manipulating the degree of  
 461 shared feature arrangement statistics (Experiment 1). **Middle:** Simulation manipulating the strength  
 462 of shared bias (Experiment 2). **Right:** Simulation manipulating the dimensionality of the target  
 463 neural network (Experiment 3).

## 464 465 466 5.3 EXTENSION TO REAL DATA

467 Experiment 2 of the previous section (simulating bias) represents the only condition where RSA  
 468 yields higher alignment than Linear Regression and where the same manipulation produces opposing  
 469 directional effects on the two metrics. As this means RSA-Linear Regression disagreement of this  
 470 nature might be a diagnostic indicator for bias, we focus our analysis on the real data in this section  
 471 on bias. We identified cases where RSA > Linear Regression in the neural space: ResNet-50 layer  
 472 4 to FFA-1 and CLIP feature layer to FFA-1. We sort neural activity for each system according  
 473 to the L-1 norm to identify the top 10 features for each system, and found they overlap in their  
 474 semantic selectivity more than features where RSA  $\leq$  Linear Regression 6. We apply the same  
 475 L1-sorting strategy to the latents of each system, finding a decrease in semantic selectivity over  
 476 the top 10 features that coincides with the decrease in RSA observed in feature-based alignment.  
 477 Visual inspection confirms the nature of this shared bias: Figure 6. All systems in this comparison  
 478 show strong selectivity for faces and human figures—a well-documented inductive bias in both deep  
 479 networks and FFA-1. This concentration of shared semantic selectivity in high-magnitude features  
 480 indicates that high RSA, coupled with RSA-Linear Regression dissociation, may be diagnostic of  
 481 shared feature-level biases.  
 482

## 483 6 LIMITATIONS

484 There are several limitations in our study. The first is our assumptions that 1) projections from the  
 485 latent to neural basis are random and 2) that all features are shared. These assumptions are purely

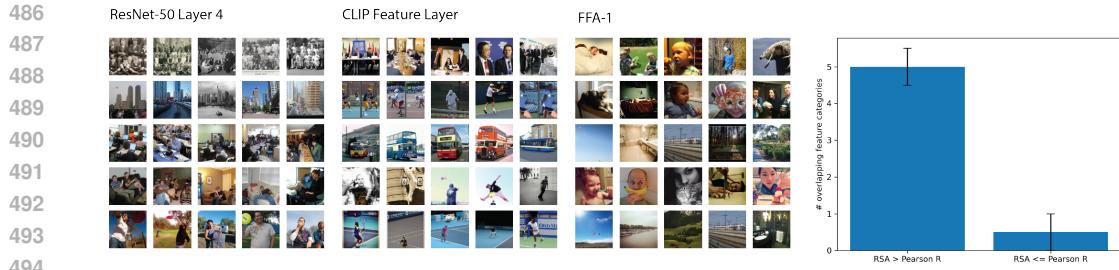


Figure 6: **Preferred features of neural networks with high baseline RSA.** **Images:** Top 5 Maximally Exciting Images (MEIs) for the top 5 features from ResNet-50 Layer 4 (Left), the CLIP feature layer (Middle) and FFA-1 (Right). **Barplot:** Degree of categorical overlap for the top 10 MEIs for high baseline RSA vs low baseline RSA comparisons.

practical; allowing us to test whether disentangling superimposed features is sufficient to increase true alignment in cases where feature arrangements obscure it. At certain scales and in certain areas, biological neural networks have a bias towards privileged, rather than random, projections (Khosla et al., 2024; Posani et al., 2025). The impact of this on alignment is likely complex and worth further exploration. It is also unlikely that all of the real networks in our study represent the exact same feature set. The second limitation stems from our use of SAEs, known to suffer various problems such as an amortization gap O’Neill et al. (2024), inconsistent latents across training seeds (Paulo & Belrose, 2025) and the sensitivity of discovered latents to dictionary dimensionality (Leask et al., 2025; Chanin et al., 2024). Further work could explore recent efforts to alleviate such problems (Fel et al., 2025), but we stress that our theory does not depend on SAEs. We pragmatically adopt SAEs as the current best method to disentangle features in superposition, and our experiments should be revisited if improved approaches are designed. The final limitation concerns scope: we only test linearly combined features. This is grounded in the superposition hypothesis (Elhage et al., 2022) and the success of linear and SAE-based probing in large models, which demonstrate that many features are linearly combined and linearly recoverable. However, the success of nonlinear metrics Huh et al. (2024); Insulla et al. (2025); Kornblith et al. (2019); Williams et al. (2021) suggests that follow-up studies may uncover additional sources of alignment obscured in neural space.

## 7 DISCUSSION

In this work, we derive analytic predictions and contribute simulation experiments demonstrating that representational alignment decreases as a function of distinct superposition arrangements of the same underlying features (i.e., compression via random projections). These experiments suggested that alignment computed over disentangled features would be higher. Based on this prediction, we used SAEs and K-Means to extract approximations of features in real neural networks, showing that alignment over latent activations is often significantly higher for the commonly used metrics of RSA and Linear Regression, particularly for early, lower-dimensional layers. We also observe a restructuring of relative representational similarities between models and across biological and artificial networks. Our findings have implications for model selection criteria. If superposition masks similarity between two systems that represent even identical features, then computing RSA or Linear Regression over raw activations of models with variable dimensionality places smaller models at a systematic disadvantage. This may explain why scaling models often produces more reliable alignment gains than designing models with more apparent alignment to human perception (Schaeffer et al., 2022; 2024). Additionally, identifying the causes of restructured representational similarity in feature space may help explain why two systems are similar in neural space, and whether this stems from a dimensionality confound or a more substantive property of the neural networks (i.e., shared inductive biases). As we seek to understand whether models and brains share representational strategies, it is important to consider the best uses of common alignment metrics. In this work, we demonstrate that performing alignment on raw neural activations imposes a systematic disadvantage for earlier, lower-dimensional models. We offer superposition disentanglement as a practical and effective solution to address this confound currently facing neural network comparisons with otherwise similar behavior.

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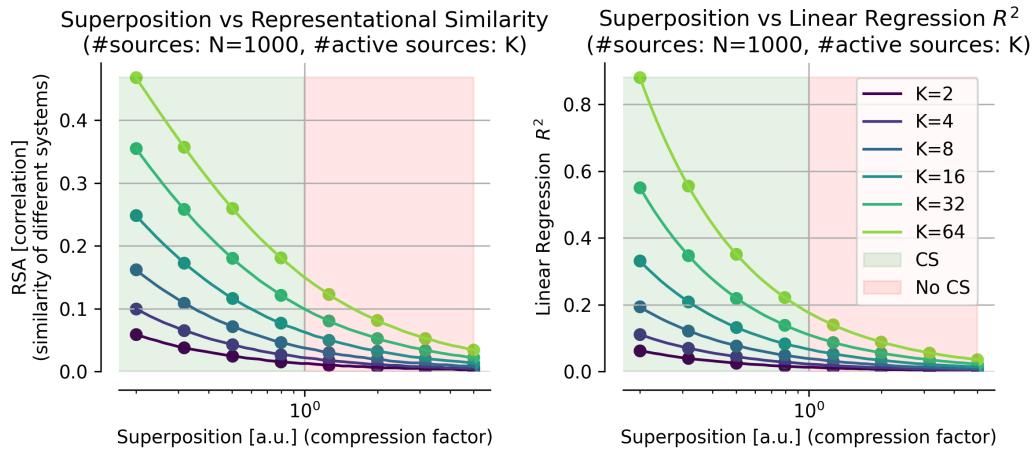
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702 A APPENDIX  
703704 B SIMULATING SUPERPOSITION’S IMPACT ON ALIGNMENT  
705706 B.1 EXPERIMENTAL SETUP  
707

708 In this section, we test our theoretical prediction that superposition is sufficient to reduce alignment  
709 in cases where two networks use an identical set of features. We generate a single feature set  $Z$   
710 of  $d \times N$  dimensional features (i.e.  $Z \in \mathbb{R}^{d \times N}$ ), which are random uniform values between 0  
711 and 1, i.e.,  $Z_{i,j} \sim \mathcal{U}(0, 1)$ . To simulate the sparsity condition, we then zero mask all but the top  $K$   
712 activating latent variables within each generated sample (i.e. individual row in  $Z$ ). Next, we generate  
713 two projection matrices, each  $N \times M$  dimensional, with elements drawn from a standard normal  
714 distribution, i.e.,  $A_0, A_1 \in \mathbb{R}^{N \times M}$  where  $A_{i,j} \sim \mathcal{N}(0, 1)$ . These matrices are used to produce two  
715 random linear projections of a shared set of features. We manipulate the degrees of superposition by  
716 varying  $M$  from  $0.2K \log(N/K)$  to  $50K \log(N/K)$ . Next, we measured alignment of the random  
717 linear projections using RSA (Experiment 1) and Linear Regression (Experiment 2). To test the  
718 effect of sparsity, we repeated these experiments across different numbers of active latents ( $K$ ). We  
719 also calculate and show the minimum dimensionality of  $M$  required for accurate latent recovery  
720 under compressed sensing as  $M = K \log(N/K)$  (Candes et al., 2006).  
721

722 B.2 RESULTS  
723

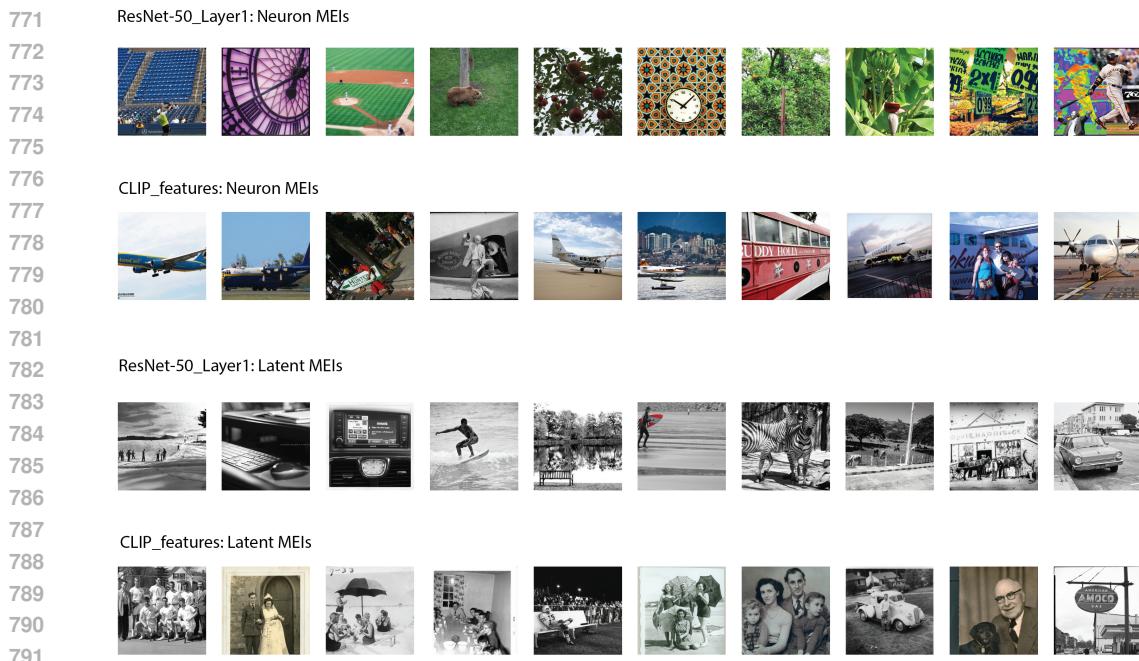
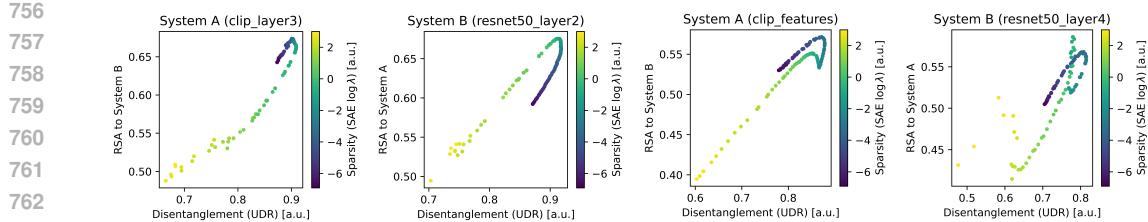
741 **Figure 7: Neural Network Alignment Decreases with Superposition.** Alignment measured with  
742 RSA (**Left**) as well as with Linear Regression (**Right**) as a function of compression ( $N/M$ ). This  
743 experiment is repeated across multiple sparsity levels ( $K$ ). Analytical predictions are represented by  
744 solid curves, while empirical results from simulation across different superposition compressions is  
745 represented by the dots. We note where accurate latent recovery from compressed representations is  
746 (CS; green shading) or is not (No CS; red shading) possible Donoho (2006).  
747

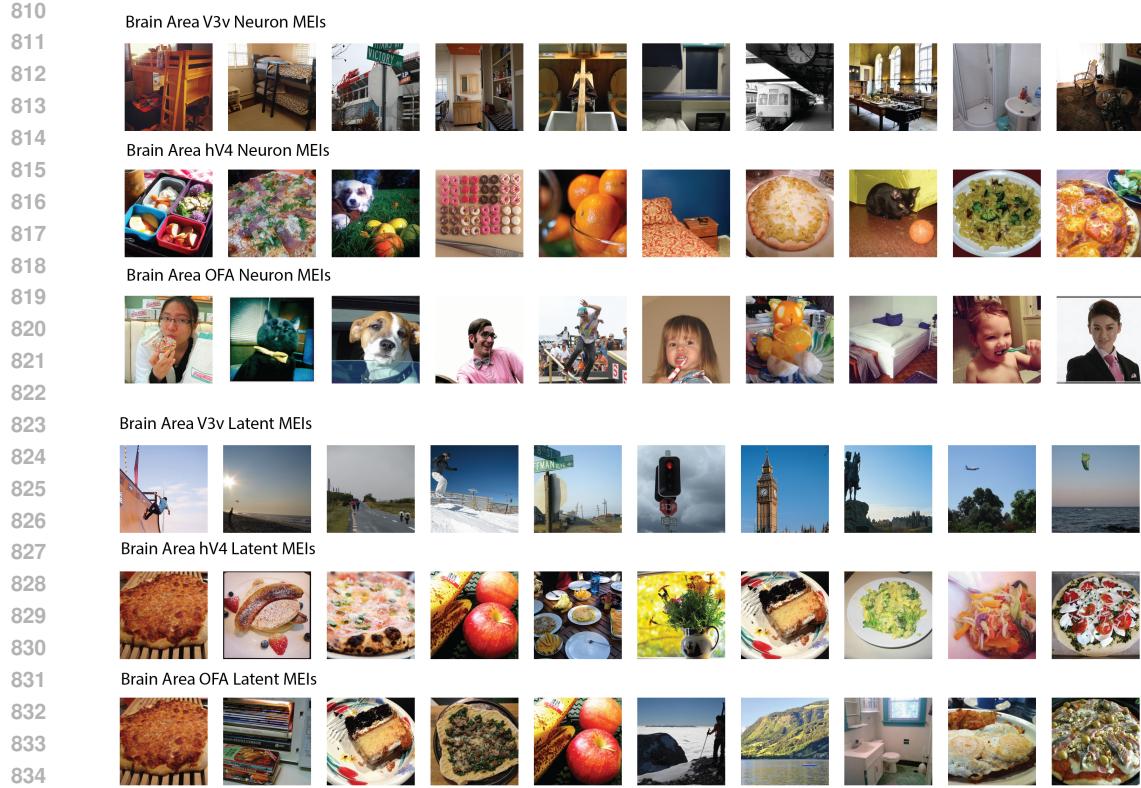
748 B.3 DERIVATION OF ANALYTICAL RSA  
749

750 To derive an analytic expression for the RSA under superposition, we first express the RSMs in  
751 terms of the Gram matrices  $G_a = A_a^\top A_a$  and  $G_b = A_b^\top A_b$ . These matrices act as metric tensors,  
752 defining the geometry of the representations.  
753

$$M(Y_a) = (A_a Z)^\top (A_a Z) = Z^\top G_a Z \quad (10)$$

$$M(Y_b) = (A_b Z)^\top (A_b Z) = Z^\top G_b Z \quad (11)$$





837 **Figure 10: K-means latents MEIs for Brain-Brain Comparisons.** **Top rows:** 10 maximally  
838 exciting images (MEIs) for the most interpretable neuron from brain areas V3v, hV4 and OFA.  
839 **Bottom rows:** 10 maximally exciting images (MEIs) for the most interpretable latent from brain  
840 areas V3v, hV4 and OFA. This supports the switch from higher hV4-V3v similarity in the neural  
841 space to higher hV4-OFA similarity in the latent space observed in Figure 5.

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845  
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847  
848 RSM matrix elements  $\mu_Y^{UT}$ , and show that in the asymptotic limit the two empirical quantities are  
849 equivalent and converge to zero:

850  
851  
852  
853  
854  
855 
$$\mu_Y \equiv \frac{1}{d^2} \sum_{i,j} M(Y)_{ij} = \frac{1}{d^2} \sum_{i,j} z_i^T G z_j \quad (12)$$

856  
857  
858 
$$= \frac{1}{d} \sum_i z_i^T G \left[ \frac{1}{d} \sum_j z_j \right] \quad (13)$$

859  
860  
861 
$$\approx \frac{1}{d} \sum_i z_i^T G \mathbb{E}[z_j] = z_i^T G \mathbf{0} \quad (14)$$

862  
863 
$$= 0 \quad (15)$$

864  $\mu_Y^{UT} \equiv \frac{1}{d(d-1)/2} \sum_{i < j} M(Y)_{ij} = \frac{1}{d(d-1)} \sum_{i \neq j} M(Y)_{ij}$  (16)  
 865  
 866  
 867  
 868  $= \frac{1}{d(d-1)} \left\{ \left[ \sum_{i,j} M(Y)_{ij} \right] - \left[ \sum_i M(Y)_{ii} \right] \right\}$  (17)  
 869  
 870  
 871  $= \frac{d^2}{d(d-1)} \mu_Y - \frac{1}{d-1} \mu_Y^{\text{diag}}$  (18)  
 872  
 873  $\approx \mu_Y$  (19)  
 874  $= 0$  (20)

875  
 876 **Covariance and Variance** Since the mean of the off-diagonal elements is zero, their covariance  
 877 for  $i \neq j$  is the empirical mean of their product: The Covariance of the off-diagonal elements of two  
 878 RSMs can then be shown as:

879  $\text{Cov}(\vec{m}_a, \vec{m}_b) = \text{Cov}(M(Y_a)^{\text{UT}}, M(Y_b)^{\text{UT}})$  (21)  
 880  
 881  $= \frac{1}{d(d-1)/2} \sum_{i < j} \{M(Y_a)_{ij} - \mu_a^{\text{UT}}\} \{M(Y_b)_{ij} - \mu_b^{\text{UT}}\}$  (22)  
 882  
 883  $\approx \frac{1}{d(d-1)/2} \sum_{i < j} M(Y_a)_{ij} M(Y_b)_{ij} = \frac{1}{d(d-1)} \sum_{i \neq j} M(Y_a)_{ij} M(Y_b)_{ij}$  (23)  
 884  
 885  
 886  $= \frac{1}{d(d-1)} \left\{ \left[ \sum_{i,j} M(Y_a)_{ij} M(Y_b)_{ij} \right] - \left[ \sum_i M(Y_a)_{ii} M(Y_b)_{ii} \right] \right\}$  (24)  
 887  
 888  
 889  $\approx \frac{1}{d(d-1)} \sum_{i,j} M(Y_a)_{ij} M(Y_b)_{ij}$  (25)  
 890  
 891  
 892  $= \frac{1}{d(d-1)} \sum_{i,j} (z_i^T G_a z_j) (z_i^T G_b z_j)$  (26)  
 893  
 894  
 895  $= \frac{1}{d(d-1)} \sum_{i,j} (z_i^T G_a z_j) (z_j^T G_b^T z_i)$  (27)  
 896  
 897  
 898  $= \frac{1}{d-1} \sum_i z_i^T G_a \left[ \frac{1}{d} \sum_j z_j z_j^T \right] G_b z_i$  (28)  
 899  
 900  
 901  $\approx \frac{1}{d-1} \sum_i z_i^T G_a \mathbb{E}[z_j z_j^T] G_b z_i$  (29)  
 902  
 903  
 904  $= \frac{1}{d-1} \sum_i z_i^T G_a G_b z_i$  (30)  
 905  
 906  $= \frac{d}{d-1} \text{Tr} \left[ G_a G_b \left( \frac{1}{d} \sum_i z_i z_i^T \right) \right]$  (31)  
 907  
 908  $\approx \text{Tr} [G_a G_b \mathbb{E}[z z^T]]$  (32)  
 909  
 910  $= \text{Tr} [G_a G_b]$  (33)

911 The variance of the elements is found by setting  $G_a = G_b$ , and can be related to the Frobenius norm  
 912 ( $\|X\|_F^2 = \text{Tr}(X^T X)$ ):

913  $\text{Var}(\vec{m}_a) = \text{Var}(M(Y_a)^{\text{UT}}) = \text{Tr}(G_a G_a) = \text{Tr}(G_a^T G_a) = \|G_a\|_F^2$  (34)  
 914  
 915

916  $\text{Var}(\vec{m}_b) = \text{Var}(M(Y_b)^{\text{UT}}) = \text{Tr}(G_b G_b) = \text{Tr}(G_b^T G_b) = \|G_b\|_F^2$  (35)

917 For a large number of data points  $d$ , the correlation of the vectorized RSMs is well-approximated  
 918 by the correlation of their constituent elements. Substituting the covariance and variance into the

918 Pearson formula yields our main result:  
 919

$$\rho(Y_a, Y_b) \approx \frac{\text{Tr}(G_a G_b)}{\sqrt{\|G_a\|_F^2 \|G_b\|_F^2}} = \frac{\langle G_a, G_b \rangle_F}{\|G_a\|_F \|G_b\|_F} \quad (36)$$

#### 923 B.4 DERIVATION OF ANALYTICAL LINEAR REGRESSION RESULTS

925 We consider a multivariate linear regression model to predict the activity of representation  $Y_b$  from  
 926  $Y_a$ :

$$Y_b = WY_a + E \quad (37)$$

928 where  $W \in \mathbb{R}^{m_b \times m_a}$  is the weight matrix and  $E$  is the matrix of residuals. The Ordinary Least  
 929 Squares (OLS) method finds the estimator  $\hat{W}$  that minimizes the sum of squared errors, given by the  
 930 squared Frobenius norm  $\|Y_b - WY_a\|_F^2$ .  
 931

932 **OLS Estimator and Asymptotic Simplification** The standard OLS solution for the weight matrix  
 933 is:

$$\hat{W} = Y_b Y_a^\top (Y_a Y_a^\top)^{-1} \quad (38)$$

935 To find an analytic expression in terms of the underlying superposition matrices, we substitute  $Y_a = A_a Z$  and  $Y_b = A_b Z$ . We then leverage the same statistical properties of the latent variables  $Z$  used  
 936 in the RSA derivation. For a large number of i.i.d. samples  $d$ , the sample covariance of the latent  
 937 variables converges to a scaled identity matrix:  
 938

$$\frac{1}{d} Z Z^\top = \frac{1}{d} \sum_{i=1}^d z_i z_i^\top \rightarrow \mathbb{E}[z z^\top] = I_n \implies Z Z^\top \approx d I_n$$

942 Using this approximation, the terms in the OLS estimator simplify:  
 943

$$Y_b Y_a^\top = (A_b Z)(A_a Z)^\top = A_b (Z Z^\top) A_a^\top \approx d (A_b A_a^\top) \quad (39)$$

$$Y_a Y_a^\top = (A_a Z)(A_a Z)^\top = A_a (Z Z^\top) A_a^\top \approx d (A_a A_a^\top) \quad (40)$$

947 Substituting these into the formula for  $\hat{W}$  gives the ideal "population" level regression coefficient,  
 948 which is free from the sampling noise of a specific  $Z$ :

$$\hat{W} \approx d (A_b A_a^\top) (d (A_a A_a^\top)^{-1})^{-1} = A_b A_a^\top (A_a A_a^\top)^{-1} \quad (41)$$

951 **Derivation of the Mean Squared Error** The Mean Squared Error (MSE) is the total squared  
 952 error divided by the total number of predicted elements,  $m_b d$ . The prediction error matrix is  $E =$   
 953  $Y_b - \hat{W} Y_a$ .  
 954

$$E \approx A_b Z - (A_b A_a^\top (A_a A_a^\top)^{-1}) A_a Z \quad (42)$$

$$= (A_b - A_b A_a^\top (A_a A_a^\top)^{-1} A_a) Z \quad (43)$$

957 The total squared error is the squared Frobenius norm of  $E$ .  
 958

$$\begin{aligned} \|E\|_F^2 &= \text{Tr}(E^\top E) \approx \text{Tr}\left(Z^\top (\dots)^\top (\dots) Z\right) \\ &= \text{Tr}\left((\dots)^\top (\dots) (Z Z^\top)\right) \quad (\text{using cyclic property of trace}) \\ &\approx d \cdot \text{Tr}\left((\dots)^\top (\dots)\right) = d \|A_b - A_b A_a^\top (A_a A_a^\top)^{-1} A_a\|_F^2 \end{aligned} \quad (44)$$

959 Dividing the total squared error by  $m_b d$  yields the final MSE expression:  
 960

$$\text{MSE}(Y_b | Y_a) \approx \frac{1}{m_b} \|A_b - A_b (A_a^\top (A_a A_a^\top)^{-1} A_a)\|_F^2 \quad (45)$$

969 Notation:  
 970

$$\hat{Y}_b = (\hat{y}_{b,(1)}, \dots, \hat{y}_{b,(d)}) \quad (46)$$

```

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974 
$$\mathbb{E}[\hat{Y}_b^i] \equiv \frac{1}{d} \sum_{k=1}^d \hat{y}_{b,(k)}^i = \frac{1}{d} \sum_{k=1}^d \sum_m \hat{W}^{im} y_{a,(k)}^m$$

975
976
977 
$$= \frac{1}{d} \sum_{k=1}^d \sum_{m,n} \hat{W}^{im} A_a^{mn} z_{(k)}^n = \sum_{m,n} \hat{W}^{im} A_a^{mn} \frac{1}{d} \sum_{k=1}^d z_{(k)}^n$$

978
979
980 
$$\approx \sum_{m,n} \hat{W}^{im} A_a^{mn} \mathbb{E}[z^n]$$

981
982 
$$= 0$$

983
984
985 
$$\mathbb{E}[y^i y^j] = \sum_{m,n} A^{im} A^{jn} \mathbb{E}[z^m z^n] = \sum_{m,n} A^{im} A^{jn} \delta_{mn} = \sum_m A^{im} A^{jm} = (AA^\top)_{ij}$$

986
987

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**Derivation of the Explained Variance  $R^2$**  The Explained Variance  $R^2$  is defined by:

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$$R^2 = 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}} \tag{47}$$

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991

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where

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995 
$$SS_{\text{res}} = \sum_{k=1}^d \|y_{b,(k)} - \hat{y}_{b,(k)}\|^2 \tag{48}$$

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997
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1000 
$$SS_{\text{tot}} = \sum_{k=1}^d \|y_{b,(k)} - \bar{y}_b\|^2 \tag{49}$$

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1005 
$$\bar{y}_b = \frac{1}{d} \sum_{k=1}^d y_{b,(k)} \tag{50}$$

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We can derive an analytical expression of  $SS_{\text{res}}$ ,  $SS_{\text{tot}}$ , and  $\bar{y}_b$  in terms of the projection matrices  $A_a$  and  $A_b$ :

$$\bar{y}_b = \frac{1}{d} \sum_{k=1}^d y_{b,(k)} = A_b \frac{1}{d} \sum_{k=1}^d z_k \approx A_b \mathbb{E}[z] \tag{51}$$

$$= 0 \tag{52}$$

$$SS_{\text{res}} = \sum_{k=1}^d \|y_{b,(k)} - \hat{y}_{b,(k)}\|^2 = \text{Tr}[(Y_b - \hat{Y}_b)^\top (Y_b - \hat{Y}_b)] = \text{Tr}[Z^\top (A_b - \hat{W} A_a)^\top (A_b - \hat{W} A_a) Z] \tag{53}$$

$$= \text{Tr}[(A_b - \hat{W} A_a)^\top (A_b - \hat{W} A_a) Z Z^\top] \approx d \cdot \text{Tr}[(A_b - \hat{W} A_a)^\top (A_b - \hat{W} A_a)] \tag{54}$$

$$SS_{\text{tot}} = \sum_{k=1}^d \|y_{b,(k)} - \bar{y}_b\|^2 \approx \sum_{k=1}^d \|y_{b,(k)}\|^2 = \text{Tr}[Y_b^\top Y_b] \tag{55}$$

$$= \text{Tr}[Z^\top A_b^\top A_b Z] = \text{Tr}[A_b^\top A_b Z Z^\top] \tag{56}$$

$$\approx d \cdot \text{Tr}[A_b^\top A_b] \tag{57}$$

1026 Thus the analytical expression of  $R^2$  can be expressed as:  
 1027

$$1028 R^2 = 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}} = 1 - \frac{\text{Tr}[(A_b - \hat{W}A_a)^T(A_b - \hat{W}A_a)]}{\text{Tr}[A_b^T A_b]} \quad (58)$$

1029  
 1030

1031 **Derivation of the Pearson Correlation** The prediction is  $\hat{Y}_b = \hat{W}Y_a$   
 1032

1033 The Pearson Correlation matrix between the prediction and the ground truth is given by:  
 1034

$$1035 \rho(\hat{Y}_b, Y_b)_{ij} \equiv \rho(\hat{Y}_b^i, Y_b^j) = \frac{\text{Cov}(\hat{Y}_b^i, Y_b^j)}{\sqrt{\text{Var}(\hat{Y}_b^i) \text{Var}(Y_b^j)}} \quad (59)$$

1036  
 1037

1038 Where indices  $i$  and  $j$  correspond to system dimensions. The Covariances can be expressed as:  
 1039

$$1040 \text{Cov}(\hat{Y}_b^i, Y_b^j) = \frac{1}{d-1} \sum_{k=1}^d \hat{y}_{b,(k)}^i y_{b,(k)}^j = \frac{1}{d-1} \sum_{k=1}^d \sum_m \hat{W}^{im} y_{a,(k)}^m y_{b,(k)}^j$$

1041

$$1042 = \frac{1}{d-1} \sum_{k=1}^d \sum_{m,n,l} \hat{W}^{im} A_a^{mn} z_{(k)}^n A_b^{jl} z_{(k)}^l = \frac{1}{d-1} \sum_{m,n,l} \hat{W}^{im} A_a^{mn} A_b^{jl} \sum_{k=1}^d z_{(k)}^n z_{(k)}^l$$

1043

$$1044 \approx \frac{1}{d-1} \sum_{m,n,l} \hat{W}^{im} A_a^{mn} A_b^{jl} d \cdot \mathbb{E}[z^n z^l] = \frac{d}{d-1} \sum_{m,n,l} \hat{W}^{im} A_a^{mn} A_b^{jl} \delta_{nl}$$

1045

$$1046 \approx \sum_{m,n} \hat{W}^{im} A_a^{mn} A_b^{jn} = (\hat{W} A_a A_b^T)_{ij} = (A_b A_a^T (A_a A_a^T)^{-1} A_a A_b^T)_{ij}$$

1047

$$1048$$

1049

1050

1051 And the Variances:  
 1052

$$1053 \text{Var}(\hat{Y}_b^i) = \frac{1}{d-1} \sum_{k=1}^d \hat{y}_{b,(k)}^i \hat{y}_{b,(k)}^i = \frac{1}{d-1} \sum_{k=1}^d \sum_{m,n} \hat{W}^{im} y_{a,(k)}^m \hat{W}^{in} y_{a,(k)}^n$$

1054

$$1055 = \frac{1}{d-1} \sum_{m,n} \hat{W}^{im} \hat{W}^{in} \sum_{k=1}^d y_{a,(k)}^m y_{a,(k)}^n$$

1056

$$1057 \approx \frac{1}{d-1} \sum_{m,n} \hat{W}^{im} \hat{W}^{in} d \cdot \mathbb{E}[y_a^m y_a^n]$$

1058

$$1059 = \frac{d}{d-1} \sum_{m,n} \hat{W}^{im} \hat{W}^{in} (A_a A_a^T)_{mn}$$

1060

$$1061 \approx (\hat{W} (A_a A_a^T) \hat{W}^T)_{ii}$$

1062

$$1063 = (A_b A_a^T (A_a A_a^T)^{-1} (A_a A_a^T) \hat{W}^T)_{ii}$$

1064

$$1065 = (A_b A_a^T (A_a A_a^T)^{-1} A_a A_b^T)_{ii}$$

1066

1067

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$$1069 \text{Var}(Y_b^j) = \frac{1}{d-1} \sum_{k=1}^d y_{b,(k)}^j y_{b,(k)}^j \approx \frac{d}{d-1} \mathbb{E}[y_b^j y_b^j]$$

1070

$$1071 \approx (A_b A_b^T)_{jj}$$

1072

1073

1074

1075 Expressed in  $A_a$  and  $A_b$ , the Pearson Correlation matrix becomes:  
 1076

$$1077 \rho(\hat{Y}_b, Y_b)_{ij} \approx \frac{(A_b A_a^T (A_a A_a^T)^{-1} A_a A_b^T)_{ij}}{\sqrt{(A_b A_a^T (A_a A_a^T)^{-1} A_a A_b^T)_{ii} (A_b A_b^T)_{jj}}} = \frac{(\hat{W} A_a A_b^T)_{ij}}{\sqrt{(\hat{W} A_a A_b^T)_{ii} (A_b A_b^T)_{jj}}} \quad (60)$$

1078

1079