

Orthogonal Contrastive Learning for Multi-Representation fMRI Analysis

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Learning By Machine



My website

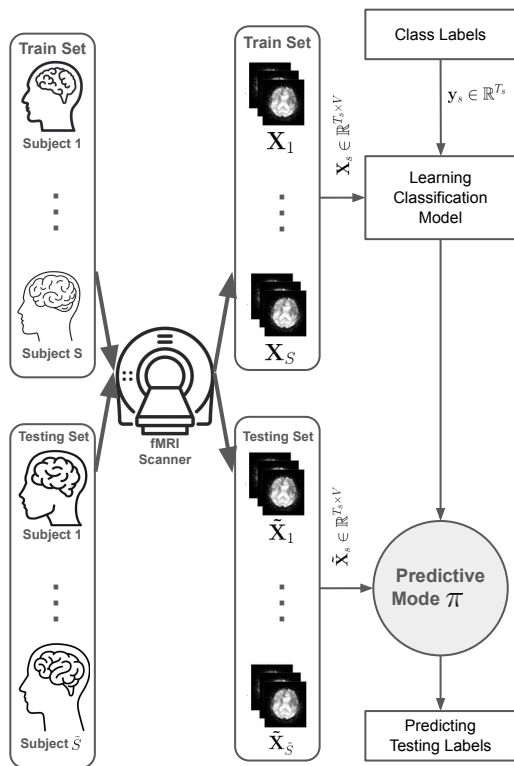


OCL GitHub

NeurIPS 2025

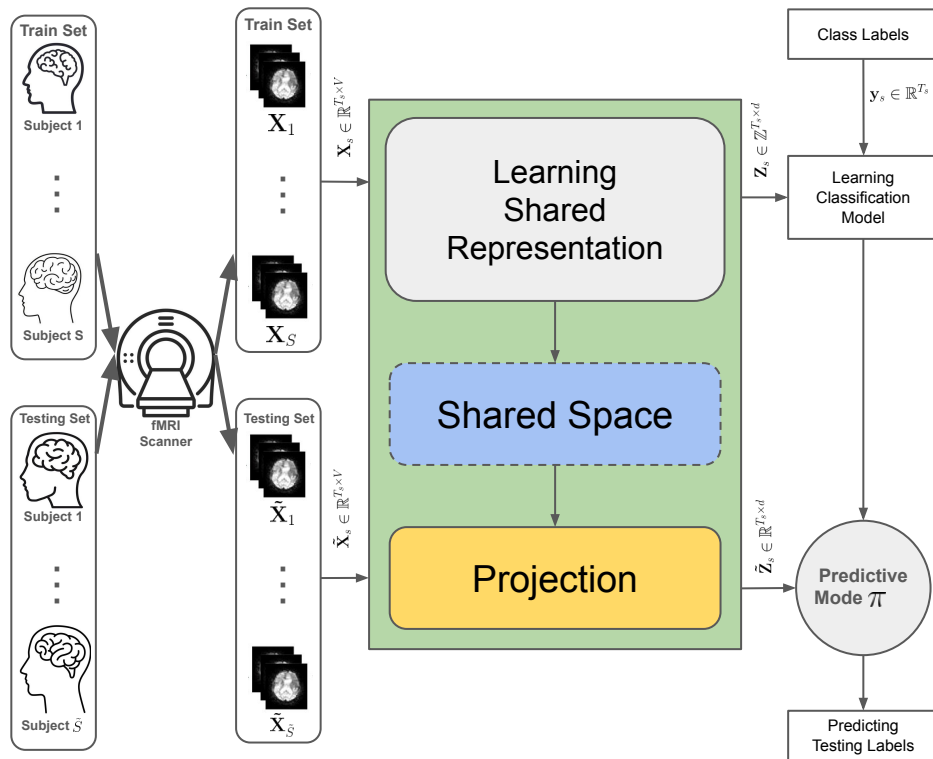


Motivation



- Developing a **neural classification model** from multi-subject task-based fMRI brain activation patterns.
- Given **labeled spatiotemporal fMRI data**, we train a classification model capable of **predicting task conditions for unseen test samples**.
- These tasks may involve *visual or auditory stimuli, movie viewing, or other sensory experiments* **performed by the subject during the fMRI scan**.
- However, multi-subject neural responses must be **functionally aligned** due to variations in individual brain connectomes.
- From a machine learning perspective, **each subject's data represents a distinct transformation of a shared underlying pattern**, which must be accounted for before training a classifier.

Functional Alignment



- Functional alignment first learns a new representation from the training fMRI data, capturing a shared underlying pattern across subjects such that neural responses to the same stimuli are aligned among all individuals.
- We then train the classifier on the newly learned representation rather than on the raw neural responses.
- A commonly used classical approach is **Generalized Canonical Correlation Analysis (GCCA)**, which has been developed in various deterministic and probabilistic forms:

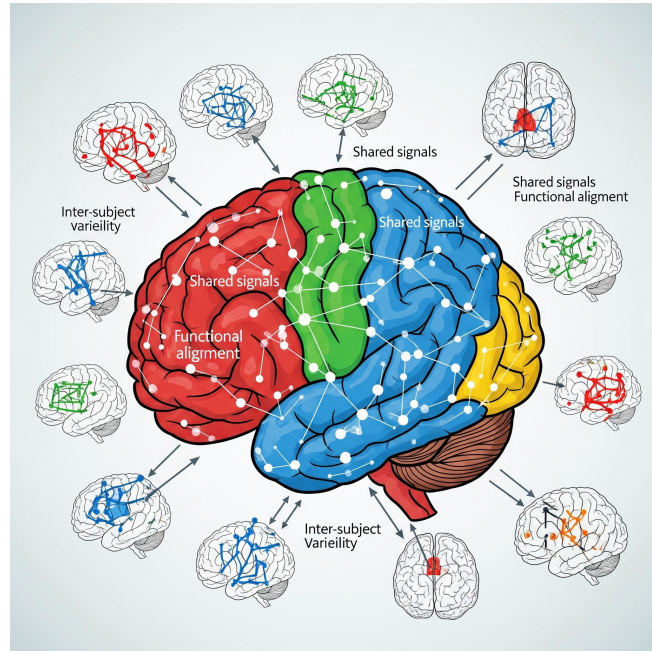
$$\arg \min_{\mathbf{R}_s, \mathbf{G}, \theta} \sum_{s=1}^S \left\| \overset{\text{Neural responses}}{f_{\theta}(\mathbf{X}_s)} \overset{\text{Shared Space}}{\mathbf{R}_s} - \overset{\text{Rotation Matrix}}{\mathbf{G}} \right\|_F^2$$

Subject to $\mathbf{G}^\top \mathbf{G} = \mathbf{I}$

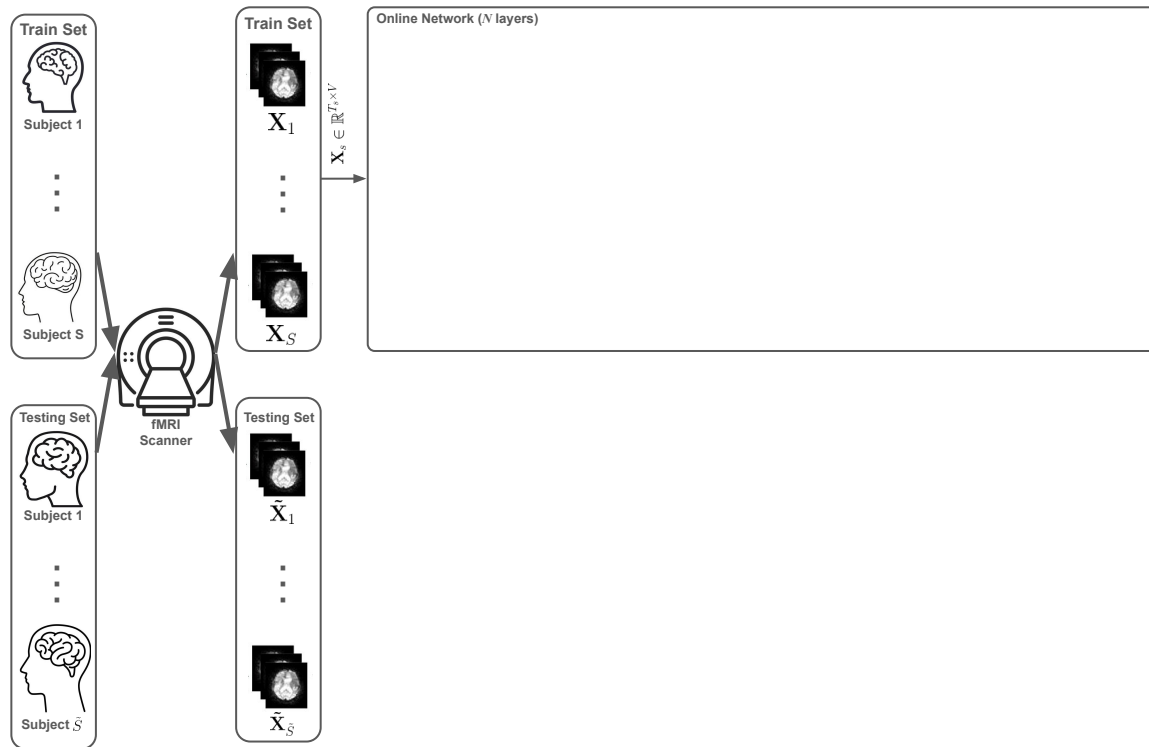
- Function f could be a linear, classic kernel function, or even a **deep neural network**

Key Challenges

- **Inter-subject variability** leads to misaligned neural representations across individuals.
- **High-dimensional, noisy, and limited-sample** fMRI data hinder effective model training and generalization.
- **Temporal misalignment** of BOLD responses remains a major issue—most CCA-based alignment methods struggle with this due to their **static shared-space structure**, which cannot fully capture temporal dynamics across subjects.
- **Cross-site heterogeneity** and scanner differences introduce domain shifts and batch effects. Lack of **domain-adaptive, multi-representation learning** frameworks limits robustness in large-scale, multi-subject fMRI analysis.
- Recent advances in **Transformer architectures** offer a promising **solution** for modeling long-term temporal dependencies and complex spatiotemporal patterns in fMRI analysis.

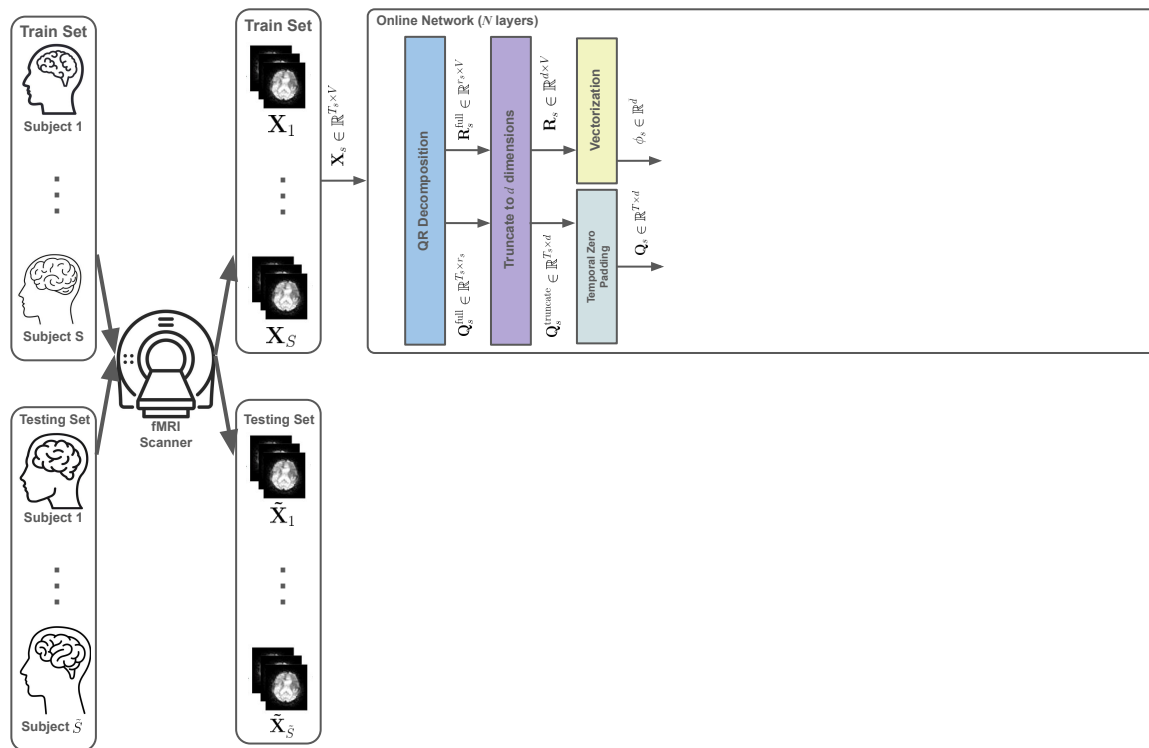


Orthogonal Contrastive Learning



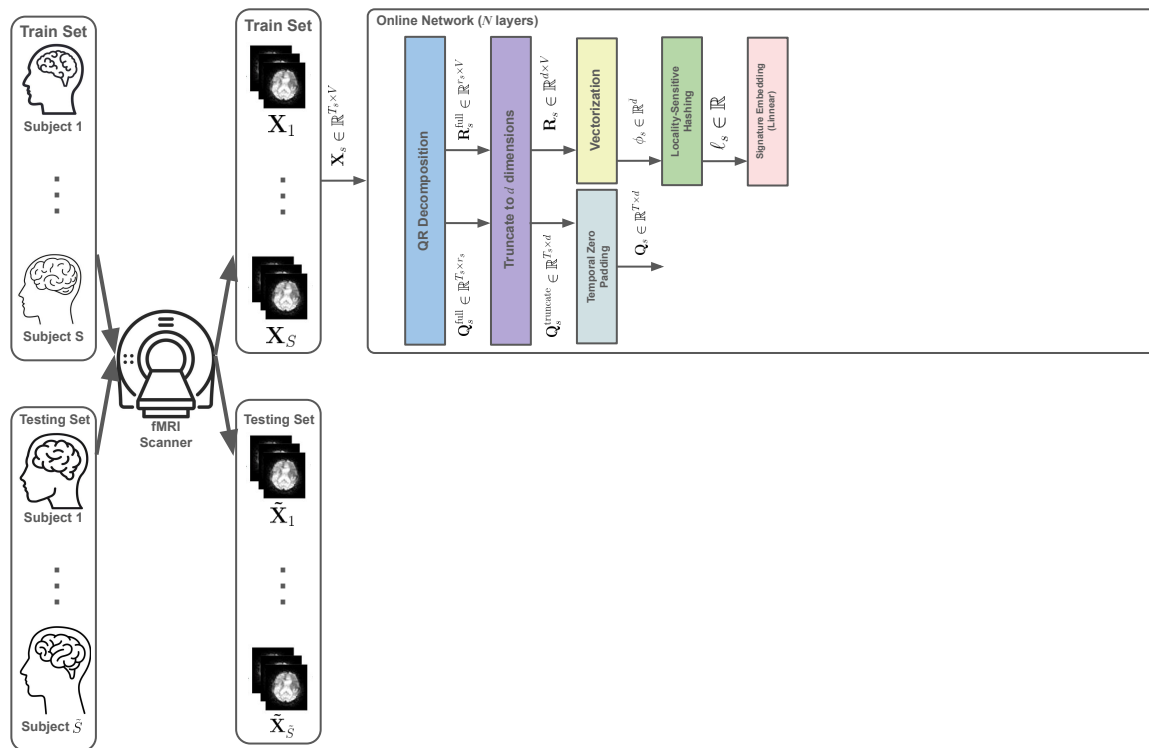
- Each OCL layer has **four primary components**:

Orthogonal Contrastive Learning - QR decomposition



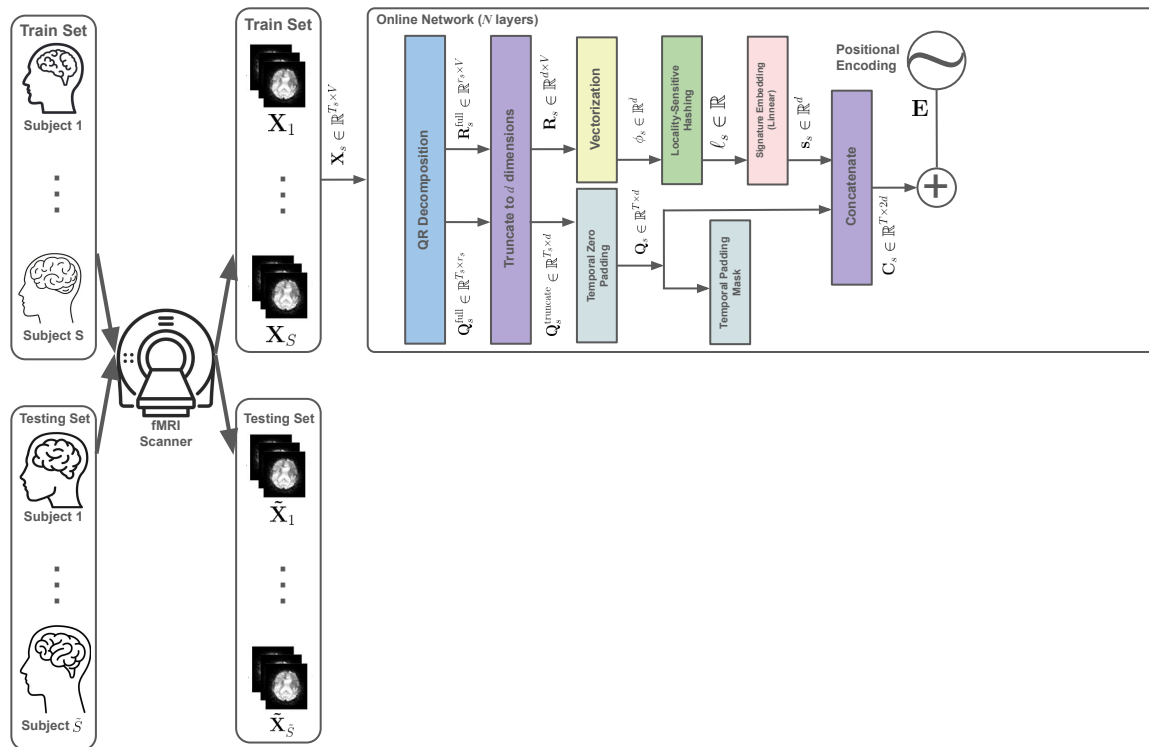
- Each OCL layer has **four primary components**:
- **QR decomposition**, which yields orthonormal feature bases to decorrelate signals and enhance the signal-to-noise ratio

Orthogonal Contrastive Learning - Locality-sensitive hashing



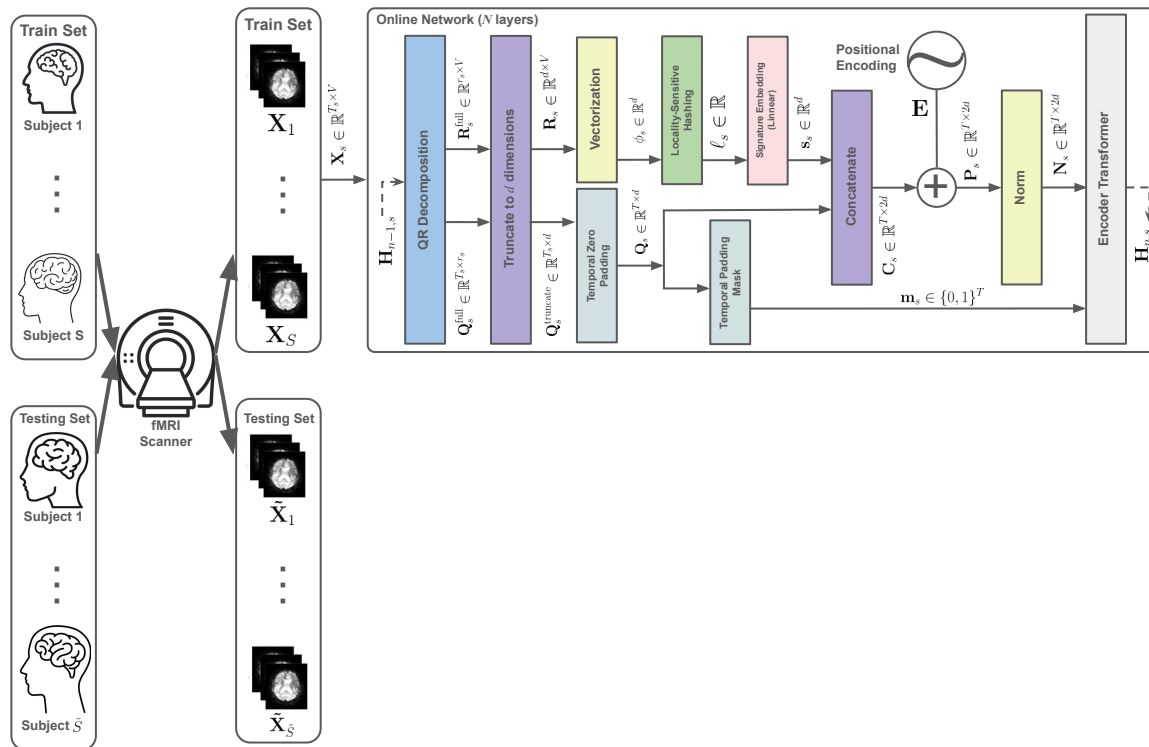
- Each OCL layer has **four primary components**:
- **QR decomposition**, which yields orthonormal feature bases to decorrelate signals and enhance the signal-to-noise ratio
- **Locality-sensitive hashing (LSH)**, which produces compact subject-specific signatures

Orthogonal Contrastive Learning - Positional encoding



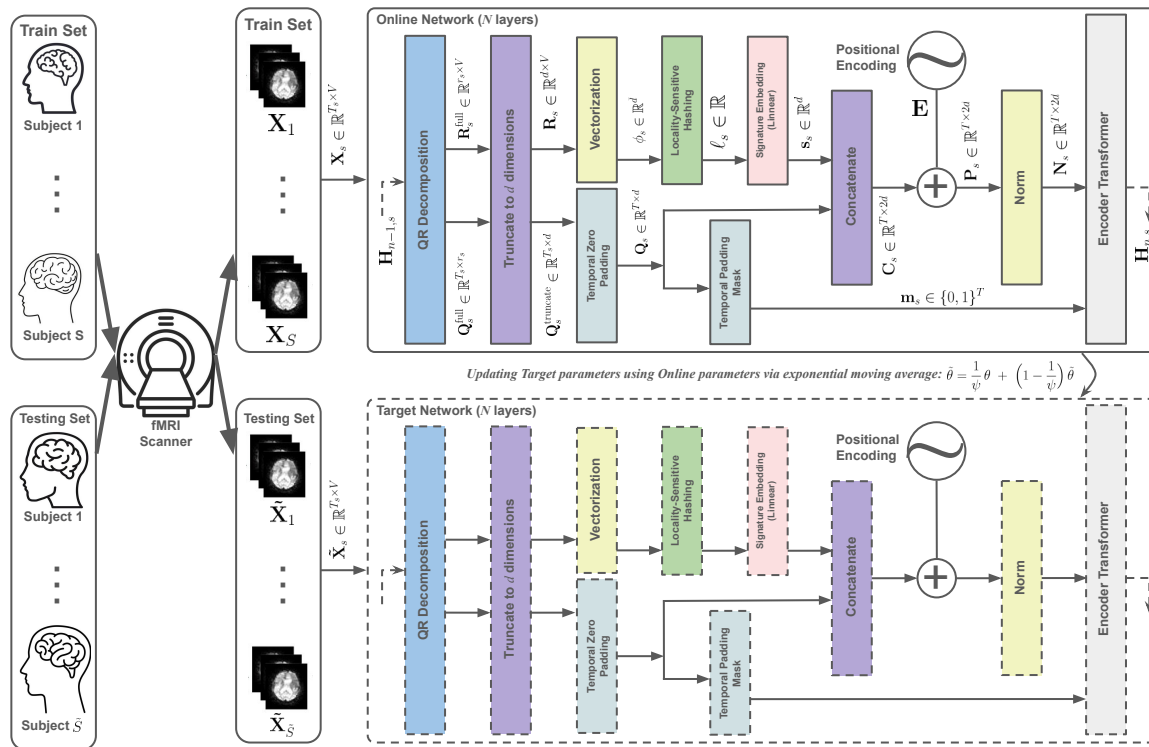
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- **Positional encoding**, which integrates fMRI temporal information into spatial feature representations

Orthogonal Contrastive Learning - Transformer encoder



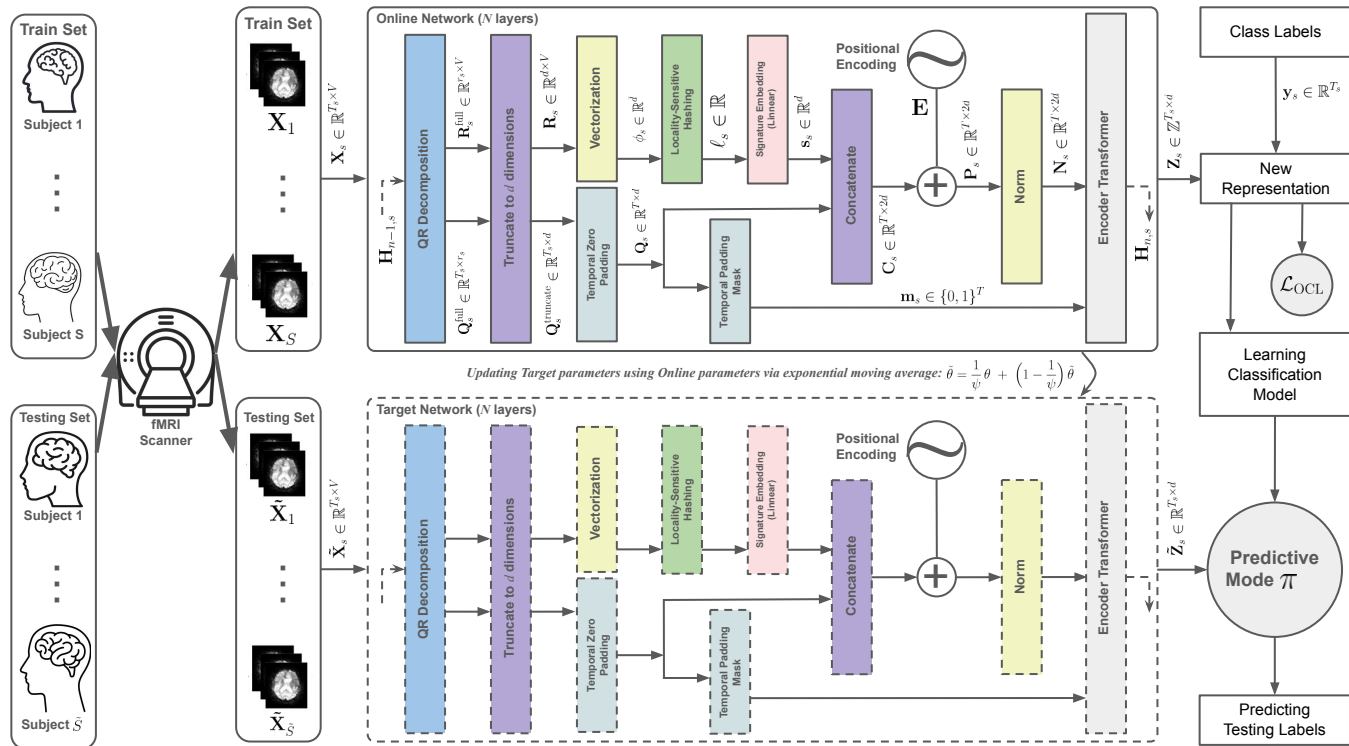
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- QR decomposition**, which yields orthonormal feature bases to decorrelate signals and enhance the signal-to-noise ratio
- Locality-sensitive hashing (LSH)**, which produces compact subject-specific signatures
- Positional encoding**, which integrates fMRI temporal information into spatial feature representations
- A **transformer encoder** integrates these inputs, ensuring that neural representations from the same stimulus become closely aligned, while representations of different stimuli remain distinct

Orthogonal Contrastive Learning - Exponential moving average



- We design a **dual-encoder architecture**:
 - An **online network**, which actively learns representations through a contrastive objective
 - A **target network**, whose parameters are gradually updated as a moving average of the online network's parameters.
- This dual-network setup **stabilizes** training and ensures consistent representations across subjects

Orthogonal Contrastive Learning



- OCL objective function:

$$\mathcal{L}_{\text{OCL}}(\tau, \mu, \lambda)(\mathbf{Z}_s, \mathbf{y}_s) = -\frac{1}{T_s} \sum_{i=1}^{T_s} \log \frac{\sum_{j=1}^{T_s} \exp(\langle z_{s,i}, z_{s,j} \rangle / \tau)}{\sum_{k=1}^{T_s} \exp(\langle z_{s,i}, z_{s,k} \rangle / \tau)}$$

$$+ \lambda \frac{1}{T_s^2} \sum_{i=1}^{T_s} \sum_{\substack{j=1 \\ y_{s,j} \neq y_{s,i}}}^{T_s} \log \left(1 + \exp(\langle z_{s,i}, z_{s,j} \rangle / \tau - \mu) \right).$$

- We learn a contrastive loss that pulls same-stimulus responses together and pushes different-stimulus responses apart

- Trained OCL models can facilitate multi-site fMRI analysis through transfer learning based on orthogonal contrastive embeddings:

$$\tilde{\theta}_{\text{sites}} = \frac{1}{B} \sum_{b=1}^B \tilde{\theta}_b \text{ Single-site parameters}$$

Experimental Setup and Methodology

- We first **pretrained** OCL using **2 million synthetic** fMRI-like data
- We compare OCL with **7 single-site** methods:
 - FastSRM and HyperHMM as baselines
 - ShIndICA as a non-CCA method;
 - DHA and DeepGeoCCA as deep multi-view learning approaches
 - MindEye2 and MindAligner as self-supervised constructive learning approaches.
- We compare OCL with **5 multi-site** techniques
 - SSTL as a baseline
 - DeepSSTL and XG-GNN as deep multi-site learning approaches
 - MindEye2 and MindAligner as self-supervised constructive methods.

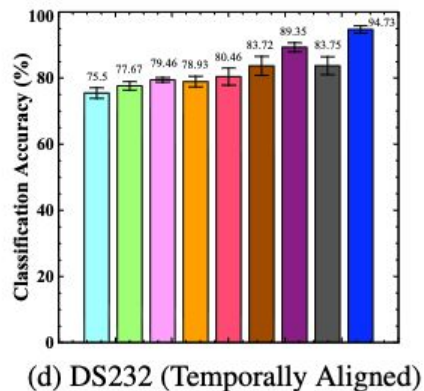
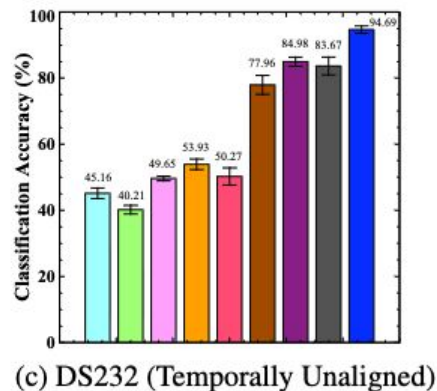
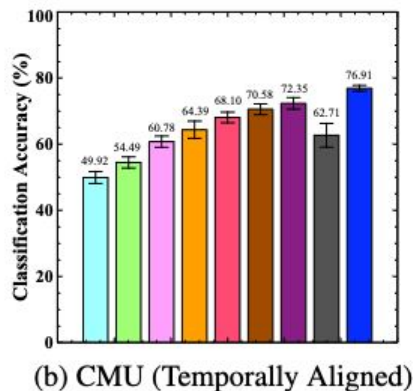
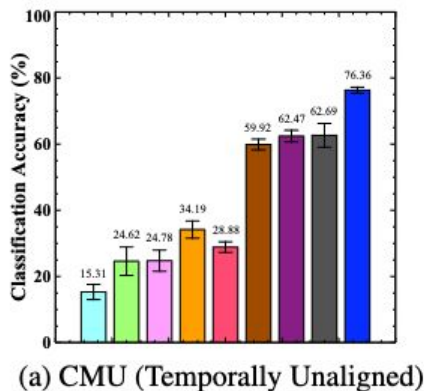
The fMRI datasets

- We used **whole-brain ROI**
- Each scan was registered to the **MNI152 T1-weighted** template
- We used 10 datasets to benchmark OCL performance

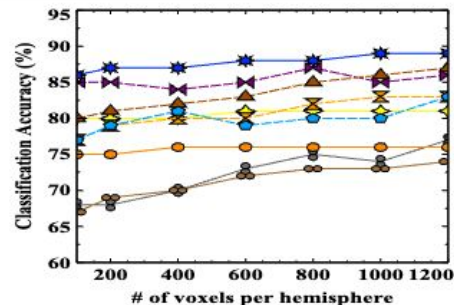
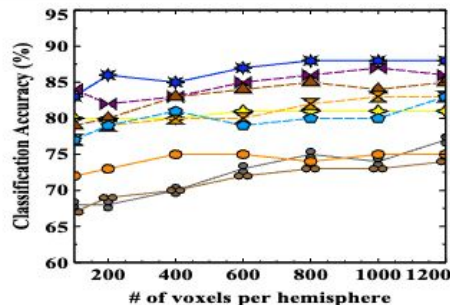
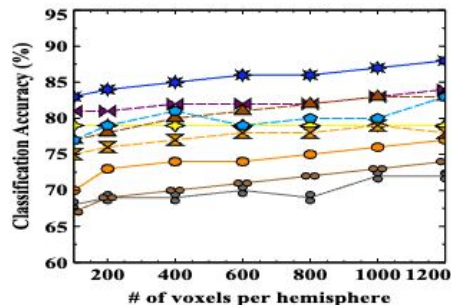
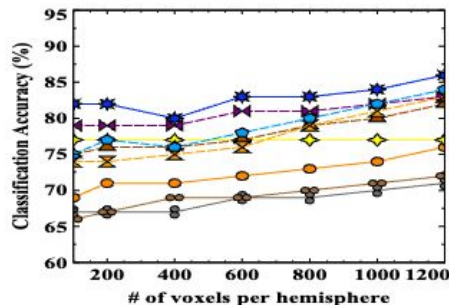
ID	Title	Type	S	$ \mathbf{y} $	T_s	Site(#)
A*	Stop signal (DS007)	Decision	20	4	472	B (3)
B	Conditional stop signal (DS008)	Decision	13	4	317	A (1)
CMU	Meanings of Nouns	Semantic	9	12	402	
C	Simon task (DS101)	Simon	21	2	302	D (1)
D	Flanker task (DS102)	Flanker	26	2	292	C (1)
DS232	Face-coding models with individual-face	Visual	10	4	760	
E	Integration of sweet taste: Study 1 (DS229)	Flavour	15	6	580	F (1)
F	Integration of sweet taste: Study 3 (DS231)	Flavour	9	6	650	E (1)
Forrest	Forrest Gump movie	Visual	20	10	451	
Raiders	Raiders movie	Visual	10	7	924	

S is the number of subjects; $|\mathbf{y}|$ is the number of stimulus categories; T_s is the number of time points per subject; *Site* lists the other datasets whose neural responses can be transferred to this dataset. # represents the number of sites in the corresponding dataset. * this dataset is partitioned into three independent ‘sites’—pseudo-word naming (A1), letter naming (A2), and manual response (A3)

Classification Analysis: Temporally Aligned versus Temporally Unaligned Data



Classification Analysis: Movie stimuli

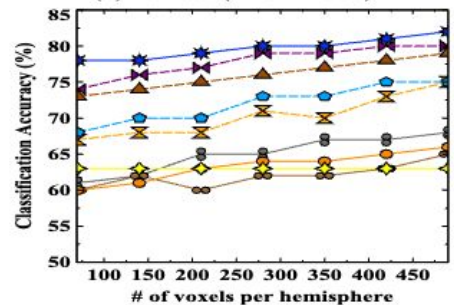
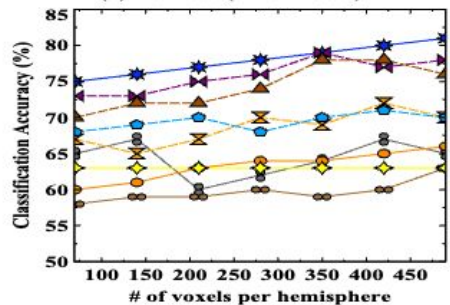
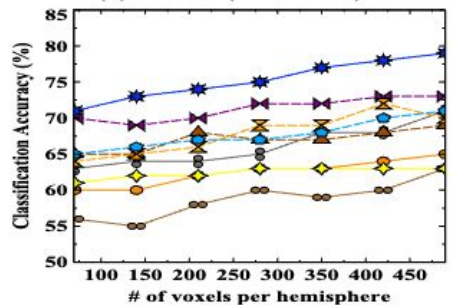
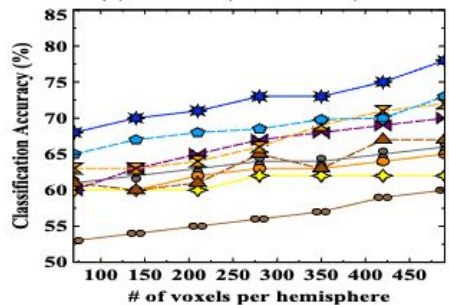


(a) Forrest (TRs = 100)

(b) Forrest (TRs = 400)

(c) Forrest (TRs = 800)

(d) Forrest (TRs = 2000)



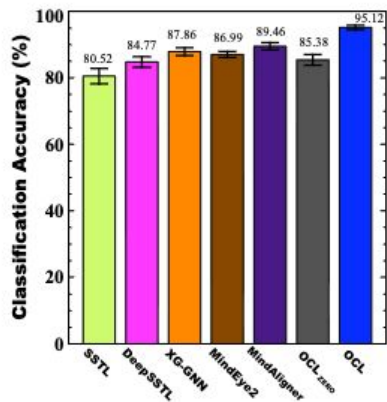
(e) Raiders (TRs = 100)

(f) Raiders (TRs = 400)

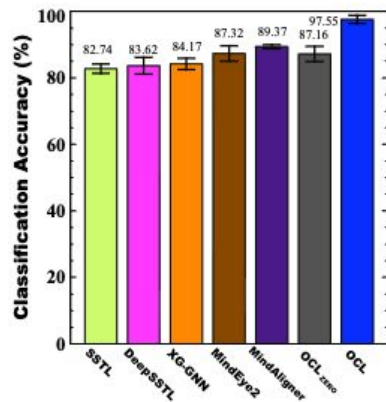
(g) Raiders (TRs = 800)

(h) Raiders (TRs = 2000)

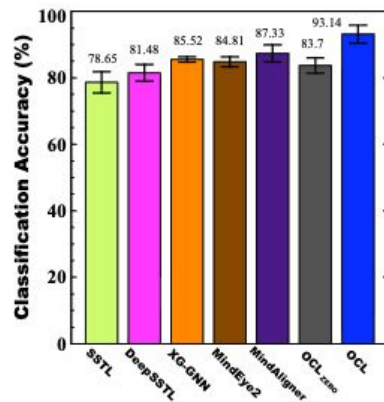
Multi-site Classification Analysis



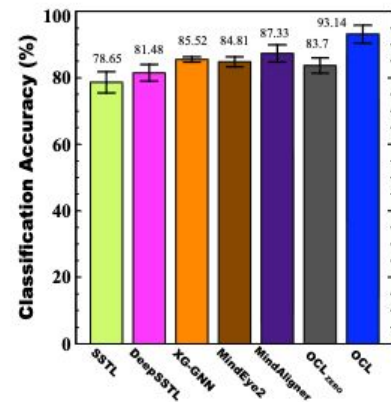
(a) $A \rightleftharpoons B$



(b) $C \rightleftharpoons D$



(c) $E \rightleftharpoons F$



(d) Pairs of {A1, A2, A3, B}

Conclusion

- We introduced **orthogonal contrastive learning (OCL)**, a unified framework that addresses task-based fMRI's key challenges:
 - Low signal-to-noise ratio
 - High dimensionality
 - Variable time-series lengths
- OCL employs a **dual-encoder** design: an **online network** and a **target network** whose weights track the online network via exponential moving average to **stabilize learning**.
- Each OCL network layer combines
 - **QR decomposition** for orthogonal feature extraction
 - **Locality-sensitive hashing (LSH)** to produce compact subject-specific signatures
 - **Positional encoding** to embed temporal structure alongside spatial features
 - A **transformer encoder** to generate discriminative, stimulus-aligned embeddings, trained with a contrastive loss that pulls together same-stimulus responses and pushes apart different-stimulus responses.

Thank You

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