
Shared Space Transfer Learning for analyzing multi-site fMRI data

Supplemental Material

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A Proofs

Lemma 1

We assume $\mathbf{R}^{(d,s)} = \left(\mathbf{X}^{(d,s)}(\mathbf{X}^{(d,s)})^\top + \epsilon \mathbf{I}_{T_d}\right)^{-1} (\mathbf{X}^{(d,s)})^\top \mathbf{G}^{(d,S_d)}$, $s = 1 \dots S_d$ are optimum transformation matrices for d -th site. Then, a regularized version of (1) can be written based on the common space $\mathbf{G}^{(d,S_d)}$ and the projection matrix $\mathbf{P}^{(d,s)}$:

$$\tilde{\mathcal{J}}_C^{(d)}\left([\mathbf{X}^{(d,s)}]_{s=1\dots S_d}\right) = \arg \max_{\mathbf{G}^{(d,S_d)}} \left(\text{tr} \left(\left(\mathbf{G}^{(d,S_d)} \right)^\top \sum_{s=1}^{S_d} \mathbf{P}^{(d,s)} \mathbf{G}^{(d,S_d)} \right) \right).$$

Proof. In this paper, we use the same procedure proposed in [1–3]. We start from (1):

$$\mathcal{J}_C^{(d)}\left([\mathbf{X}^{(d,s)}]_{s=1\dots S_d}\right) = \arg \min_{\mathbf{R}^{(d,s)}, \mathbf{G}^{(d,S_d)}} \sum_{s=1}^{S_d} \left\| \mathbf{G}^{(d,S_d)} - \mathbf{X}^{(d,s)} \mathbf{R}^{(d,s)} \right\|_F^2 \quad (1)$$

By substituting $\mathbf{R}^{(d,s)} = \left(\mathbf{X}^{(d,s)}(\mathbf{X}^{(d,s)})^\top + \epsilon \mathbf{I}_{T_d}\right)^{-1} (\mathbf{X}^{(d,s)})^\top \mathbf{G}^{(d,S_d)}$, we have:

$$\begin{aligned} \mathcal{J}_C^{(d)}\left([\mathbf{X}^{(d,s)}]_{s=1\dots S_d}\right) &\approx \tilde{\mathcal{J}}_C^{(d)}\left([\mathbf{X}^{(d,s)}]_{s=1\dots S_d}\right) \\ &= \arg \min_{\mathbf{G}^{(d,S_d)}} \sum_{s=1}^{S_d} \left\| \mathbf{G}^{(d,S_d)} - \mathbf{X}^{(d,s)} \left(\mathbf{X}^{(d,s)}(\mathbf{X}^{(d,s)})^\top + \epsilon \mathbf{I}_{T_d}\right)^{-1} (\mathbf{X}^{(d,s)})^\top \mathbf{G}^{(d,S_d)} \right\|_F^2 \end{aligned}$$

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Algorithm 1 Shared Space Transfer Learning (SSTL)

Input:

- Training set $[\mathbf{X}^{(d,s)}]_{d=1\dots\tilde{D},s=1\dots S_d}$,
- Training labels $[\mathbf{y}^{(d,s)}]_{d=1\dots\tilde{D},s=1\dots S_d}$,
- Testing set $[\mathbf{X}^{(d,s)}]_{d=1\dots\hat{D},s=1\dots S_d}$,
- Testing labels $[\mathbf{y}^{(d,s)}]_{d=1\dots\hat{D},s=1\dots S_d}$,
- Regularized parameter ϵ ,
- Number of features k .

Output:

- Classification Model Π ,
- Site-specific common features $[\mathbf{G}^{(d,S_d)}]_{d=1\dots\tilde{D}+\hat{D}}$,
- Global shared space transformation \mathbf{W} ,
- and the model evaluation (accuracy, precision, etc.).

Method:
Common Phase — must run for each dataset separately

01. $D = \tilde{D} + \hat{D}$
02. Initialize $\mathbf{G}^{(d,0)} = \{0\}^{T_d \times k}$ and $\tilde{\Sigma}^{(d,0)} = \text{diag}(\{0\}^k)$ for $d = 1 \dots D$.
03. Generate $\mathbf{G}^{(d,S_d)}$ and $\mathbf{R}^{(d,s)}$ for $d = 1 \dots D$ and $s = 1 \dots S_d$ by using (1) to (8).

Training Phase

04. Concatenate $\mathbf{G} = [\mathbf{G}^{(d,S_d)}]_{d=1\dots\tilde{D}}$ based on (9).
05. Calculate the second moment $\mathbf{C} = \frac{1}{T-1} (\mathbf{G} - \mathbf{1}_T \mu^\top)^\top (\mathbf{G} - \mathbf{1}_T \mu^\top)$ based on (12).
06. Calculate \mathbf{W} as eigenvectors of \mathbf{C} .
07. Train a classification model $\Pi([\mathbf{X}^{(d,s)} \mathbf{R}^{(d,s)} \mathbf{W}]_{d=1\dots\tilde{D},s=1\dots S_d}, [\mathbf{y}^{(d,s)}]_{d=1\dots\tilde{D},s=1\dots S_d})$.

Testing Phase

08. Predict based on model $[\hat{\mathbf{p}}^{(d,s)}]_{d=1\dots\hat{D},s=1\dots S_d} = \Pi([\mathbf{X}^{(d,s)} \mathbf{R}^{(d,s)} \mathbf{W}]_{d=1\dots\hat{D},s=1\dots S_d})$.
 09. Evaluate accuracy of the model — *i.e.*, $[\hat{\mathbf{p}}^{(d,s)}]_{d=1\dots\hat{D},s=1\dots S_d}$ vs. $[\mathbf{y}^{(d,s)}]_{d=1\dots\hat{D},s=1\dots S_d}$.
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By considering the definition of the regularized projection matrix $\mathbf{P}^{(d,s)}$, we have:

$$\begin{aligned}
 \arg \min_{\mathbf{G}^{(d,S_d)}} \sum_{s=1}^{S_d} \left\| \mathbf{G}^{(d,S_d)} - \mathbf{P}^{(d,s)} \mathbf{G}^{(d,S_d)} \right\|_F^2 &= \arg \min_{\mathbf{G}^{(d,S_d)}} \sum_{s=1}^{S_d} \left\| (\mathbf{I}_{T_d} - \mathbf{P}^{(d,s)}) \mathbf{G}^{(d,S_d)} \right\|_F^2 \\
 &= \arg \min_{\mathbf{G}^{(d,S_d)}} \sum_{s=1}^{S_d} \text{tr} \left(\left((\mathbf{I}_{T_d} - \mathbf{P}^{(d,s)}) \mathbf{G}^{(d,S_d)} \right)^\top (\mathbf{I}_{T_d} - \mathbf{P}^{(d,s)}) \mathbf{G}^{(d,S_d)} \right) \\
 &= \arg \min_{\mathbf{G}^{(d,S_d)}} \sum_{s=1}^{S_d} \text{tr} \left(\left(\mathbf{G}^{(d,S_d)} \right)^\top (\mathbf{I}_{T_d} - \mathbf{P}^{(d,s)})^\top (\mathbf{I}_{T_d} - \mathbf{P}^{(d,s)}) \mathbf{G}^{(d,S_d)} \right) \\
 &= \arg \min_{\mathbf{G}^{(d,S_d)}} \sum_{s=1}^{S_d} \text{tr} \left(\left(\mathbf{G}^{(d,S_d)} \right)^\top (\mathbf{I}_{T_d} - \mathbf{P}^{(d,s)})^2 \mathbf{G}^{(d,S_d)} \right) \\
 &= \arg \min_{\mathbf{G}^{(d,S_d)}} \sum_{s=1}^{S_d} \text{tr} \left(\left(\mathbf{G}^{(d,S_d)} \right)^\top (\mathbf{I}_{T_d}^2 + (\mathbf{P}^{(d,s)})^2 - 2\mathbf{I}_{T_d} \mathbf{P}^{(d,s)}) \mathbf{G}^{(d,S_d)} \right)
 \end{aligned}$$

Since $\mathbf{P}^{(d,s)}$ is idempotent ($(\mathbf{P}^{(d,s)})^2 = \mathbf{P}^{(d,s)}$) [1–3], we have:

$$\begin{aligned}
 &= \arg \min_{\mathbf{G}^{(d,S_d)}} \sum_{s=1}^{S_d} \text{tr} \left(\left(\mathbf{G}^{(d,S_d)} \right)^\top (\mathbf{I}_{T_d}^2 + \mathbf{P}^{(d,s)} - 2\mathbf{P}^{(d,s)}) \mathbf{G}^{(d,S_d)} \right) \\
 &= \arg \min_{\mathbf{G}^{(d,S_d)}} \sum_{i=s}^{S_d} \text{tr} \left(\left(\mathbf{G}^{(d,S_d)} \right)^\top (\mathbf{I}_{T_d} - \mathbf{P}^{(d,s)}) \mathbf{G}^{(d,S_d)} \right)
 \end{aligned}$$

$$\begin{aligned}
&= \arg \min_{\mathbf{G}^{(d,S_d)}} \left(\text{tr} \left(\left(\mathbf{G}^{(d,S_d)} \right)^\top \left(\sum_{s=1}^{S_d} \mathbf{I}_{T_d} - \mathbf{P}^{(d,s)} \right) \mathbf{G}^{(d,S_d)} \right) \right) \\
&\equiv \arg \max_{\mathbf{G}^{(d,S_d)}} \left(\text{tr} \left(\left(\mathbf{G}^{(d,S_d)} \right)^\top \left(\sum_{s=1}^{S_d} \mathbf{P}^{(d,s)} \right) \mathbf{G}^{(d,S_d)} \right) \right) \quad \blacksquare
\end{aligned}$$

B SSTL Algorithm

Algorithm 1 shows the Shared Space Transfer Learning (SSTL) learning procedure.

C Notations

Table 1 and Table 2 respectively show all variables and functions that are used in our paper.

Table 1: Variables

Variable or Function	Description
\mathbb{R}	The set of real numbers.
\mathbf{I}_k	The identity matrix in size k .
$\mathbf{1}_T$	All-ones vector in size T .
d	Index of the d -th site index.
D	Total of all sites in a multi-site fMRI analysis.
\tilde{D}	Number of training sites in a multi-site fMRI analysis.
\hat{D}	Number of testing sites in a multi-site fMRI analysis.
s	Index of the s -th subject.
S_d	Total of all subjects in the d -th site.
v	Index of the v -th voxel or feature.
V	Total of all voxels in each dataset.
k	Total of all extracted features.
T_d	Total of all time points for the s -th subject in the d -th dataset.
ϵ	A regularization term.
L	Maximum number of iterations (for other TL techniques)
$\tilde{T} = \sum_{d=1}^{\tilde{D}} T_d$	Total of all time points in the training sites.
$\mathbf{X}^{(d,s)} \in \mathbb{R}^{T_d \times V}$	Matrix of neural responses for s -th subject in d -th site.
$\mathbf{y}^{(d,s)} \in \mathbb{R}^{T_d}$	Label vector for s -th subject in d -th site.
$x_{tv}^{(d,s)}$	A neural response scalar for t -th time point, v -th voxel, s -th subject, d -th site.
$\mathbf{R}^{(d,s)} \in \mathbb{R}^{V \times k}$	Site-specific mapping matrix for s -th subject in d -th site.
$\mathbf{G}^{(d,s)} \in \mathbb{R}^{T_d \times k}$	Site-specific common feature for s -th subject in d -th site.
$\mathbf{G}^{(d,S_d)} \in \mathbb{R}^{T_d \times k}$	Final site-specific common feature for d -th site.
$g_{tv}^{(d,S_d)}$	Final site-specific scalar for t -th time point, v -th voxel, d -th site.
$\mathbf{G} \in \mathbb{R}^{\tilde{T} \times k}$	A concatenated version of all common features in the training set.
$\mathbf{g}_t, \bar{\mathbf{g}}_t$	The common feature for t -th time point, v -th voxel, d -th site.
$\mathbf{P}^{(d,s)}$	Projection matrix for s -th subject in d -th site.
$\Phi^{(d,s)}$	A diagonal matrix is used for calculating projection for s -th subject in d -th site.
$\mathbf{H}^{(d,s)}, \mathbf{A}^{(d,s)}, \mathbf{B}^{(d,s)}$	Matrices used for optimization procedure for s -th subject in d -th site.
$\mathbf{U}^{(d,s)}, \tilde{\mathbf{U}}^{(d,s)}$	Left unitary matrices generated respectively by SVD decomposition of $\mathbf{X}^{(d,s)}$ and $\mathbf{A}^{(d,s)}$
$\Sigma^{(d,s)}, \tilde{\Sigma}^{(d,s)}$	Rectangular diagonal matrices generated respectively by SVD decomposition of $\mathbf{X}^{(d,s)}$ and $\mathbf{A}^{(d,s)}$
$\mathbf{V}^{(d,s)}, \tilde{\mathbf{V}}^{(d,s)}$	Right unitary matrices generated respectively by SVD decomposition of $\mathbf{X}^{(d,s)}$ and $\mathbf{A}^{(d,s)}$
$\mathbf{M}^{(d,s)} \mathbf{N}^{(d,s)}$	QR decomposition of $\mathbf{H}^{(d,s)}$; $\mathbf{N}^{(d,s)} \in \mathbb{R}^{T_d \times T_d}$ is an upper triangular matrix.
\mathbf{C}	Zero-mean second moment of the matrix \mathbf{G}
$\mathbf{W} \in \mathbb{R}^{k \times k}$	A linear transformation to a global shared space; Eigenvectors of \mathbf{C}
$\mathbf{Q} \in \mathbb{R}^{\tilde{T} \times k}$	Mapped common features in the global shared space; $\mathbf{Q} = \mathbf{G}\mathbf{W}$
Λ	Eigenvalues of \mathbf{C} .
$\mu \in \mathbb{R}^{k \times 1}$	The mean vector from each row of the matrix \mathbf{G} .

Table 2: Functions

Variable or Function	Description
$\mathcal{J}_C^{(d)}$	The general objective function for extracting site-specific common space for d -th site.
$\tilde{\mathcal{J}}_C^{(d)}$	The regularized function for extracting site-specific common space for d -th site.
\mathcal{J}_G	The general objective function for extracting global shared space.
$\tilde{\mathcal{J}}_G$	The Karhunen–Loeve transformation (KLT) for extracting global shared space.
$\mathcal{N}(0, 1)$	Normalized distribution with zero mean and unit variance.
$diag()$	Diagonal function convert a vector to a diagonal matrix.
$tr()$	Trace function.
$\Omega()$	Regularization function over hyper-parameters.
$\Pi()$	A classification model.
$\ \cdot\ _F$	The Frobenius norm.

Table 3: Accuracy of classification analysis (mean±std). The best result for each task is in **bold**, and the second best is underlined.

Datasets	MNI	MIDA	SIDeR	SRM	MDDL	MDMS	SSTL
A → B	62.51±2.4	65.44±4.21	78.01±2.7	75.64±2.41	78.97±1.89	81.34±1.73	94.65±1.42
B → A	59.17±3.7	70.98±3.69	80.1±3.1	76.99±1.67	82.04±1.21	84.8±2.00	92.40±1.02
A → C	67.31±1.6	77.19±3.46	67.39±4.01	75.27±2.17	84.00±1.04	90.69±1.37	98.18±0.26
C → A	60.47±5.14	69.24±3.76	69.12±3.91	74.86±1.98	83.99±1.47	89.43±1.94	96.42±0.59
B → C	69.18±2.47	79.26±4.1	91.02±1.24	81.45±2.39	90.47±1.27	93.23±1.64	95.72±1.07
C → B	61.82±1.93	72.35±3.47	78.96±2.50	79.99±1.01	83.29±1.37	89.60±1.53	94.18±0.81
H → G	25.11±3.07	71.24±3.81	70.04±2.17	65.33±1.87	69.61±1.14	70.96±1.20	78.35±1.04
G → H	27.38±4.26	63.51±3.07	75.10±2.71	62.34±3.92	70.16±1.72	72.46±1.00	79.14±0.98
(A, B) → C	67.34±2.71	66.59±2.07	88.99±1.91	81.36±2.37	85.94±2.16	90.00±1.46	94.62±1.02
C → (A, B)	52.73±4.51	53.29±3.88	84.38±2.69	79.37±2.31	82.64±2.53	88.16±1.45	91.33±1.10
(A, C) → B	64.94±2.01	62.46±2.94	79.50±2.00	65.12±3.46	69.38±1.91	77.81±1.53	90.03±0.81
B → (A, C)	58.39±3.64	60.08±3.92	69.41±4.61	64.78±4.13	72.84±1.43	70.21±2.10	89.41±2.06
(B, C) → A	59.27±4.00	52.94±2.76	81.23±3.41	82.99±1.27	85.34±2.86	91.81±1.84	94.05±1.04
A → (B, C)	57.37±5.41	53.03±4.11	78.61±4.52	80.79±2.13	82.19±3.24	92.04±2.59	91.84±1.36
A → D	73.33±3.11	67.70±5.10	86.26±1.95	N/A	N/A	N/A	92.09±0.74
D → A	62.45±5.94	53.64±4.01	66.15±3.20	N/A	N/A	N/A	90.84±1.05
B → D	74.61±4.15	61.78±4.72	93.81±2.17	N/A	N/A	N/A	92.17±2.07
D → B	65.07±2.46	68.51±3.17	75.42±3.0	N/A	N/A	N/A	91.04±2.37
C → D	73.91±3.67	74.16±4.60	88.52±2.02	N/A	N/A	N/A	90.41±1.40
D → C	70.57±2.85	75.07±3.88	87.69±2.17	N/A	N/A	N/A	89.39±1.97
E → F	66.07±1.81	69.55±3.70	74.00±3.87	N/A	N/A	N/A	85.39±1.07
F → E	54.66±2.46	63.17±3.05	55.37±5.64	N/A	N/A	N/A	88.01±0.79
(A, B, C) → D	54.58±4.38	78.91±2.83	75.42±3.95	N/A	N/A	N/A	95.29±1.21
D → (A, B, C)	60.99±3.51	70.52±3.68	74.82±2.16	N/A	N/A	N/A	89.41±2.38
(A, B, D) → C	57.71±2.09	78.77±2.41	<u>80.57±2.09</u>	N/A	N/A	N/A	94.36±1.27
C → (A, B, D)	59.08±4.83	75.30±2.91	<u>79.62±1.26</u>	N/A	N/A	N/A	88.71±1.47
(A, C, D) → B	61.83±3.81	70.39±3.12	<u>76.97±2.05</u>	N/A	N/A	N/A	92.69±1.35
B → (A, C, D)	59.41±2.56	68.29±2.71	<u>73.80±2.25</u>	N/A	N/A	N/A	90.36±1.28
(B, C, D) → A	58.39±2.71	77.92±3.63	<u>76.18±2.91</u>	N/A	N/A	N/A	94.45±1.84
A → (B, C, D)	60.02±3.92	75.22±4.41	<u>76.08±1.46</u>	N/A	N/A	N/A	87.24±2.25
(A, B) → (C, D)	62.49±2.74	81.51±2.47	<u>88.09±1.56</u>	N/A	N/A	N/A	92.13±1.75
(C, D) → (A, B)	66.18±3.63	80.37±3.00	<u>89.01±1.18</u>	N/A	N/A	N/A	90.83±1.62
(A, C) → (B, D)	63.80±2.48	79.15±3.85	<u>85.21±2.04</u>	N/A	N/A	N/A	89.61±1.56
(B, D) → (A, C)	68.73±2.95	81.59±2.71	<u>88.88±1.36</u>	N/A	N/A	N/A	88.17±1.02
(A, D) → (B, C)	71.96±2.17	83.15±2.76	<u>80.69±1.11</u>	N/A	N/A	N/A	91.52±1.27
(B, C) → (A, D)	69.03±1.99	<u>82.99±2.73</u>	<u>84.28±2.01</u>	N/A	N/A	N/A	92.48±1.07

D Results

Table 3 reports five different types of results for multi-site fMRI analysis. The first section of rows shows the results for peer to peer TL models — *i.e.*, applied to datasets where some subjects appear in each pair of sites. The second section of rows analyzes the situation where either the testing set, or

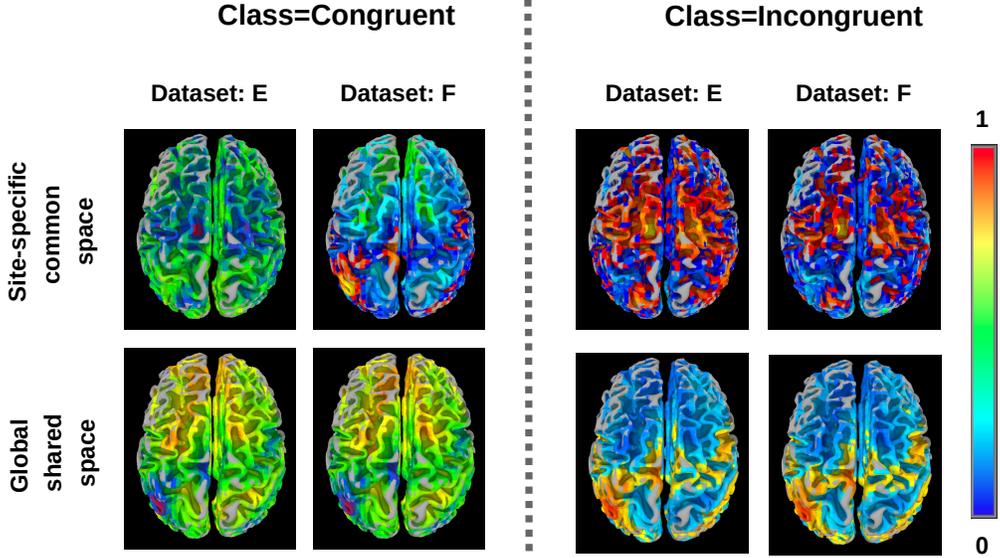


Figure 1: Comparing the site-specific common space in datasets E and F with the global shared space.

the training set, involves two datasets. The third section analyzes peer to peer TL where no subject appears in each pair of sites. This means we cannot use SRM, MDDL, and MDMS as these methods can only transfer cognitive tasks between multi-site fMRI datasets (with overlap) if some subjects appear in each pair of sites. The last two sections repeat experiments on the third section datasets, but using multi-site analysis.

This results reported here are more detailed than in the Experiment section of the main text, which just reports the average each pair of one-way analysis — *e.g.*, $acc(A \rightarrow B)$ and $acc(B \rightarrow A)$ are shown as $acc(A \rightleftharpoons B)$.

E Visualizing transferred neural responses

This section visualizes both the site-specific common space ($\mathbf{G}^{(d,S_d)}$) and the global shared space ($\mathbf{G}^{(d,S_d)}\mathbf{W}$) generated by SSTL for the dataset E and F. We chose these datasets as they include only 2 classes (*i.e.*, Congruent, and Incongruent) — allowing us to visualize all of the stimulus categories. Here, SSTL first generates the site-specific common space in voxel space ($k = V$) for datasets E and F separately. The first row of Figure 1 illustrates the average of these site-specific common space across time points belonging to each category of stimuli — *i.e.*, $\sum_{t \in Y} \mathbf{g}_t^{(d,S_d)}$ for $Y = \{\text{Congruent, Incongruent}\}$, and $d = \{E, F\}$. We then transfer these site-specific common space to global shared space. The second row of Figure 1 shows the average of the transformed common features across time points belonging to each category of stimuli — *i.e.*, $\sum_{t \in Y} \mathbf{q}_t^{(d,S_d)}$ for $\mathbf{Q}^{(d,S_d)} = \mathbf{G}^{(d,S_d)}\mathbf{W}$, $Y = \{\text{Congruent, Incongruent}\}$, and $d = \{E, F\}$. While the average of these site-specific common features are significantly distinctive for sites E and F, they are highly correlated after transforming to the global shared space.

F SRM versus SSTL

The first difference between the earlier SRM [4] versus our SSTL lies in defining the shared space. SRM uses $\min \sum_{s=1}^{S_d} \|\mathbf{X}^{(d,s)} - \mathbf{R}^{(d,s)}\mathbf{G}^{(d,S_d)}\|_F^2$ as the objective function, where $\mathbf{G}^{(d,S_d)} = \sum_{s=1}^{S_d} (\mathbf{R}^{(d,s)})^\top \mathbf{X}^{(d,s)}$ and $(\mathbf{R}^{(d,s)})^\top \mathbf{R}^{(d,s)} = \mathbf{I}$. Instead, SSTL utilizes $\min \sum_{s=1}^{S_d} \|\mathbf{X}^{(d,s)}\mathbf{R}^{(d,s)} - \mathbf{G}^{(d,S_d)}\|_F^2$ as objective function, where $(\mathbf{G}^{(d,S_d)})^\top \mathbf{G}^{(d,S_d)} = \mathbf{I}$. Note that both the site-dependents ($\mathbf{G}^{(d,S_d)}$) and the global shared space (\mathbf{W}) in SSTL are orthonormal;

thus, transformation for each site ($\mathbf{W} \mathbf{G}^{(d, S_a)}$) is also orthonormal. Like [5], these transformation matrices only apply standard rotations on the neural responses and will preserve the general shape of the data distribution during the transformation procedure. Empirical studies in [6] also showed that the original forms of SRM and HA (*i.e.*, the shared space) can rapidly reduce the performance of multi-site fMRI analysis. Moreover, SRM uses a probabilistic, iterative optimization approach that may coverage to a different $\mathbf{G}^{(d, S_a)}$ in each independent run. We instead propose a single-iteration optimization approach that our empirical studies demonstrate to be more time-efficient and robust.

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