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Shared Space Transfer Learning

for analyzing multi-site fMRI data

Tony M. Yousefnezhad, Alessandro M. Selvitella, Daoqiang Zhang, Andrew J. Greenshaw, Russell Greiner

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NeurIPS 2020

easy fMRI

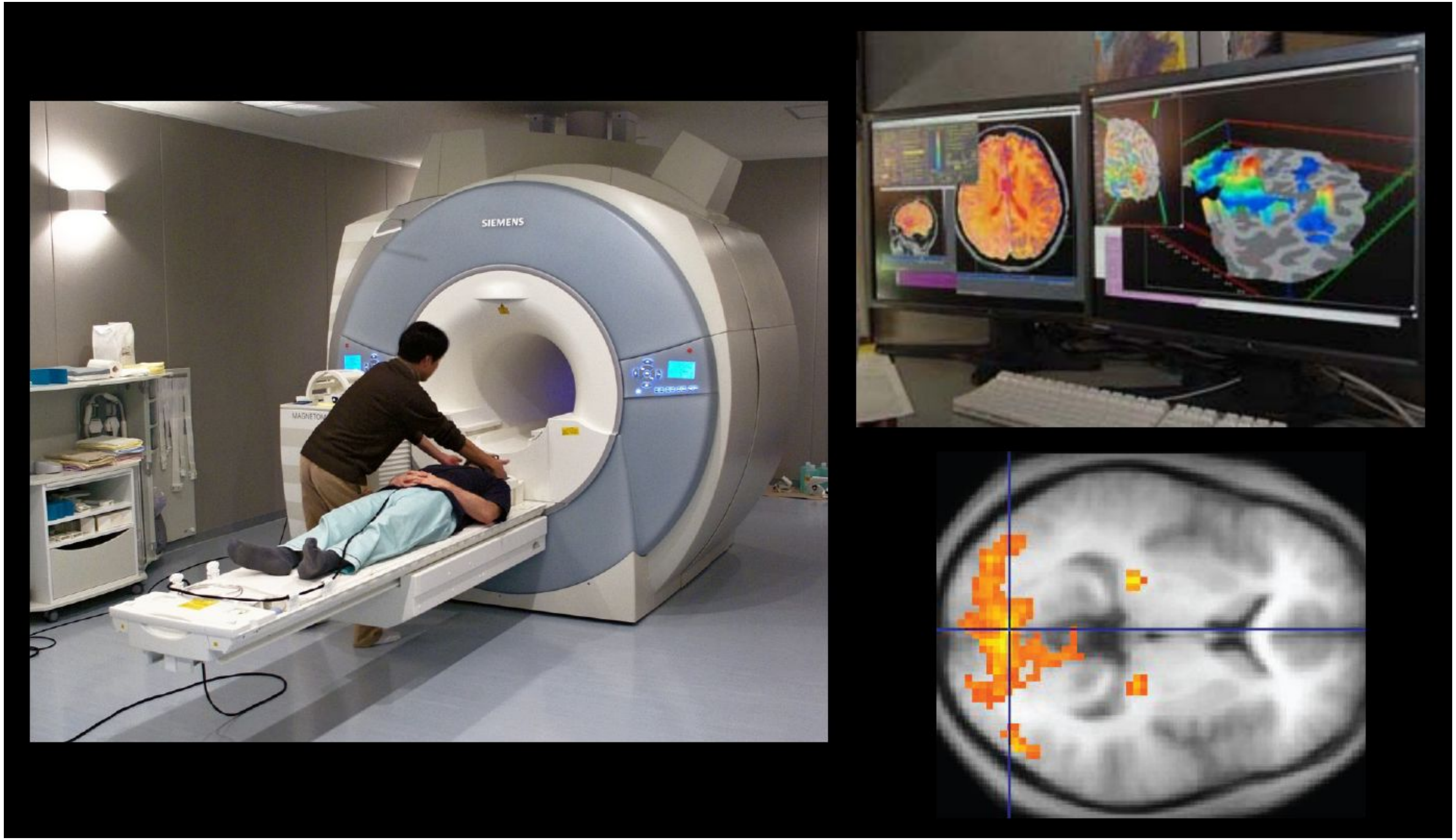
Paper link: https://papers.nips.cc/paper/2020/hash/b837305e43f7e535a1506fc263eee3ed-Abstract.html

Outline

- Task-based fMRI analysis
  - Representational Space
- *Single-site* Functional Alignment
  - Multi-view Learning
- Multi-site fMRI analysis
  - Challenges
  - Our proposed Shared Space Transfer Learning (SSTL)
- SSTL: Algorithm
- Empirical Studies
- Feature Works

Task-based fMRI analysis

functional Magnetic Resonance Imaging (fMRI) machine



Task-based fMRI dataset

Subject

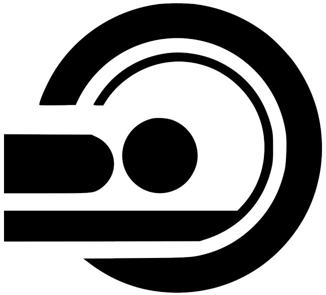
Subject

Task-based fMRI dataset

Subject

Subject

fMRI scan



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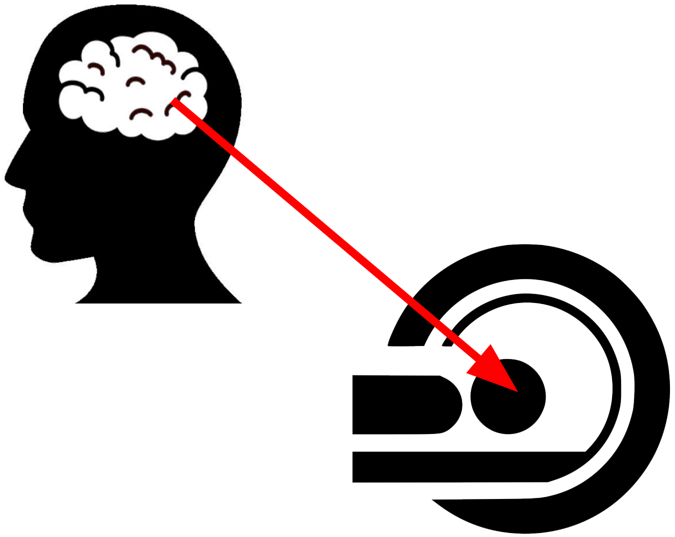
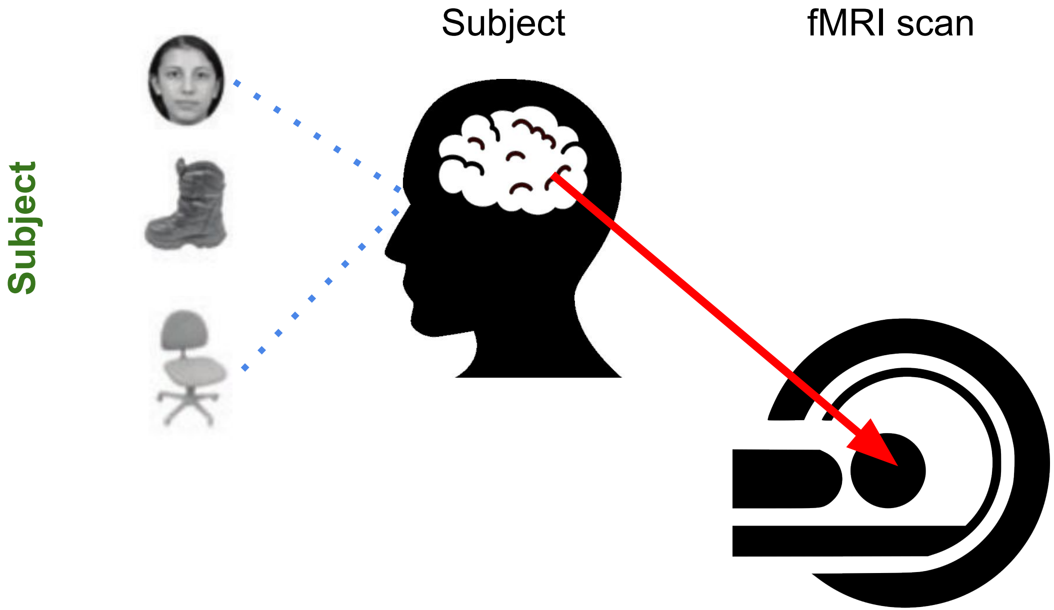
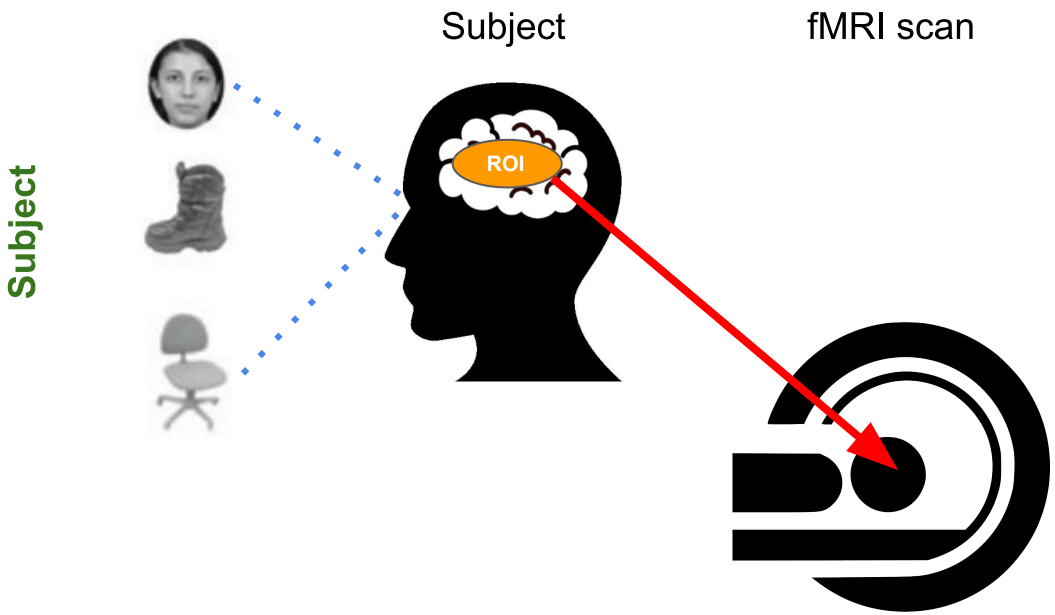


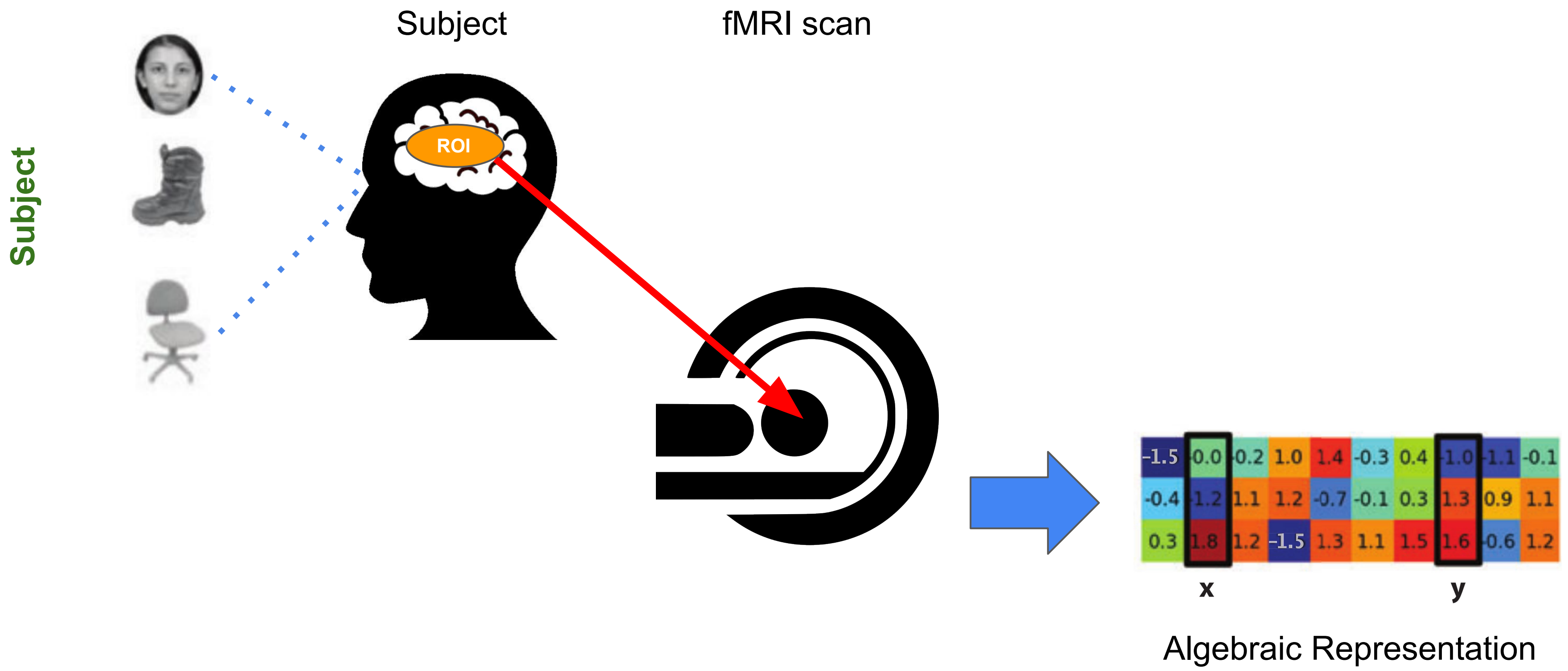
Task-based fMRI dataset



Task-based fMRI dataset



Task-based fMRI dataset



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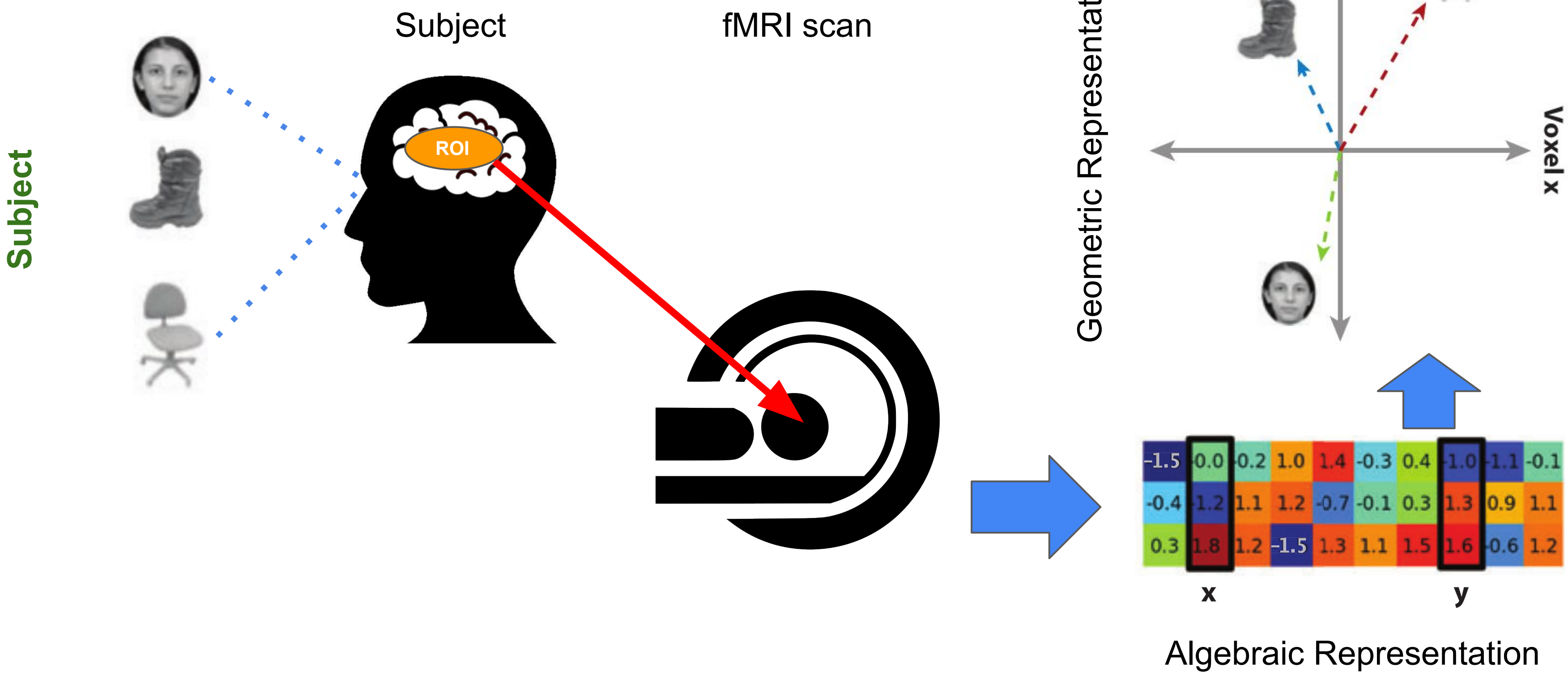
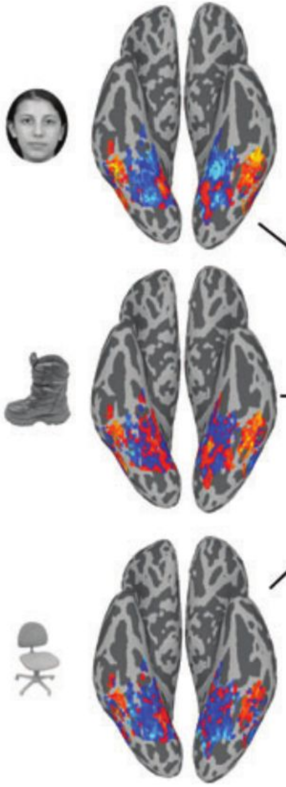
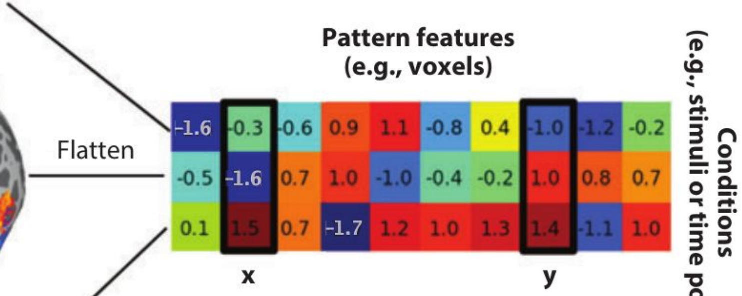


Representational (or Vector) Space

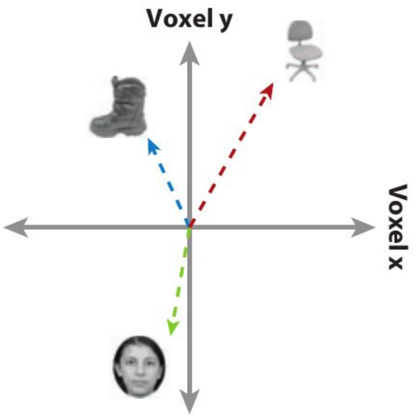
Algebraic Representation

Geometric Representation





E.g., $\mathbf{X}^{(d,s)} \in \mathbb{R}^{3\times 10}$



- Let $d=1 \ldots D$ be the number of sites
- S_d is the number of subjects in *d-th* site
- Let T_d be the number of time point in *d-th* site
- V is the number of voxel
- The brain image for *s-th* subject in *d-th* site: $\mathbf{X}^{(d,s)} \in \mathbb{R}^{T_d \times V}$

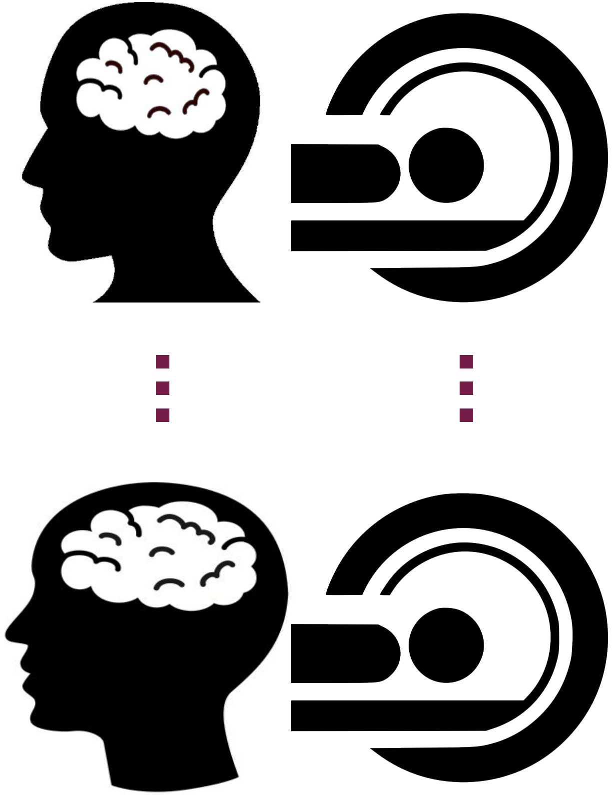
Functional Alignment

single-site

Multi-subject fMRI dataset

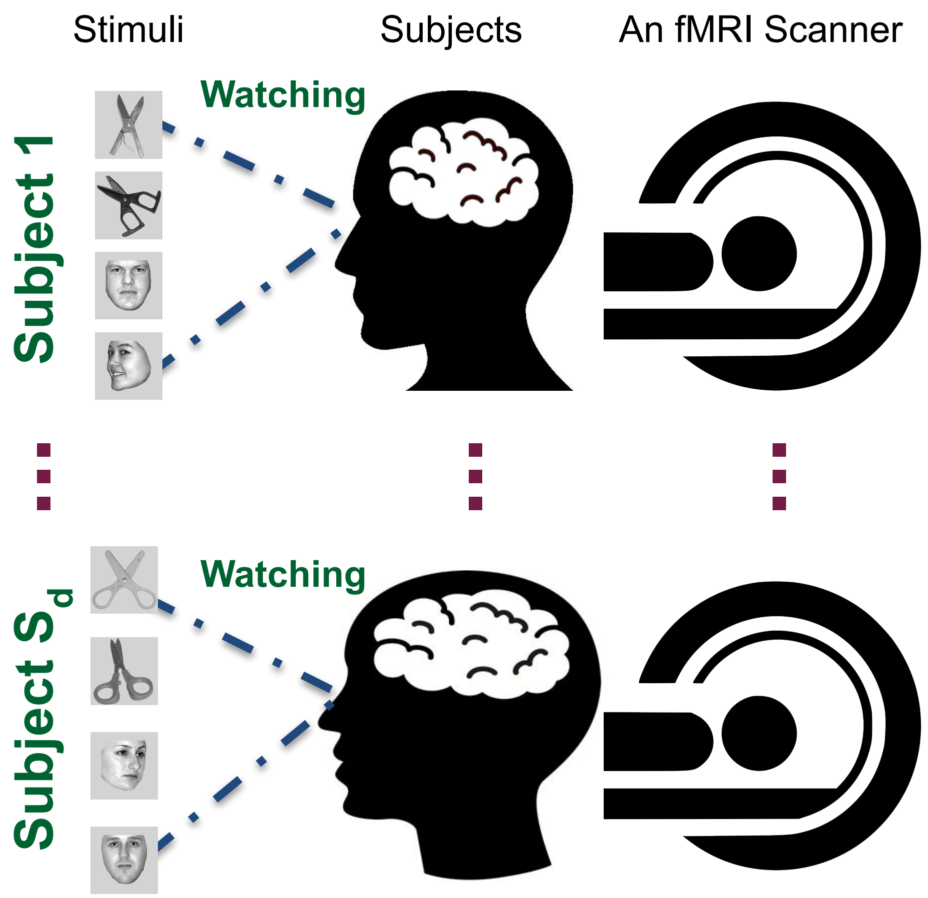
Subjects An fMRI Scanner

Subject 1



Subject S_d

Multi-subject fMRI dataset



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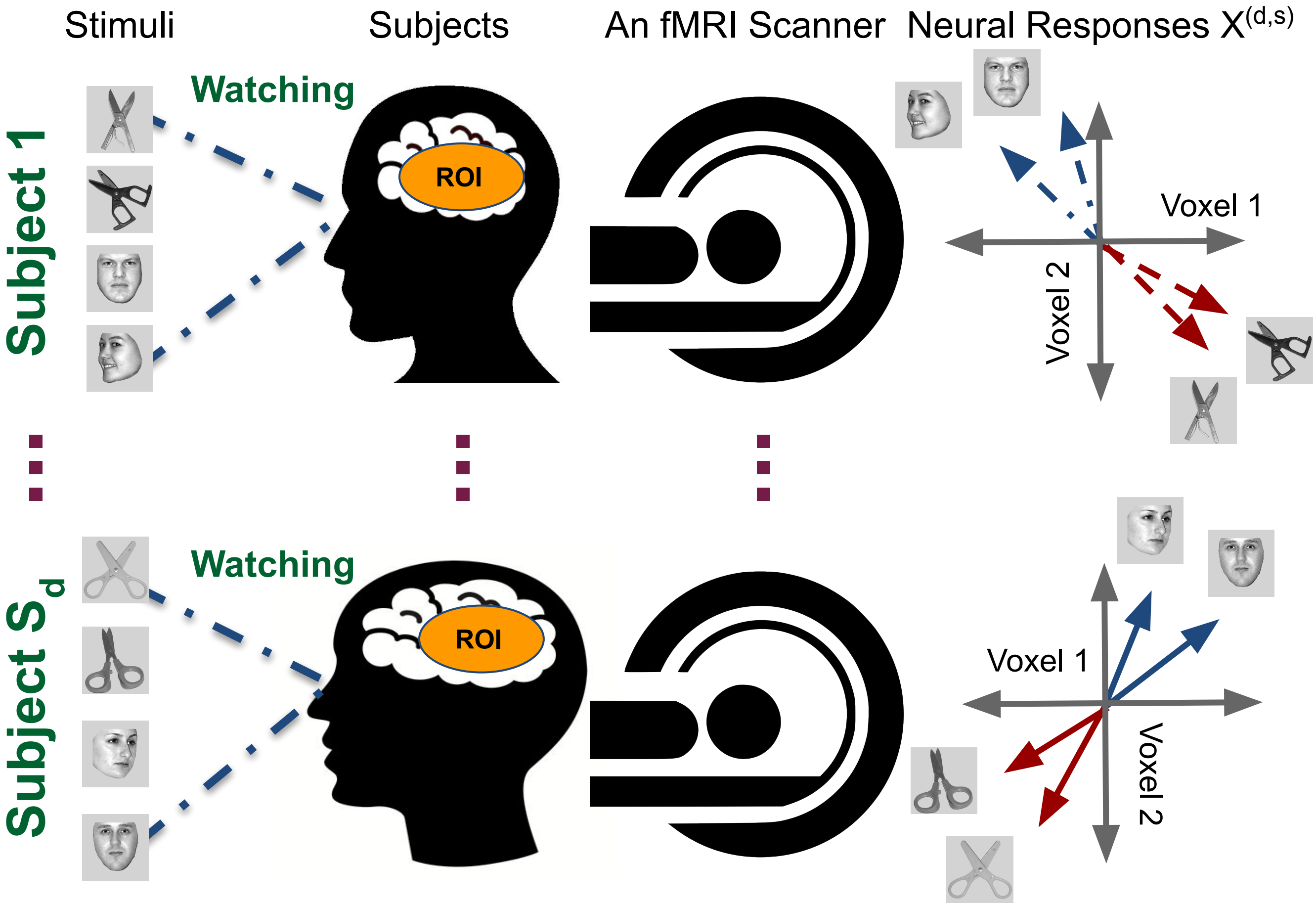

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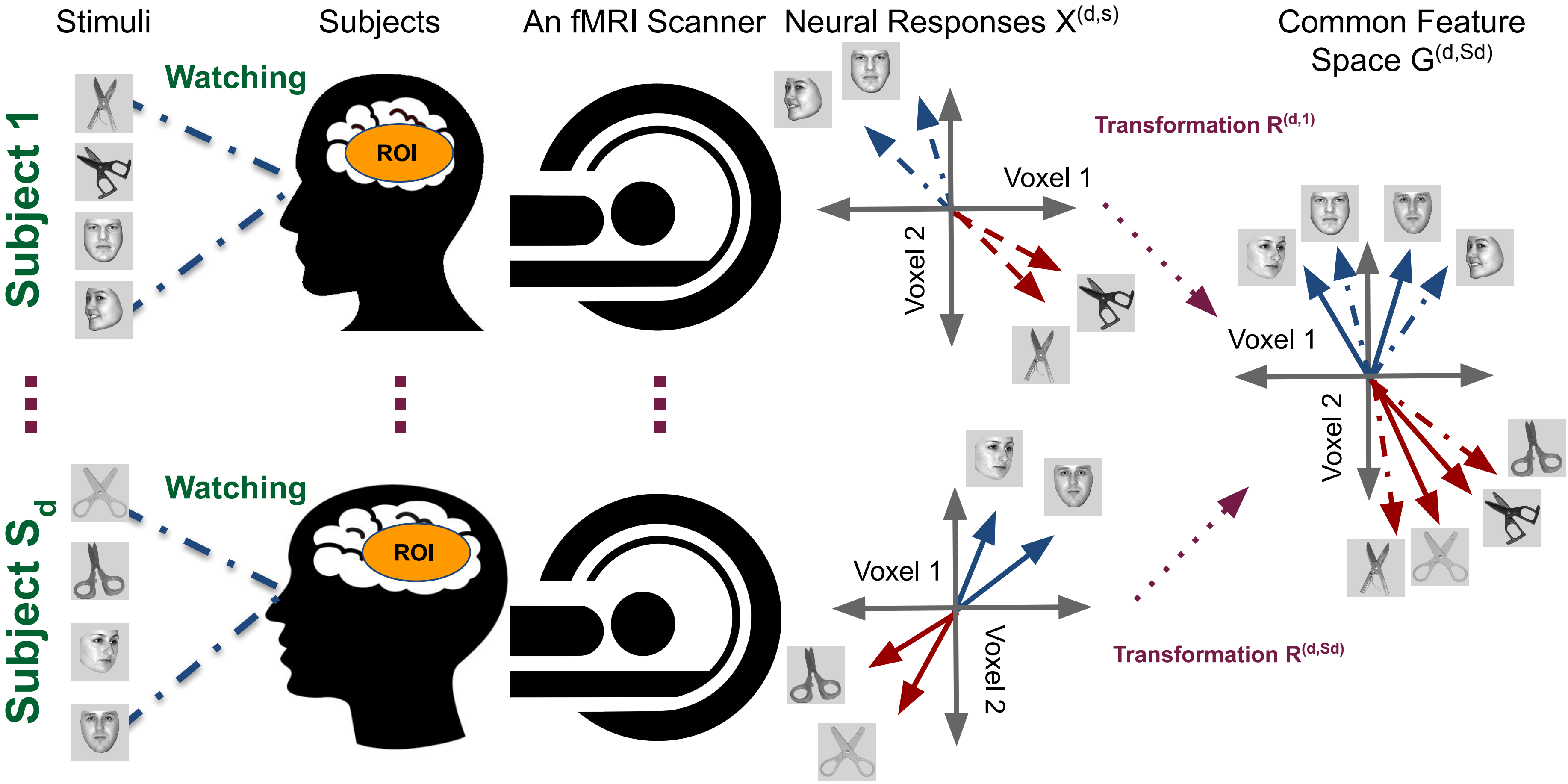
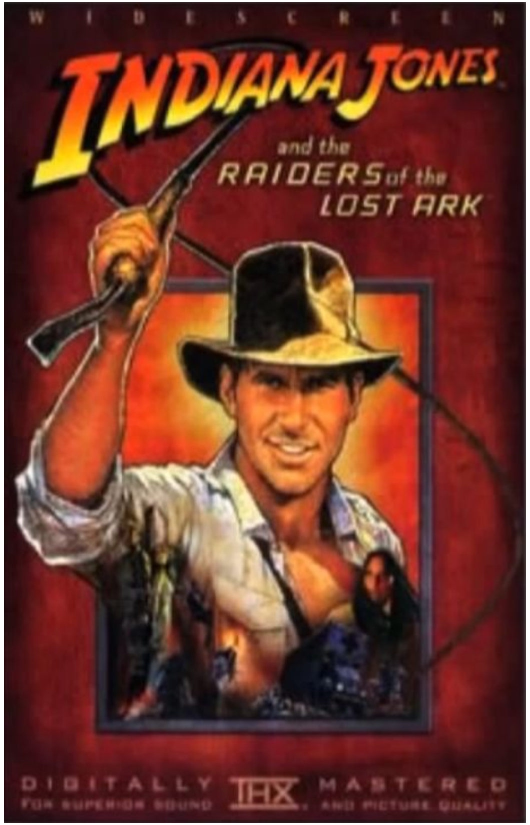
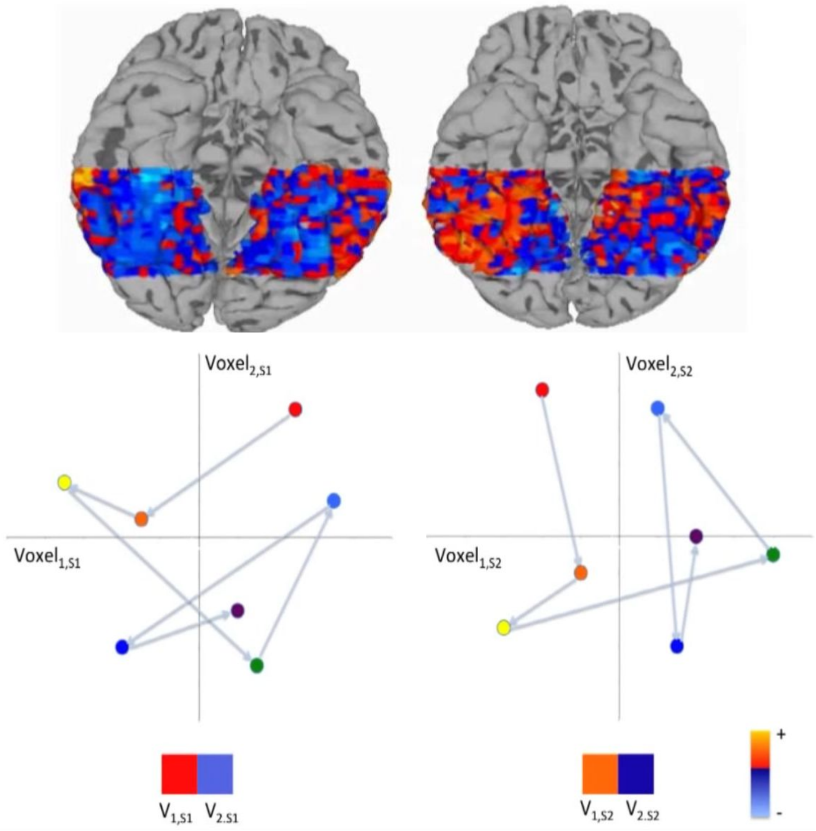


Pattern vector trajectories for 2 subjects in a 2-voxel representation space





Subject 1

Subject 2

This slide is part of [Haxby, 2011] talk in Dartmouth College
Link https://youtu.be/jaR9PmlaIPs

Single-site functional alignment for multi-subject fMRI

➢ **Generating the common space for *each site:***

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

$$\text{subject to} \quad \left(\mathbf{G}^{(d,S_d)}\right)^\top \mathbf{G}^{(d,S_d)} = \mathbf{I}_k.$$

- Let $d=1 \dots D$ be the number of sites
- $s=1 \dots S_d$ is the number of subjects in *d-th* site
- Let $t=1 \dots T_d$ be the number of time point in *d-th* site
- $v=1 \dots V$ is the number of voxel
- We let $k << V$ be the number of components

- The brain image for *s-th* subject in *d-th* site: $\mathbf{X}^{(d,s)} \in \mathbb{R}^{T_d \times V}$
- The mapping matrix for *s-th* subject in *d-th* site: $\mathbf{R}^{(d,s)} \in \mathbb{R}^{V \times k}$
- The common space for *d-th* site: $\mathbf{G}^{(d,S_d)} \in \mathbb{R}^{T_d \times k}$

An insight for the optimization procedure

- We define the regularized projection (hat) matrix for *s-th* subject in *d-th* site:

$$\mathbf{P}^{(d,s)} = \mathbf{X}^{(d,s)} \left(\mathbf{X}^{(d,s)} \left(\mathbf{X}^{(d,s)} \right)^{\top} + \epsilon \mathbf{I}_{T_d} \right)^{-1} \left(\mathbf{X}^{(d,s)} \right)^{\top}$$

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- We also define the mapping matrix for *s-th* subject in *d-th* site:

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

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- By these assumptions, we can rewrite the objective function only based on the common space:

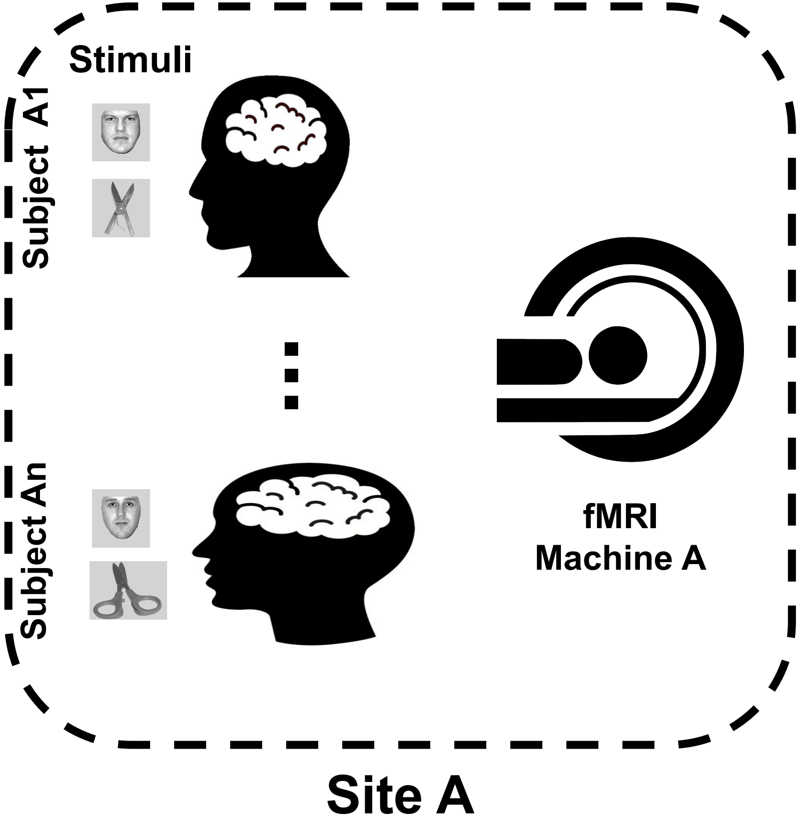
$$\underset{\mathbf{R}^{(d,s)},\mathbf{G}^{(d,S_d)}}{\arg\min} \sum_{s=1}^{S_d}\left\|\mathbf{G}^{(d,S_d)} - \mathbf{X}^{(d,s)}\mathbf{R}^{(d,s)}\right\|_F^2 \approx \underset{\mathbf{G}^{(d,S_d)}}{\arg\max}\left(\mathrm{tr}\left(\left(\mathbf{G}^{(d,S_d)}\right)^{\top}\sum_{s=1}^{S_d}\mathbf{P}^{(d,s)}\mathbf{G}^{(d,S_d)}\right)\right)$$

- We can calculate the common space by solving an *eigendecomposition* problem

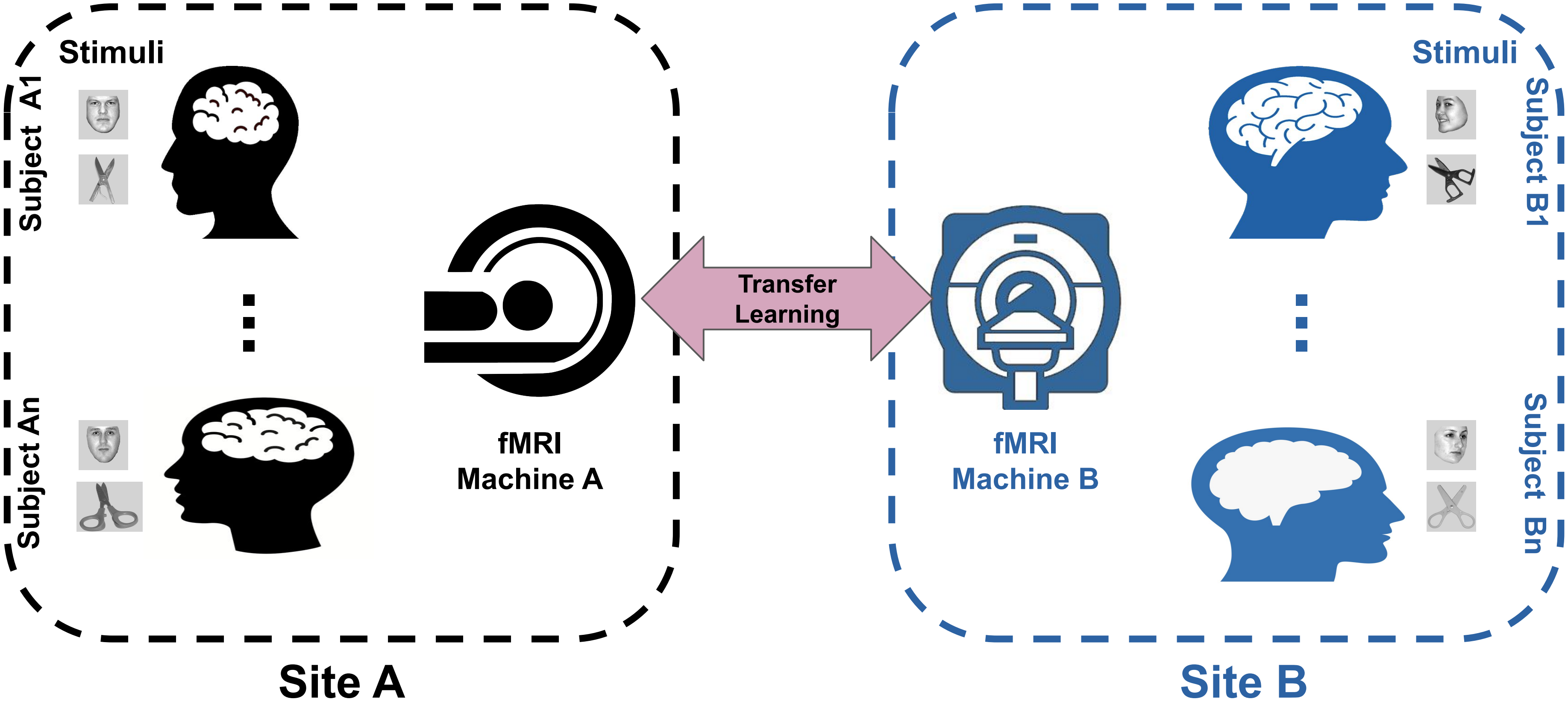
Multi-site fMRI analysis

Our SSTL algorithm

Multi-site fMRI analysis



Multi-site fMRI analysis



SSTL: Motivation

- Challenging issues in most fMRI studies:
    - **High-dimensionality** and **noisy**
    - **Expensive to collect** with **small sample** sizes

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  - **Temporal alignment**: a unique time-point shows the same stimulus for all subjects
  - **Batch effects**: a set of external elements that may affect the distribution of fMRI datasets
    - The **environment** noise
    - Standards that are used by **vendors** of fMRI machines

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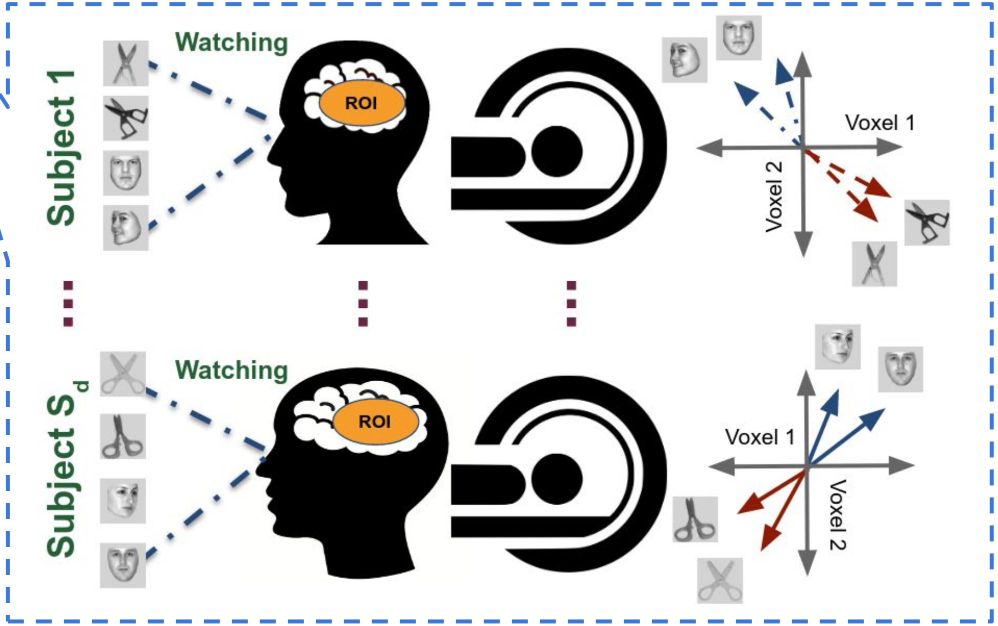
    - Standards that are used by **vendors** of fMRI machines
- Shared Space Transfer Learning (SSTL)
  - A novel **Transfer Learning (TL)** approach for multi-site fMRI analysis
  - It can functionally **align homogeneous multi-site** fMRI datasets
  - It **IS NOT LIMITED** to overlapped datasets (*i.e.*, share some subjects)
  - It can improve the **prediction performance** in every site.

SSTL: Learning pipeline

Site d=1
(with labels)

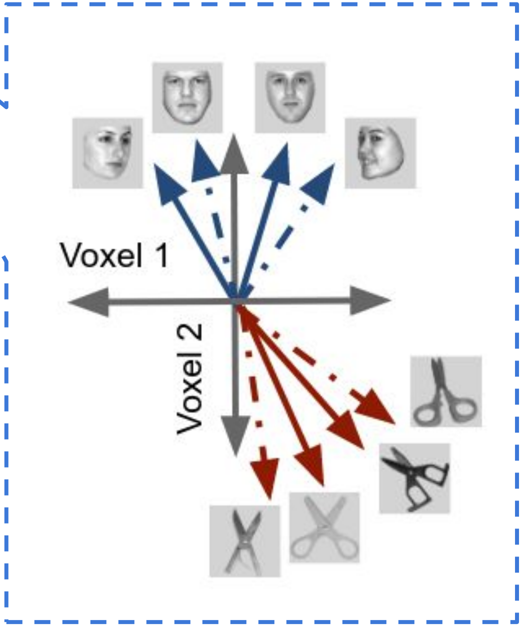


SSTL: Learning pipeline

Site d=1
(with labels)

→

Common Space $\mathbf{G}^{(1,S_1)}$



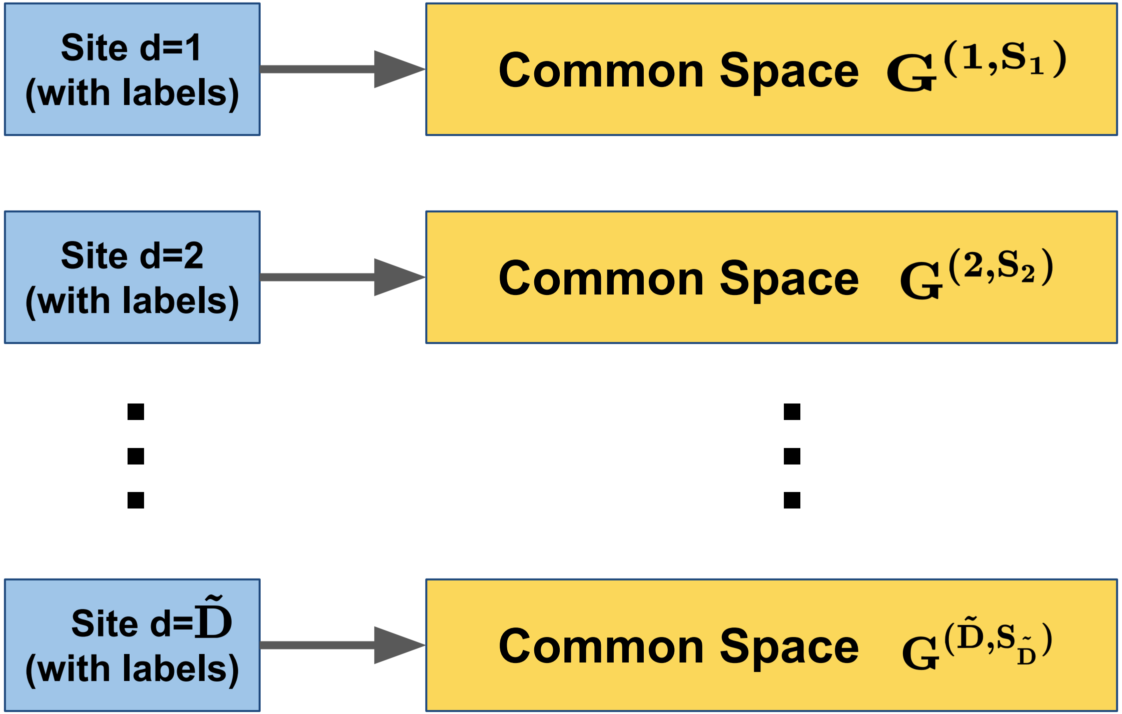
SSTL: Learning pipeline

Site d=1 (with labels) → **Common Space $\mathbf{G}^{(1,S_1)}$**

Site d=2 (with labels)

- This site can have:
  - different set of subjects
  - different temporal alignment
  - different vendors of fMRI machine
- **BUT** it must have homogeneous cognitive tasks
  - all performing the same set of fMRI tasks

SSTL: Learning pipeline



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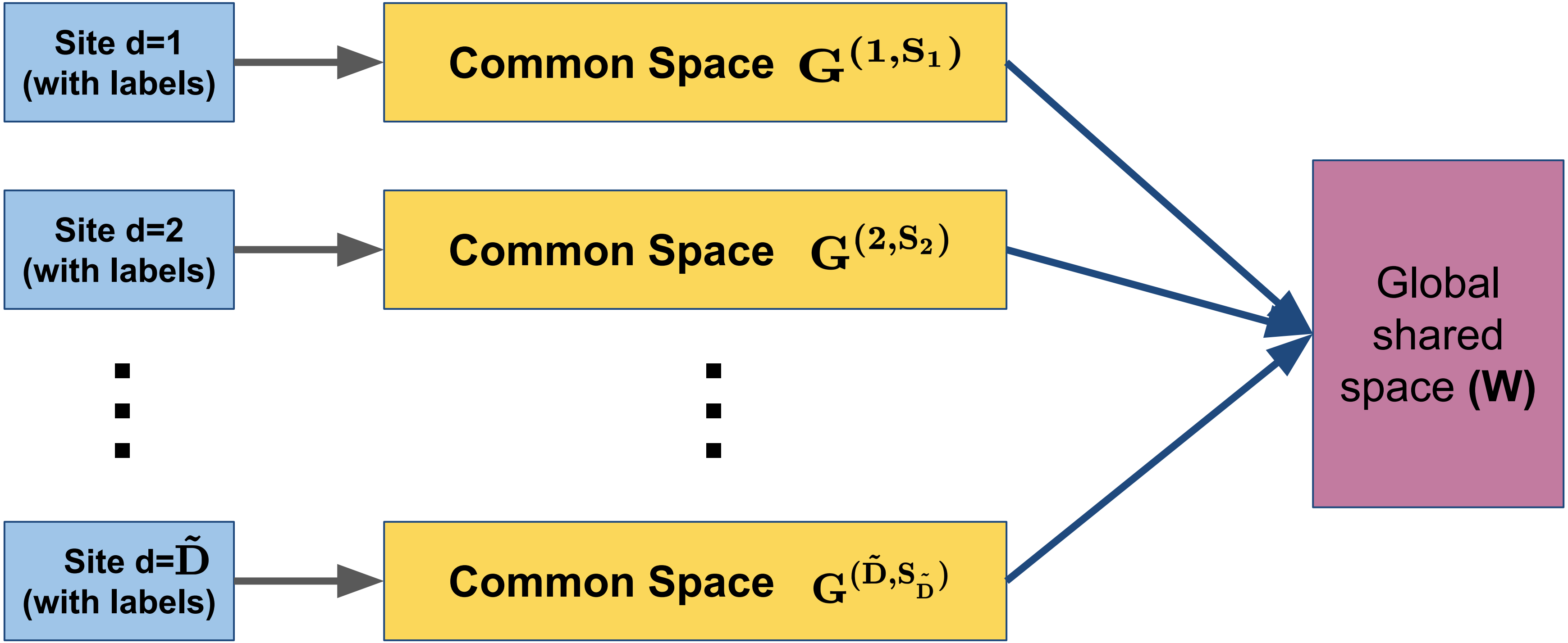

Generating the Global Shared Space (training phase)

- We denote a concatenated version of all common spaces in the training set as follows:

$$\mathbf{G} \quad = \quad \begin{bmatrix} \mathbf{G}^{(1,S_1)} \\ \mathbf{G}^{(2,S_2)} \\ \vdots \\ \mathbf{G}^{(\widetilde{D},S_{\widetilde{D}})} \end{bmatrix}$$

- We use linear Karhunen–Loeve transformation (KLT) for learning the global shared space:

$$\widetilde{\mathcal{T}}_G\left(\mathbf{G}\right) \quad = \quad \underset{\mathbf{W}}{\arg\min}\left\|\mathbf{G} - \mathbf{G}\mathbf{W}\mathbf{W}^\top\right\|_F^2,$$

$$\text{subject to} \quad \mathbf{W}^\top\mathbf{W} = \mathbf{I}_k$$

SSTL: Algorithm

SSTL: Objective Functions

➢ **STEP 1: Generating the common space for *each site:***

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

$$\text{subject to} \quad \left(\mathbf{G}^{(d,S_d)}\right)^\top \mathbf{G}^{(d,S_d)} = \mathbf{I}_k.$$

- $X^{(d,s)}$ denotes the **neural responses** for *s-th* subject in *d-th* site
- $R^{(d,s)}$ denotes the **mapping matrices** for *s-th* subject in *d-th* site
- $G^{(d,sd)}$ denotes **the common space** for *d-th* site

➢ **STEP 2: Generating the global shared space**

$$\widetilde{\mathcal{J}}_G\left(\mathbf{G}\right) = \underset{\mathbf{W}}{\arg\min} \left\| \mathbf{G} - \mathbf{G}\mathbf{W}\mathbf{W}^\top \right\|_F^2,$$

$$\text{subject to} \quad \mathbf{W}^\top\mathbf{W} = \mathbf{I}_k.$$

- G denotes the concatenated version of **all common spaces in the training set**
- W is the **global shared space**

SSTL: Algorithm

Algorithm 1 Shared Space Transfer Learning (SSTL)

Input:

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

Output:

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

Method:

 # Common Phase — must run for each dataset separately

01. $D = \widetilde{D} + \widehat{D}$
02. Initialize $\mathbf{G}^{(d,0)} = \{0\}^{T_d \times k}$ and $\widetilde{\mathbf{\Sigma}}^{(d,0)} = \text{diag}(\{0\}^k)$ 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 $\mathbf{G} = [\mathbf{G}^{(d,S_d)}]_{d=1\dots\widetilde{D}}$ based on (9).
05. Calculate the second moment $\mathbf{C} = \frac{1}{T-1}\left(\mathbf{G} - \mathbf{1}_T\mu^\top\right)^\top\left(\mathbf{G} - \mathbf{1}_T\mu^\top\right)$ based on (12).
06. Calculate $\mathbf{W}$ as eigenvectors of $\mathbf{C}$.
07. Train a classification model $\mathbf{\Pi}\left([\mathbf{X}^{(d,s)}\mathbf{R}^{(d,s)}\mathbf{W}]_{d=1\dots\widetilde{D},s=1\dots S_d}, [\mathbf{y}^{(d,s)}]_{d=1\dots\widetilde{D},s=1\dots S_d}\right)$.

 # Testing Phase

08. Predict based on model $[\widehat{\mathbf{p}}^{(d,s)}]_{d=1\dots\widehat{D},s=1\dots S_d} = \mathbf{\Pi}\left([\mathbf{X}^{(d,s)}\mathbf{R}^{(d,s)}\mathbf{W}]_{d=1\dots\widehat{D},s=1\dots S_d}\right)$.
09. Evaluate accuracy of the model — *i.e.*, $[\widehat{\mathbf{p}}^{(d,s)}]_{d=1\dots\widehat{D},s=1\dots S_d}$ vs. $[\mathbf{y}^{(d,s)}]_{d=1\dots\widehat{D},s=1\dots S_d}$.

Empirical Studies

Scheme of experiments: Algorithm

- We compare SSTL with **6 different** existing methods:
  - Baseline:
    - Raw neural responses in **MNI** space without using TL methods

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    - Shared response model (**SRM**)
    - Multi-dataset dictionary learning (**MDDL**)
    - Multi-dataset multi-subject (**MDMS**)

Scheme of experiments: Algorithm

- We compare SSTL with **6 different** existing methods:
  - Baseline:
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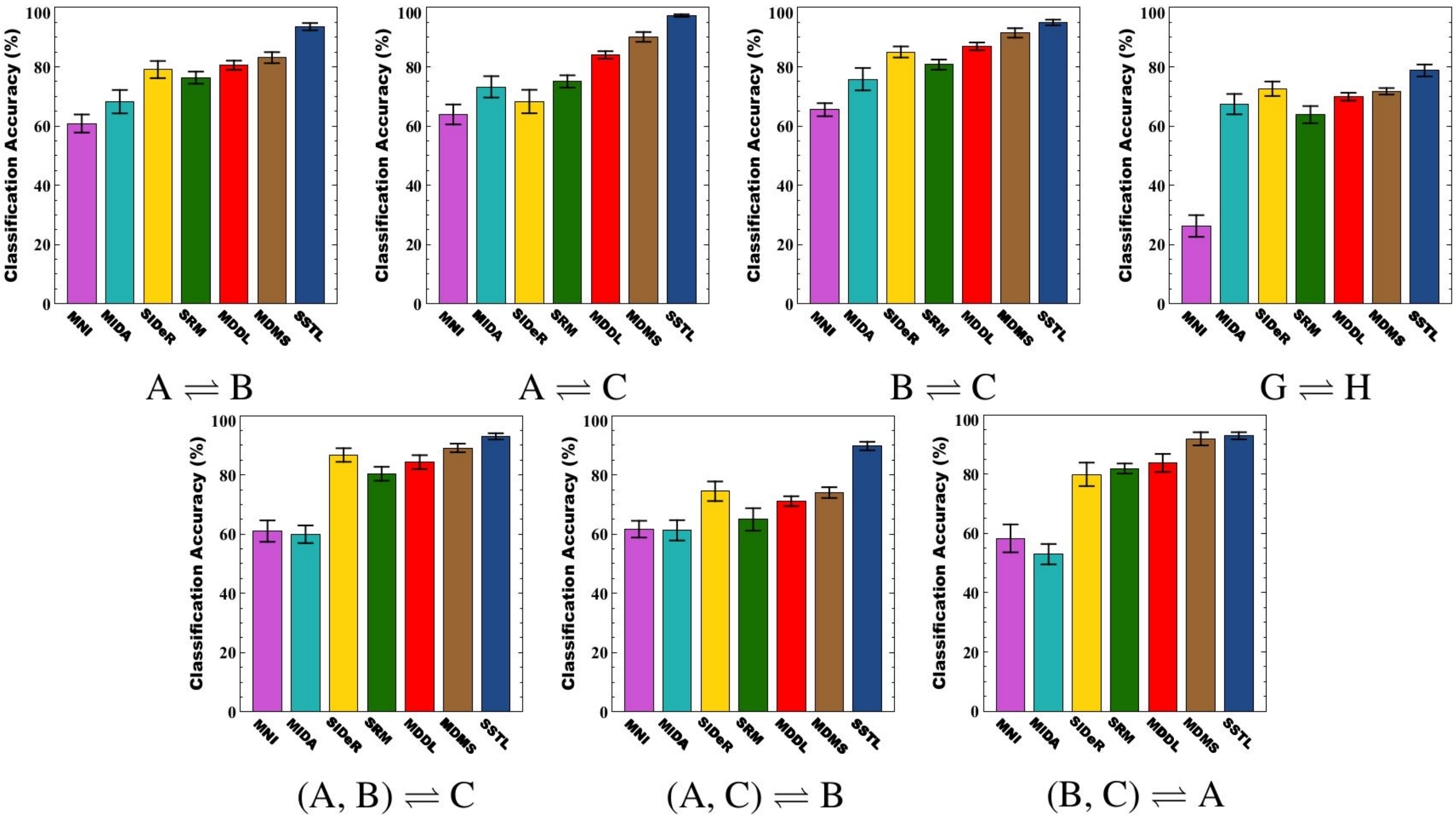
  - Methods need pair-site subjects:
    - Shared response model (**SRM**)
    - Multi-dataset dictionary learning (**MDDL**)
    - Multi-dataset multi-subject (**MDMS**)
  - Methods based on general TL algorithms:
    - Maximum independence domain adaptation (**MIDA**)
    - Side Information Dependence Regularization (**SIDeR**)

Scheme of experiments: Datasets

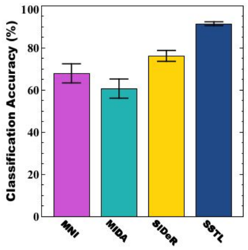
ID	Title (Open NEURO ID)	Type	S_d	#1	T_d	#2	#3
A	Stop signal with spoken pseudo word naming (DS007)	Decision	20	4	149	B, C	B, C, D
B	Stop signal with spoken letter naming (DS007)	Decision	20	4	112	A, C	A, C, D
C	Stop signal with manual response (DS007)	Decision	20	4	211	A, B	A, B, D
D	Conditional stop signal (DS008)	Decision	13	4	317		A, B, C
E	Simon task (DS101)	Simon	21	2	302		F
F	Flanker task (DS102)	Flanker	26	2	292		E
G	Integration of sweet taste – study 1 (DS229)	Flavour	15	6	580	H	H
H	Integration of sweet taste – study 3 (DS231)	Flavour	9	6	650	G	G

S_d is the number of subject; #1 is the number of stimulus categories; T_d is the number of time points per subjects; #2 lists the other datasets that overlap with this dataset; #3 lists the other datasets whose neural responses can be transferred to this dataset.

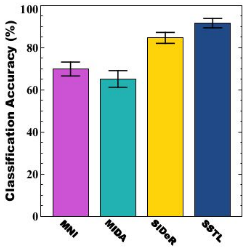
Multi-site classification analysis for pairs of datasets that overlap



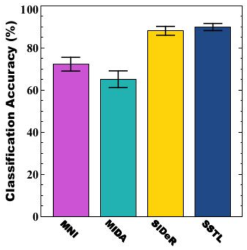
Multi-site classification analysis for sets of datasets that do not overlap



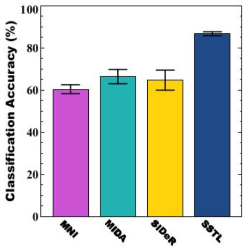
$A \rightleftharpoons D$



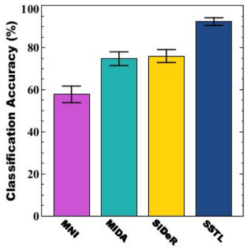
$B \rightleftharpoons D$



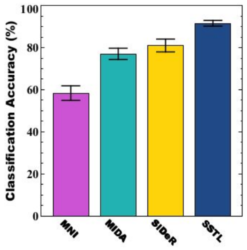
$C \rightleftharpoons D$



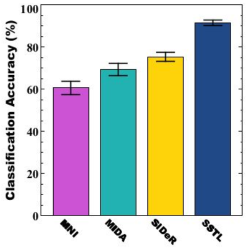
$E \rightleftharpoons F$



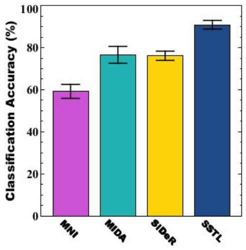
$(A, B, C) \rightleftharpoons D$



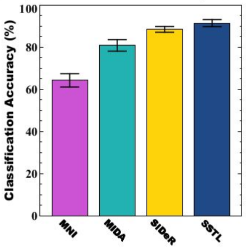
$(A, B, D) \rightleftharpoons C$



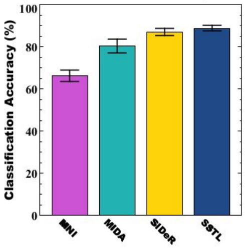
$(A, C, D) \rightleftharpoons B$



$(B, C, D) \rightleftharpoons A$



$(A, B) \rightleftharpoons (C, D)$



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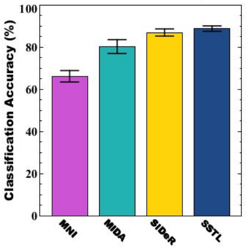
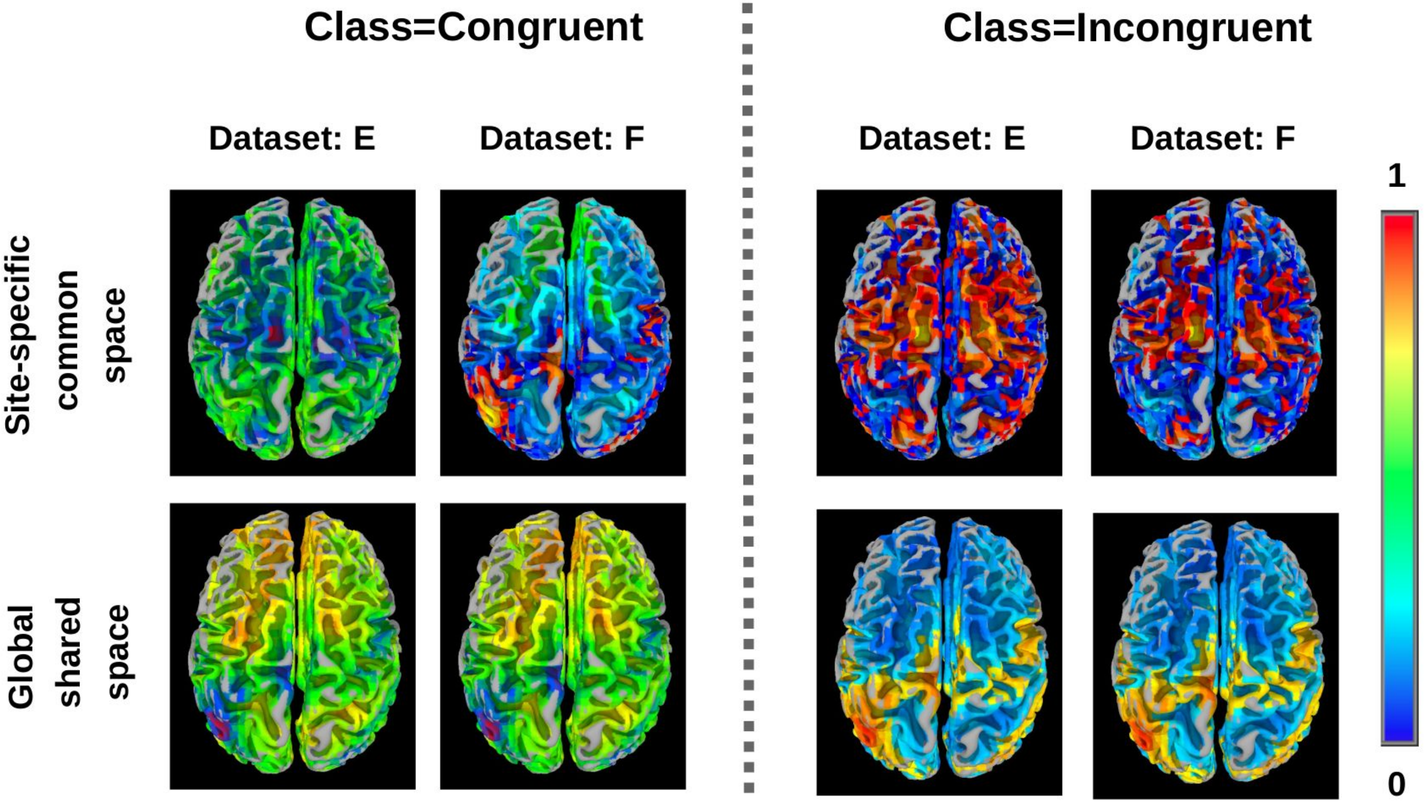
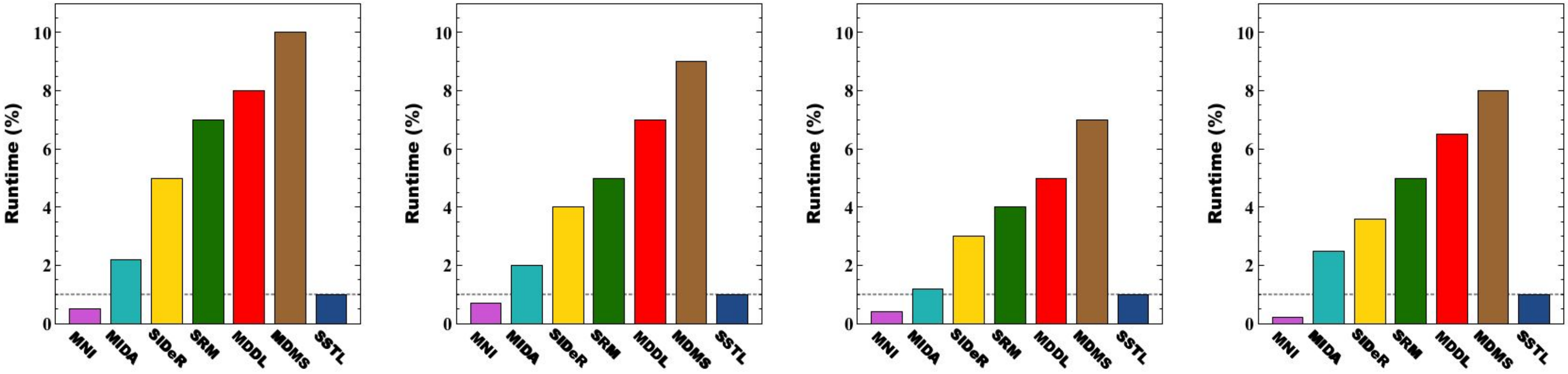


$(A, D) \rightleftharpoons (B, C)$

Visualizing transferred neural responses



Runtime



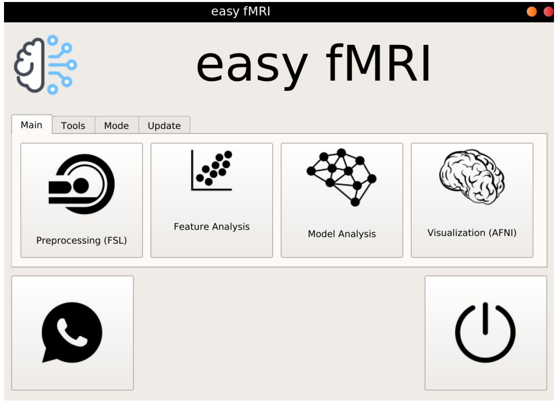
(A, B) ⇌ C (A, C) ⇌ B (B, C) ⇌ A G ⇌ H

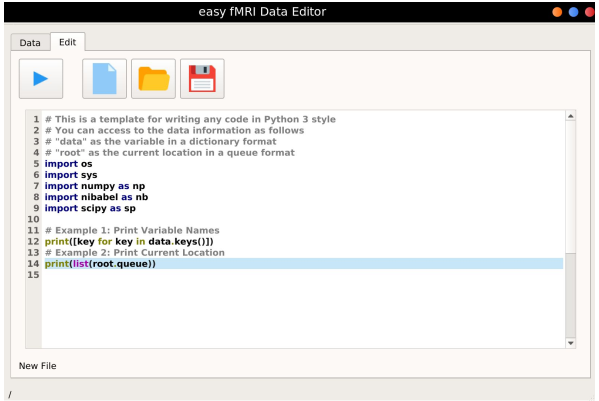
- SSTL uses a **single-iteration optimization** approach

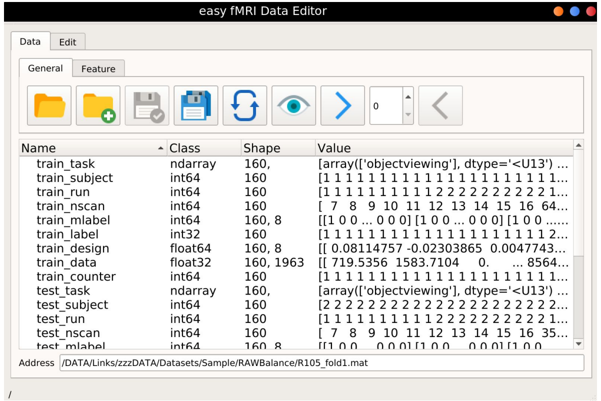
Future Works

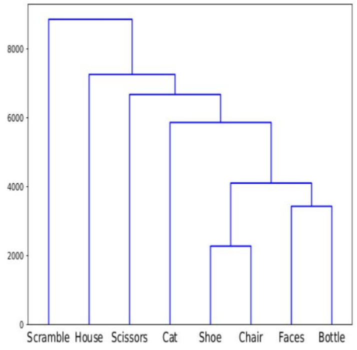
Conclusion

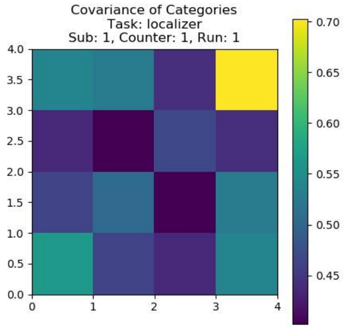
- We propose the Shared Space Transfer Learning (SSTL) as a novel transfer learning (TL) technique that can be used for homogeneous multi-site fMRI analysis.
- Our comprehensive experiments confirmed that SSTL achieves superior performance to other state-of-the-art TL analysis methods.
- We anticipate that SSTL's multi-view technique for transfer learning will have strong practical applications in neuroscience --- such as functional alignment of multi-site fMRI data, perhaps of movie stimuli.

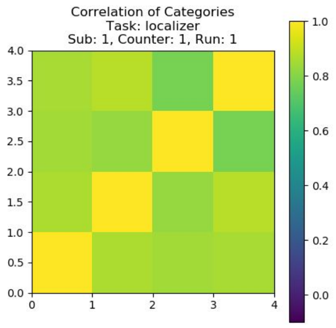


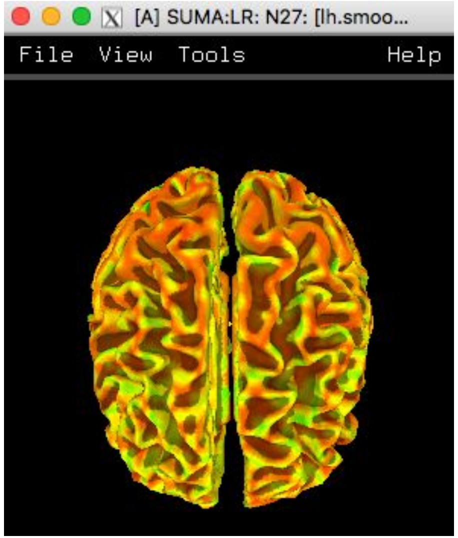






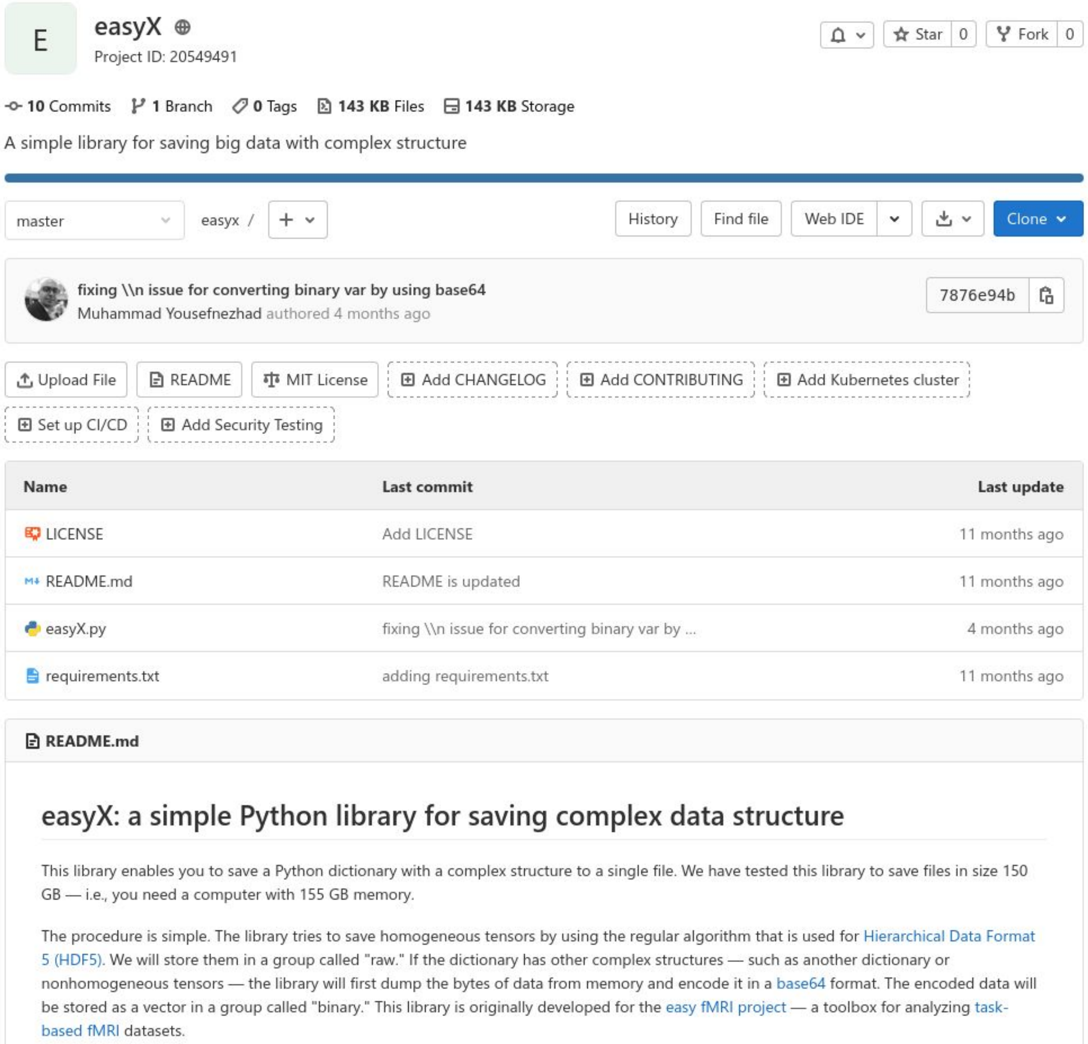






Available at https://easyfmri.learningbymachine.com/

easyX: a simple Python library for saving big complex data structure



Available at
https://gitlab.com/myousefnezhad/easyx

Research Topic on Frontiers in Neuroinformatics

Multi-Site Neuroimage Analysis: Domain Adaptation and Batch Effects

About this Research Topic

Neuroimaging is a vital tool for brain science in both basic and applied studies — including, for example, studies of cognitive processes and neurodevelopmental trends, and prediction or diagnosis of brain pathology. Despite the advantages of modern imaging technologies, this is still challenging as the data is noisy, high-dimensional, and typically only small sample sizes (as it is expensive to acquire).

Increased access to public neuroimaging datasets has motivated the field to investigate multi-site datasets, which promise an improvement of accuracy rates in the application of advanced computational learning procedures (i.e., machine learning). However, forming a dataset by merely concatenating data from various sites/sources often fails due to batch effects, where the accuracy on a dataset of a model trained on a multi-site dataset is often worse than the accuracy of a model trained on that single site. A promising area for tackling these issues is that of domain adaptation techniques — e.g., transfer learning, which leverages source data to improve related target data performance.

This Research Topic calls for papers focusing on advanced machine learning approaches that can address current challenges in multi-site neuroimaging analysis. Contributions may address homogeneous domain adaptation problems, where the source and target sites have the same modularity of neuroimage data — e.g., multi-site fMRI analysis. Another class of submissions may tackle nonhomogeneous problems, where the source and target sites have different modalities of images. One prevalent use of nonhomogeneous approaches is to improve the quality of low-resolution medical images (such as CT scans) through leveraging high-resolution features (e.g., MRIs). This Research Topic will also cover theoretical studies, which may focus on the development of novel machine learning techniques for multi-site neuroimage analysis — such as probabilistic graphical models, deep learning, multi-view methods, reinforcement learning, etc. Basic and applied studies should indicate successful analyses that relied on advanced domain adaptation techniques to improve the performance of analysis in real-world applications.

Keywords: Multi-Site Neuroimage Analysis, Domain Adaptation, Batch Effects, Transfer Learning

Important Note: All contributions to this Research Topic must be within the scope of the section and journal to which they are submitted, as defined in their mission statements. Frontiers reserves the right to guide an out-of-scope manuscript to a more suitable section or journal at any stage of peer review.

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