Canonical Correlation Analysis on Riemannian Manifolds and its Applications

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The motivating problem

- Canonical correlation analysis (CCA) based statistical analysis of images where voxel-wise measurement is manifold valued.
- CCA on the *product Riemannian manifold* representing SPD matrix-valued fields
- Correlations between diffusion tensor images (DTI) and Cauchy deformation tensor fields derived from T1-weighted magnetic resonance (MR) images

What's new?

- Extensions of CCA to nonlinear spaces e.g., KCCA, ANN, Deep CCA (ICML 2013)
- Adaptive CCA (ICML 2012) uses matrix manifold optimization but it's NOT for manifold-valued data
- **This paper : generalization of CCA for Riemannian manifolds**
- **Main technical highlight:** Exact iterative method as well as single path algorithms with approximate projections (inner product and log-Euclidean)
- Relationship between transformations on SPD(n) for more accurate approximation

CCA in Euclidean space

Pearson correlation for $x \in \mathbf{R}$ and $y \in \mathbf{R}$

$$\rho_{x,y} = \frac{\mathrm{COV}(x,y)}{\sigma_x\sigma_y} = \frac{\mathbb{E}[(x-\mu_x)(y-\mu_y)]}{\sigma_x\sigma_y} = \frac{\sum_{i=1}^N (x_i-\mu_x)(y_i-\mu_y)}{\sqrt{\sum_{i=1}^N (x_i-\mu_x)^2}\sqrt{\sum_{i=1}^N (y_i-\mu_y)^2}} \quad (1)$$

Canonical Correlation for $\mathbf{x} \in \mathbf{R}^m$ and $\mathbf{y} \in \mathbf{R}^n$

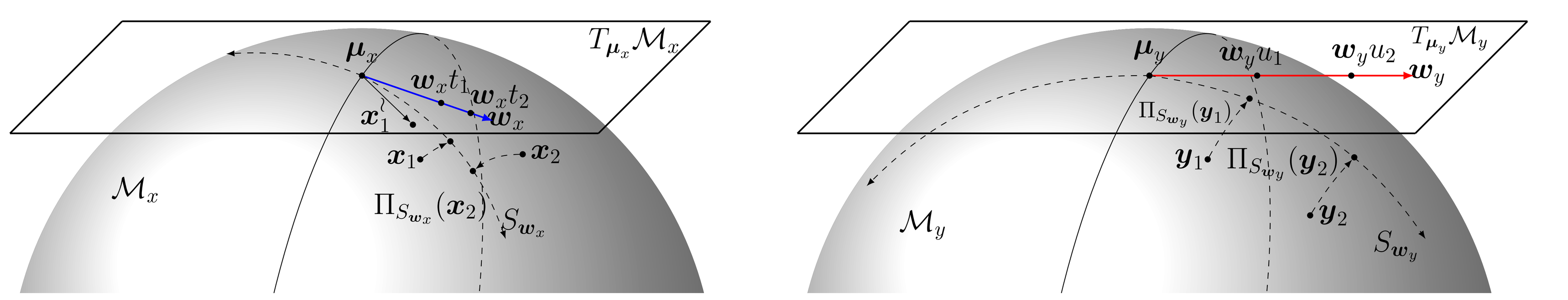
$$\max_{\mathbf{w}_x,\mathbf{w}_y} \mathrm{corr}(\pi_{\mathbf{w}_x}(\mathbf{x}), \pi_{\mathbf{w}_y}(\mathbf{y})) = \max_{\mathbf{w}_x,\mathbf{w}_y} \frac{\sum_{i=1}^N \mathbf{w}_x^T(\mathbf{x}_i-\mu_x)\mathbf{w}_y^T(\mathbf{y}_i-\mu_y)}{\sqrt{\sum_{i=1}^N (\mathbf{w}_x^T(\mathbf{x}_i-\mu_x))^2}\sqrt{\sum_{i=1}^N (\mathbf{w}_y^T(\mathbf{y}_i-\mu_y))^2}} \quad (2)$$

where *projection coefficient* $\pi_{\mathbf{w}_x}(\mathbf{x}) := \arg\min_{t\in\mathbf{R}} \mathrm{d}(t\mathbf{w}_x + \mu_x, \mathbf{x})^2$.

CCA on Manifolds: Basic Operations

Operation	Subtraction	Addition	Distance	Mean	Covariance
Euclidean	$\overrightarrow{x_ix_j} = x_j - x_i$	$x_i + \overrightarrow{x_jx_k}$	$\lVert\overrightarrow{x_ix_j}\rVert$	$\sum_{i=1}^n \overrightarrow{\bar{x}x_i} = 0$	$\mathbb{E}[(x_i-\bar{x})(x_i-\bar{x})^T]$
Riemannian	$\overrightarrow{x_ix_j} = \mathrm{Log}(x_i, x_j)$	$\mathrm{Exp}(x_i, \overrightarrow{x_jx_k})$	$\lVert\mathrm{Log}(x_i,x_j)\rVert_{x_i}$	$\sum_{i=1}^n \mathrm{Log}(\bar{x}, x_i) = 0$	$\mathbb{E}[\mathrm{Log}(\bar{x},x_i)\mathrm{Log}(\bar{x},x_i)^T]$

$$\pi_{\mathbf{w}_x}(\mathbf{x}) := \arg\min_{t\in\mathbb{R}} \mathrm{d}(\mathrm{Exp}(\mu_x, t\mathbf{w}_x), \mathbf{x})^2 \quad (3)$$



CCA on manifolds

Input: $x_1,\dots,x_N \in \mathcal{M}$, $y_1,\dots,y_N \in \mathcal{M}$
Output: $\mathbf{w}_x \in T_{\mu_x}\mathcal{M}$, $\mathbf{w}_y \in T_{\mu_y}\mathcal{M}$ (submanifolds), $t_i, u_i \in \mathbf{R}$ (projection coefficients)

$$\rho_{\mathbf{x},\mathbf{y}} = \max_{\mathbf{w}_x,\mathbf{w}_y,\mathbf{t},\mathbf{u}} \frac{\sum_{i=1}^N (t_i-\bar{t})(u_i-\bar{u})}{\sqrt{\sum_{i=1}^N (t_i-\bar{t})^2}\sqrt{\sum_{i=1}^N (u_i-\bar{u})^2}}$$

$$\text{s.t.} \quad t_i = \arg\min_{t_i\in(-\epsilon,\epsilon)} \lVert\mathrm{Log}(\mathrm{Exp}(\mu_x, t_i\mathbf{w}_x), \mathbf{x}_i)\rVert^2, \forall i \in \{1,\dots,N\}$$
$$u_i = \arg\min_{u_i\in(-\epsilon,\epsilon)} \lVert\mathrm{Log}(\mathrm{Exp}(\mu_y, u_i\mathbf{w}_y), \mathbf{y}_i)\rVert^2, \forall i \in \{1,\dots,N\} \quad (4)$$

Formulation with first order optimality conditions

$$\rho(\mathbf{w}_x,\mathbf{w}_y) = \max_{\mathbf{w}_x,\mathbf{w}_y,\mathbf{t},\mathbf{u}} f(\mathbf{t},\mathbf{u}) \text{ s.t. } \nabla_{t_i} g(t_i,\mathbf{w}_x) = 0, \nabla_{u_i} g(u_i,\mathbf{w}_y) = 0, \forall i \in \{1,\dots,N\} \quad (5)$$

$$f(\mathbf{t},\mathbf{u}) := \frac{\sum_{i=1}^N (t_i-\bar{t})(u_i-\bar{u})}{\sqrt{\sum_{i=1}^N (t_i-\bar{t})^2}\sqrt{\sum_{i=1}^N (u_i-\bar{u})^2}}$$

$$g(t_i,\mathbf{w}_x) := \lVert\mathrm{Log}(\mathrm{Exp}(\mu_x, t_i\mathbf{w}_x), \mathbf{x}_i)\rVert^2, \; g(u_i,\mathbf{w}_y) := \lVert\mathrm{Log}(\mathrm{Exp}(\mu_y, u_i\mathbf{w}_y), \mathbf{y}_i)\rVert^2$$

Objective function for CCA on Manifolds

Given a constrained optimization problem $\max f(\mathbf{x})$ s.t. $c_i(\mathbf{x}) = 0, \forall i$, the **augmented Lagrangian method (ALM)** solves a sequence of the following models increasing ν_k.

$$\max f(\mathbf{x}) + \sum_i \lambda_i c_i(\mathbf{x}) - \nu^k \sum_i c_i(\mathbf{x})^2 \quad (6)$$

The augmented Lagrangian formulation for our CCA formulation (5) is

$$\max_{\mathbf{w}_x,\mathbf{w}_y,\mathbf{t},\mathbf{u}} \mathcal{L}_A(\mathbf{w}_x,\mathbf{w}_y,\mathbf{t},\mathbf{u},\lambda^k;\nu^k) = \max_{\mathbf{w}_x,\mathbf{w}_y,\mathbf{t},\mathbf{u}} f(\mathbf{t},\mathbf{u}) + \sum_i^N \lambda_{t_i}^k \nabla_{t_i} g(t_i,\mathbf{w}_x) + \sum_i^N \lambda_{u_i}^k \nabla_{u_i} g(u_i,\mathbf{w}_y) - \frac{\nu^k}{2}\left(\sum_{i=1}^N \nabla_{t_i} g(t_i,\mathbf{w}_x)^2 + \nabla_{u_i} g(u_i,\mathbf{w}_y)^2\right) \quad (7)$$

Iterative algorithm by augmented Lagrangian method

$\mathbf{x}_1,\dots,\mathbf{x}_N \in \mathcal{M}_x$, $\mathbf{y}_1,\dots,\mathbf{y}_N \in \mathcal{M}_y$
Given $\nu^0 > 0$, $\tau^0 > 0$, starting points $(\mathbf{w}_x^0, \mathbf{w}_y^0, \mathbf{t}^0, \mathbf{u}^0)$ and λ^0
for $k = 0, 1, 2\dots$ **do**
 Start at $(\mathbf{w}_x^k, \mathbf{w}_y^k, \mathbf{t}^k, \mathbf{u}^k)$
 Find an approximate minimizer $(\mathbf{w}_x^k, \mathbf{w}_y^k, \mathbf{t}^k, \mathbf{u}^k)$ of $\mathcal{L}_A(\cdot, \lambda^k; \nu^k)$, and terminate when $\lVert\nabla\mathcal{L}_A(\mathbf{w}_x^k, \mathbf{w}_y^k, \mathbf{t}^k, \mathbf{u}^k, \lambda^k; \nu^k)\rVert \le \tau^k$
 if a convergence test is satisfied **then**
  Stop with approximate feasible solution
 end if
 $\lambda_{t_i}^{k+1} = \lambda_{t_i}^k - \nu^k \nabla_{t_i} g(t_i, \mathbf{w}_x), \forall i$ and $\lambda_{u_i}^{k+1} = \lambda_{u_i}^k - \nu^k \nabla_{u_i} g(u_i, \mathbf{w}_y), \forall i$
 Choose new penalty parameter $\nu^{k+1} \ge \nu^k$
 Set starting point for the next iteration
 Select tolerance τ^{k+1}
end for

Single path algorithm with approximate projection

$$\Pi_S(\mathbf{x}) \approx \mathrm{Exp}(\mu, \sum_{i=1}^d \mathbf{v}_i \langle \mathbf{v}_i, \mathrm{Log}(\mu, \mathbf{x})\rangle_\mu) \quad (8)$$

Input $X_1,\dots,X_N \in \mathcal{M}_y$, $Y_1,\dots,Y_N \in M_y$
Compute intrinsic mean μ_x, μ_y of $\{X_i\}, \{Y_i\}$
Compute $X_i' = \mathrm{Log}(\mu_x, X_i)$, $Y_i' = \mathrm{Log}(\mu_y, Y_i)$
Transform (using **group action**) $\{X_i'\}, \{Y_i'\}$ to the $T_I\mathcal{M}_x$, $T_I\mathcal{M}_y$
Perform CCA between $T_I\mathcal{M}_x$, $T_I\mathcal{M}_y$ and get axes $W_a \in T_I\mathcal{M}_x$, $W_b \in T_I\mathcal{M}_y$
Transform (using **group action**) W_a, W_b to $T_{\mu_x}\mathcal{M}_x$, $T_{\mu_y}\mathcal{M}_y$

Why group action is needed?

- Transformations to the Identity of SPD(n) for more accurate projection
- Group action is equivalent to the parallel transport from $T_p\mathcal{M}$ to $T_I\mathcal{M}$ on SPD(n)
- Group action is computationally more efficient

Theorem

On SPD manifold, let $\Gamma_{p\to I}(w)$ denote the parallel transport of $w \in T_p\mathcal{M}$ along the geodesic from $p \in \mathcal{M}$ to $I \in \mathcal{M}$. The parallel transport is equivalent to group action by $p^{-1/2}wp^{-T/2}$, where the inner product $\langle u, v\rangle_p = \mathrm{tr}(p^{-1/2}up^{-1}vp^{-1/2})$.

Synthetic Experiments: Riemannian vs. Euclidean CCA

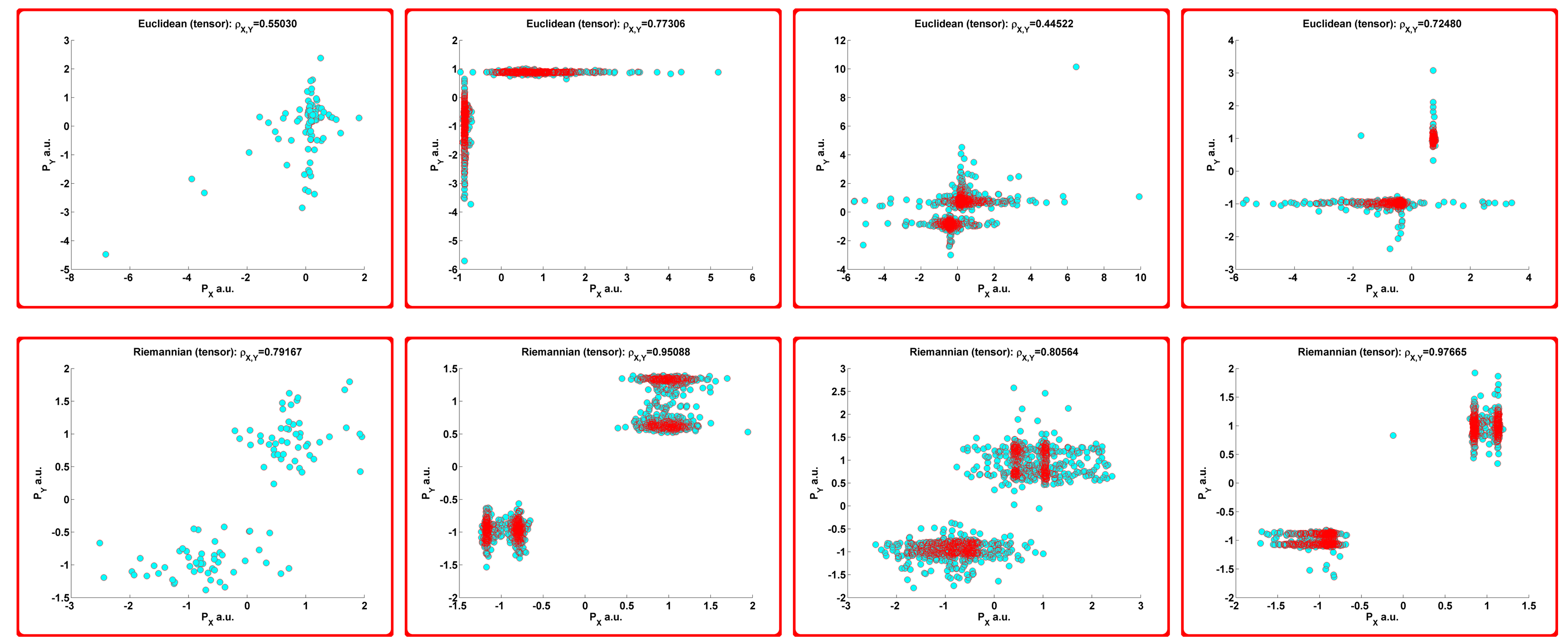


Figure : Improvements in $\rho_{x,y}$ using Riemannian CCA. Each column represents a synthetic experiment with a specific set of $\{\mu_{x_j}, \epsilon_{x_j}; \mu_{y_j}, \epsilon_{y_j}\}$. The first column has 100 samples while the other columns have 1000 samples.

Neuroimaging Experiments: CCA for Multi-modal Analysis

Task: Detect gender and age effects on white and gray matter interactions. The white matter is characterized by diffusion tensors (Y_{DTI}) while the gray matter by Cauchy deformation tensors ($X_{\mathrm{T1W}} = \sqrt{J^TJ}$).

$$Y_{\mathrm{DTI}} = \beta_0 + \beta_1 \mathrm{Gender} + \beta_2 X_{\mathrm{T1W}} + \beta_3 X_{\mathrm{T1W}} \cdot \mathrm{Gender} + \varepsilon,$$
$$Y_{\mathrm{DTI}} = \beta_0' + \beta_1' \mathrm{AgeGroup} + \beta_2' X_{\mathrm{T1W}} + \beta_3' X_{\mathrm{T1W}} \cdot \mathrm{AgeGroup} + \varepsilon,$$

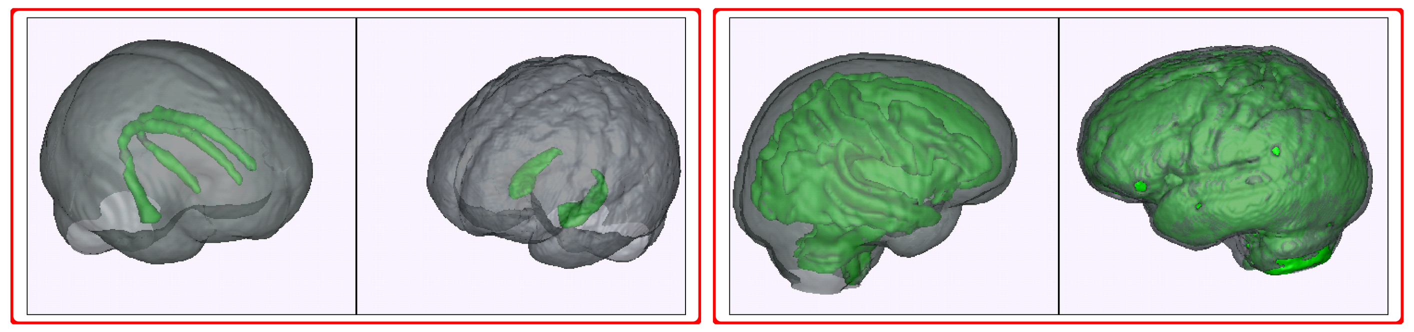


Figure : Regions of interest in which the interaction models are tested. From left to right, cingulum bundle (DTI), hippocampus (T1W), entire white matter (DTI) and entire gray matter (T1W).

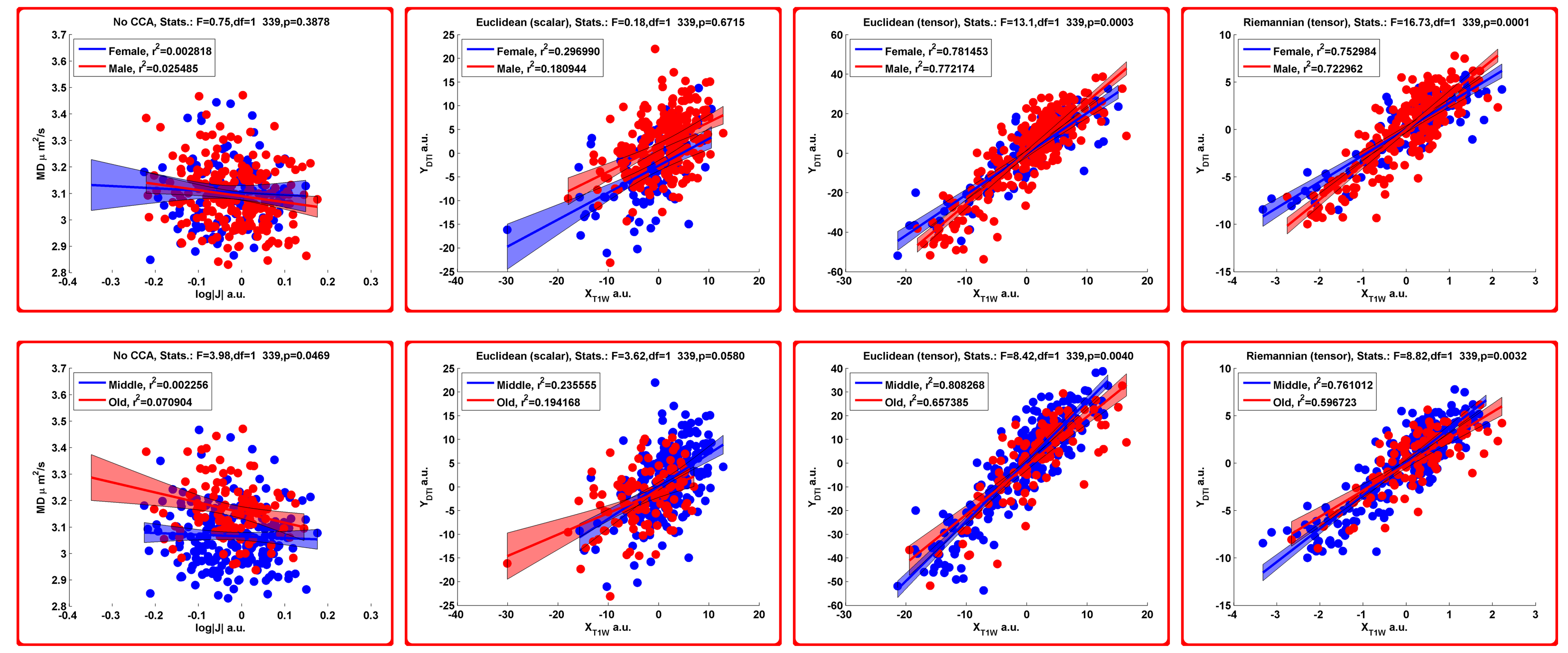
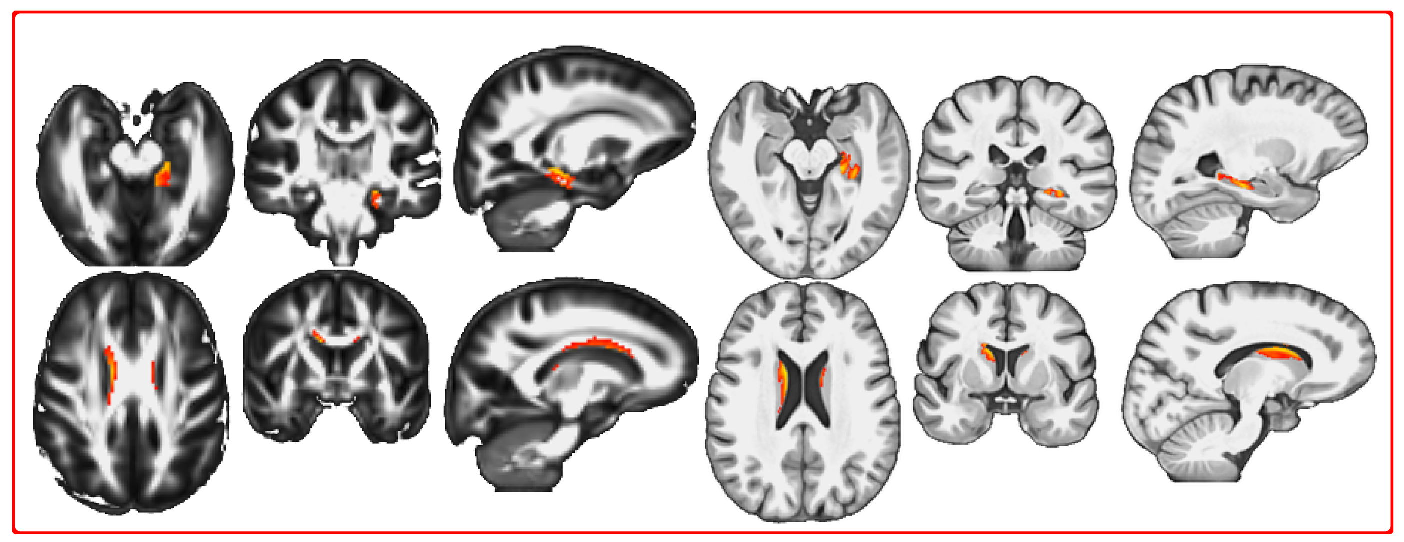


Figure : Riemannian CCA weight vectors for DTI ($\mathbf{w}_y$) and T1W ($\mathbf{w}_x$) when using the cingulum (left) and hippocampal (right) ROIs. Bottom row shows the same when using entire white and gray matter ROIs.



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