Multivariate General Linear Models (MGLM) on Riemannian Manifolds

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http://pages.cs.wisc.edu/∼hwkim/projects/riem-mglm/

The Motivating Problem

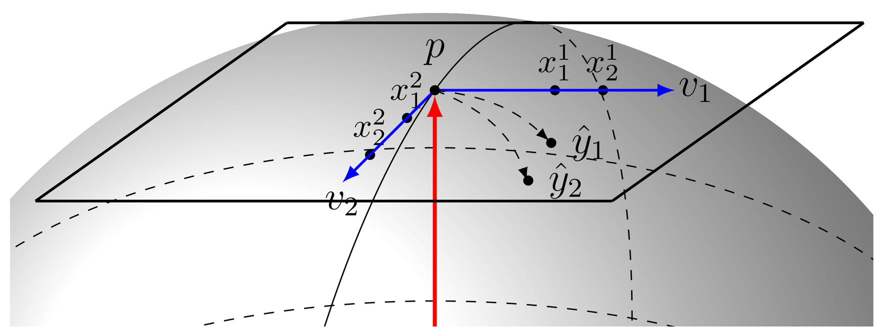
- General linear model (GLM) based statistical analysis of images where voxel-wise measurement is manifold valued.
- Identify how the relationships of voxels **differ** across clinically disparate groups, *while controlling for one or more nuisance variables*.

What is new?

- Fletcher (IJCV, 2013) provides methods for geodesic regression for $f : \mathbf{R} \to \mathcal{M}$.
- Extended for regressing $f : \mathbf{R} \to S^\infty$ by Du et al. (NeuroImage, 2014).
- This paper: multivariate multiple linear regression on manifold data, $f : \mathbf{R}^n \to \mathcal{M}$.
- The same general recipe works for both cases: $y \in \mathrm{SPD}(3)$ for diffusion tensor images (DTI) and $y \in S^\infty$ for orientation distribution functions (ODFs).
- **Main technical highlight:** Exact variational framework for $\mathbf{R}^n$ where $n > 1$ as well as a faster (but approximate) Log-Euclidean framework for optimization.

Regression on Manifolds: Basic Operations

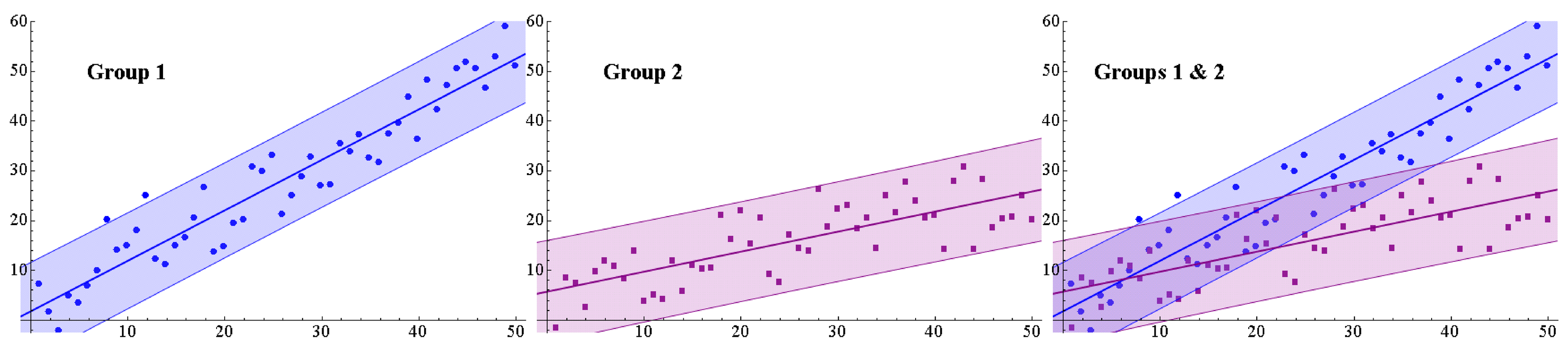
Operation	Subtraction	Addition	Distance	Mean	Covariance
Euclidean	$\overrightarrow{x_i x_j} = x_j - x_i$	$x_i + \overrightarrow{x_j x_k}$	$\lVert\overrightarrow{x_i x_j}\rVert$	$\sum_{i=1}^n \overrightarrow{\bar{x} x_i} = 0$	$\mathbb{E}\left[(x_i - \bar{x})(x_i - \bar{x})^T\right]$
Riemannian	$\overrightarrow{x_i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



v^1, v^2 are tangent vectors. Each entry of independent variables $(x^1, x^2) \in \mathbf{R}^2$, is multiplied by v_1 and v_2 respectively in $T_p\mathcal{M}$. Here, x_i^j denotes j-th entry of the i-th instance.

Multivariate General Linear Models (MGLM)

High level goal: Identify relationship of response variables with covariates; assess statistical significance of differences of regression coefficients across disparate groups.



Euclidean and Riemannian MGLMs

Euclidean

$$y = \alpha + \beta^1 x^1 + \beta^2 x^2 + \ldots + \beta^n x^n + \epsilon,$$

where $x \in \mathbf{R}^n$ and $y \in \mathbf{R}^m$ and $\epsilon \sim \frac{1}{\sqrt{(2\pi)^m|\Sigma|}} \exp\left(-\frac{1}{2}(y-\mu)^T \Sigma^{-1} (y-\mu)\right)$.

Riemannian

$$y = \mathrm{Exp}\left(\mathrm{Exp}\left(p, v^1 x^1 + v^2 x^2 + \ldots + v^n x^n\right), \epsilon\right),$$

where $\epsilon \sim \frac{1}{Z(\mu,\sigma)} \exp\left(-\frac{d(y,\mu)^2}{2\sigma^2}\right)$ and $Z(\mu,\sigma) = \int_{\mathcal{M}} \exp\left(-\frac{d(y,\mu)^2}{2\sigma^2}\right)$ is the normalization factor.

Objective Function for MGLMs on Manifolds

Input: $x_1, \ldots, x_N \in \mathbf{R}^n$, $y_1, \ldots, y_N \in \mathcal{M}$
Output: $p \in \mathcal{M}$ (the anchor point), $v^1, \ldots, v^n \in T_p\mathcal{M}$

$$\min_{p \in \mathcal{M}, \forall j, v^j \in T_p\mathcal{M}} \frac{1}{2} \sum_{i=1}^N d(\mathrm{Exp}(p, Vx_i), y_i)^2, \text{ where } Vx_i := \sum_{j=1}^n v^j x_i^j$$

High Level Summary of Optimization Scheme

Main decision variables to estimate: p and $v^1, \ldots, v^n$

$$E(p, v) = \frac{1}{2}\sum_i \langle \mathrm{Log}(\hat{y}_i, y_i), \mathrm{Log}(\hat{y}_i, y_i)\rangle_{\hat{y}_i} = \frac{1}{2}\sum_i \langle \Gamma_{\hat{y}_i \to p}\mathrm{Log}(\hat{y}_i, y_i), \Gamma_{\hat{y}_i \to p}\mathrm{Log}(\hat{y}_i, y_i)\rangle_p, \quad (1)$$

where $\hat{y}_i = \mathrm{Exp}(p, \sum_j x_i^j v^j)$. The model in tangent space $T_p\mathcal{M}$ is given as

$$\min_{p, v} E^\prime(p^\prime, v) := \min_{p^\prime, v} \frac{1}{2}\sum_i \lVert (\sum_j v^j x_i^j + p^\prime) - y_i^\prime \rVert^2 \quad (2)$$

Procedure: Given a current estimate of p and V, first update p by calculating error in $\hat{y}$ followed by a parallel transport to p. Same procedure for V but slightly more involved (involves a gradient projection type step). All details in the paper.

Optimization Algorithms

Exact Variational Method

Initialize p, v, α, α_{max} and center x
while termination condition **do**
  $p_{new} = \mathrm{Exp}(p, -\alpha \nabla_p E)$
  $V_{new} = \Gamma_{p \to p_{new}}(V - \alpha \nabla_V E)$
  if $E(p_{new}, V_{new}) < E(p, V)$ **then**
    $V \leftarrow V_{new}$ and $P \leftarrow P_{new}$
    $\alpha = \min(2\alpha, \alpha_{max})$
  else
    $\alpha = \alpha/2$
  end if
end while

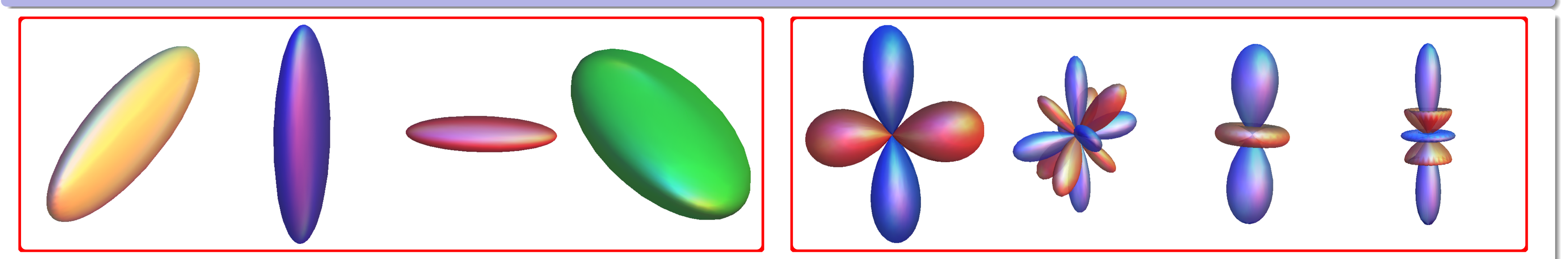
Faster Log-Euclidean Approximation

- Compute $x_i^\prime = x_i - \bar{x}$, ▷ center x
- Compute Karcher mean $\bar{y}$ of $\{y_i\}_{i=1}^n$, ▷ $p^* \approx \bar{y}$
- Compute $y_i^\prime = \mathrm{Log}(\bar{y}, y_i)$
- Parallel transport $y_i^\prime$ from $T_{\bar{y}}\mathcal{M}$ to $T_I\mathcal{M}$
- $\boldsymbol{V} = Y^\prime X^{\prime T}(X^\prime X^{\prime T})^{-1}$, ▷ $\boldsymbol{V}^* \approx \boldsymbol{V}$
- Parallel transport $\boldsymbol{V}$ from $T_I\mathcal{M}$ to $T_{\bar{y}}\mathcal{M}$

Proposition

Let $Y = \{y_1, \ldots, y_N\}$ be a subset of a manifold $\mathcal{M}$. Suppose that Y is in a sufficiently small open cover $\mathcal{B}$ such that the exponential and logarithm maps are bijections. Suppose that all $y \in Y$ are on a curve Ω that is the unique geodesic curve between some y_i and y_j in Y. Then there exists $\bar{y}$ in Ω such that $\sum_{y \in Y} Log_{\bar{y}} y = 0$ (the first order condition for Karcher mean).
Further, if $\bar{y}$ is the unique Karcher mean of $Y \subset \Omega$, and it is obtained in $\mathcal{B}$, then $\bar{y} \in \Omega$. And for some $v \in T_{\bar{y}}\mathcal{M}$ and each y, there exists $x \in \mathbf{R}$ such that $y = Exp(\bar{y}, vx)$.

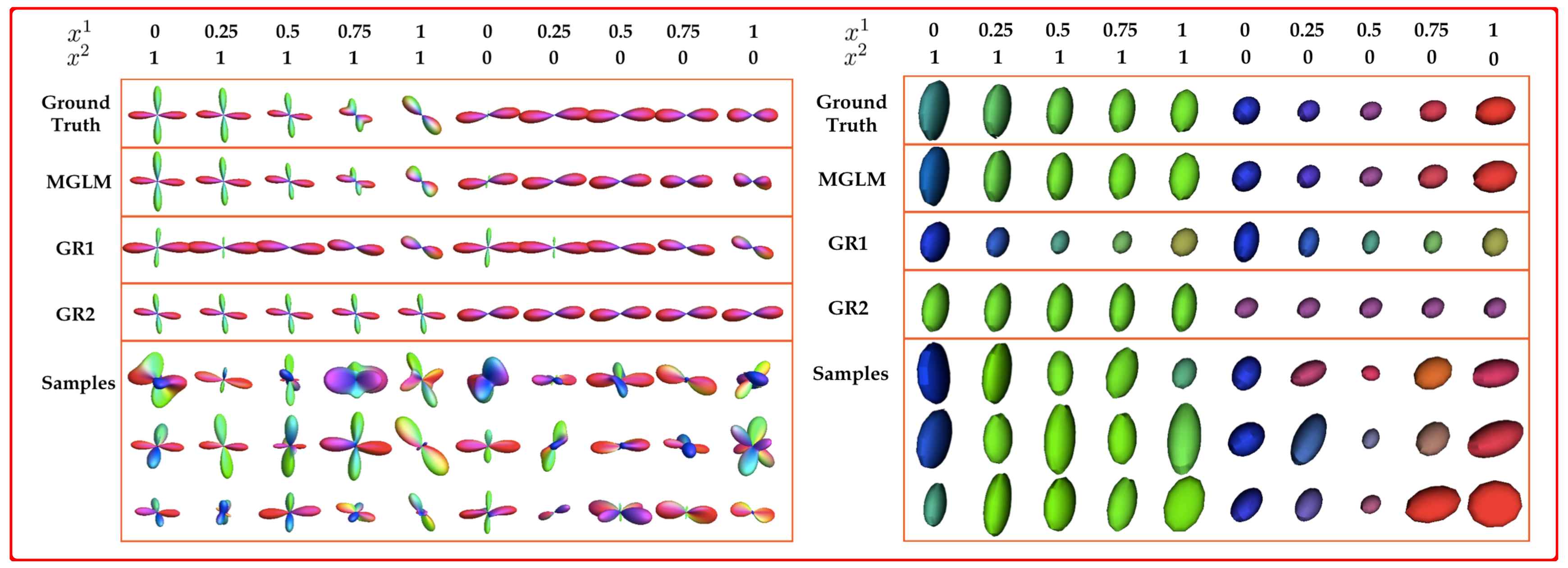
Manifolds in Diffusion Weighted Image Analysis



- Diffusion tensors: Symmetric positive definite (SPD) matrix estimated at each voxel, $\mathrm{SPD}(n)$. Forms a quotient space $\mathrm{GL}(n)/\mathrm{O}(n)$.
- Orientation distributions: Using the square root parameterization, ODFs form a unit Hilbert sphere (S^∞), $\Psi = \{\psi : \mathbb{S}^2 \to \mathbb{R}^+ | \forall s \in \mathbb{S}^2, \psi(s) \geq 0; \int_{s \in \mathbb{S}^2} \psi^2(s) ds = 1\}$.

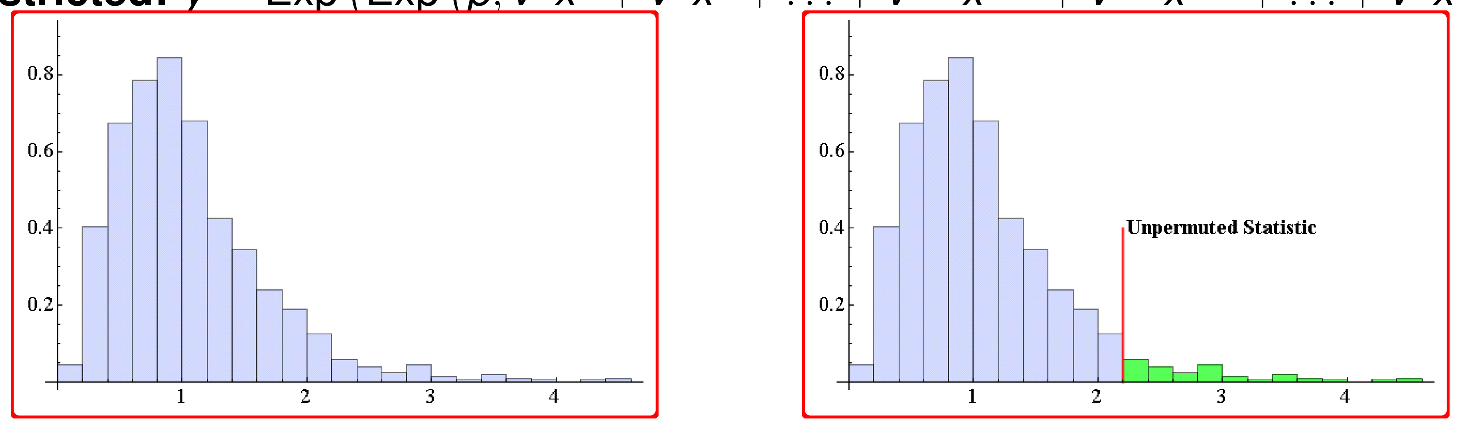
Synthetic Experiments for $f : \mathbf{R}^2 \to \mathcal{M}$

If the response variable y has a dependence on two covariates, x^1 and x^2, a multivariate GLM model is essential; geodesic regression solving for $f : \mathbf{R} \to \mathcal{M}$ will not suffice.



Permutation Testing for Statistical Significance, P-value maps

- **Full:** $y = \mathrm{Exp}\left(\mathrm{Exp}\left(p, v^1x^1 + v^2x^2 + \ldots + v^{i-1}x^{i-1} + v^i x^i + v^{i+1}x^{i+1} + \ldots + v^n x^n\right), \epsilon\right)$
- **Restricted:** $y = \mathrm{Exp}\left(\mathrm{Exp}\left(p, v^1x^1 + v^2x^2 + \ldots + v^{i-1}x^{i-1} + v^{i+1}x^{i+1} + \ldots + v^n x^n\right), \epsilon\right)$



Neuroimaging Experiments: Data and Design

- **Data**: (a) **AD Risk:** Group $\in$ {APOE+, APOE-}, $y \in \mathrm{SPD}(3)$, $N = 343$; (b) **Contemplative Neuroscience (CN):** Group $\in$ {LTM, WLC}, $y \in S^{14}$, $N = 49$.
- **MGLMs**: **Full:** $y = \mathrm{Exp}(p, v^1\mathrm{Group} + v^2\mathrm{Gender} + v^3\mathrm{Age})$; **For group effect:** $y = \mathrm{Exp}(p, v^2\mathrm{Gender} + v^3\mathrm{Age})$; **For age effect:** $y = \mathrm{Exp}(p, v^1\mathrm{Group} + v^2\mathrm{Gender})$

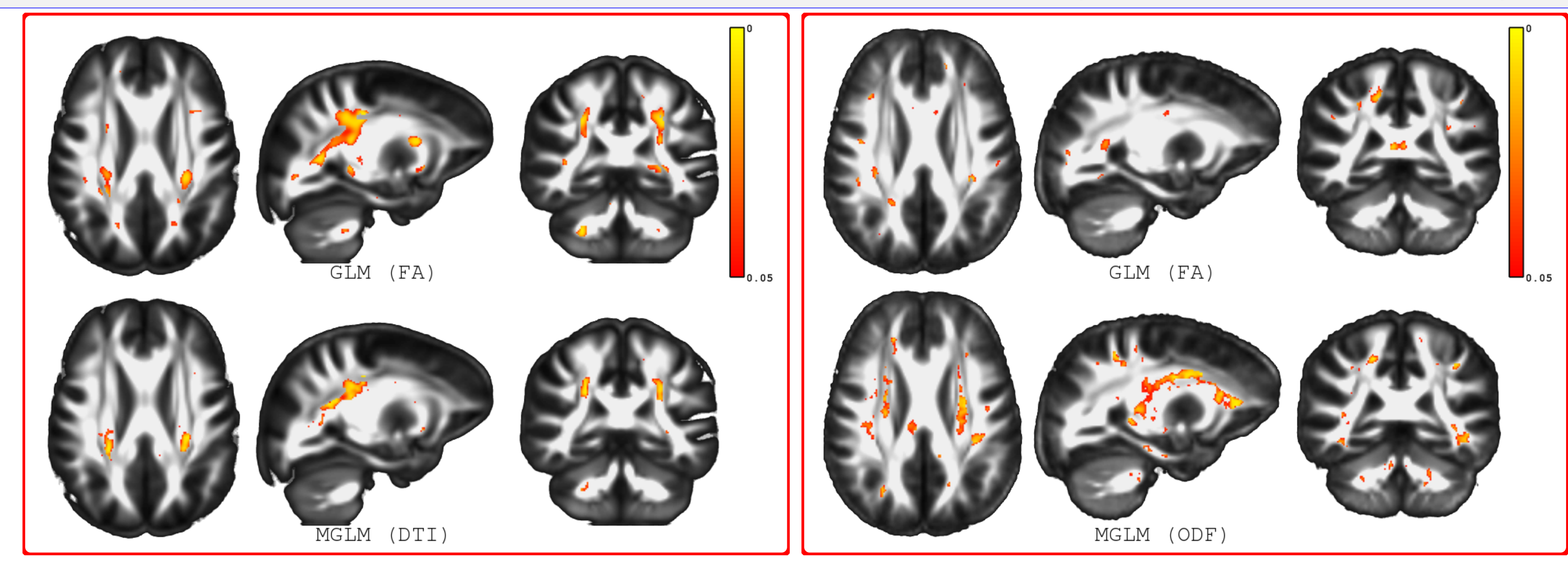


Figure : Effect of Group *controlling for age and gender.* AD study (left); CN study (right).

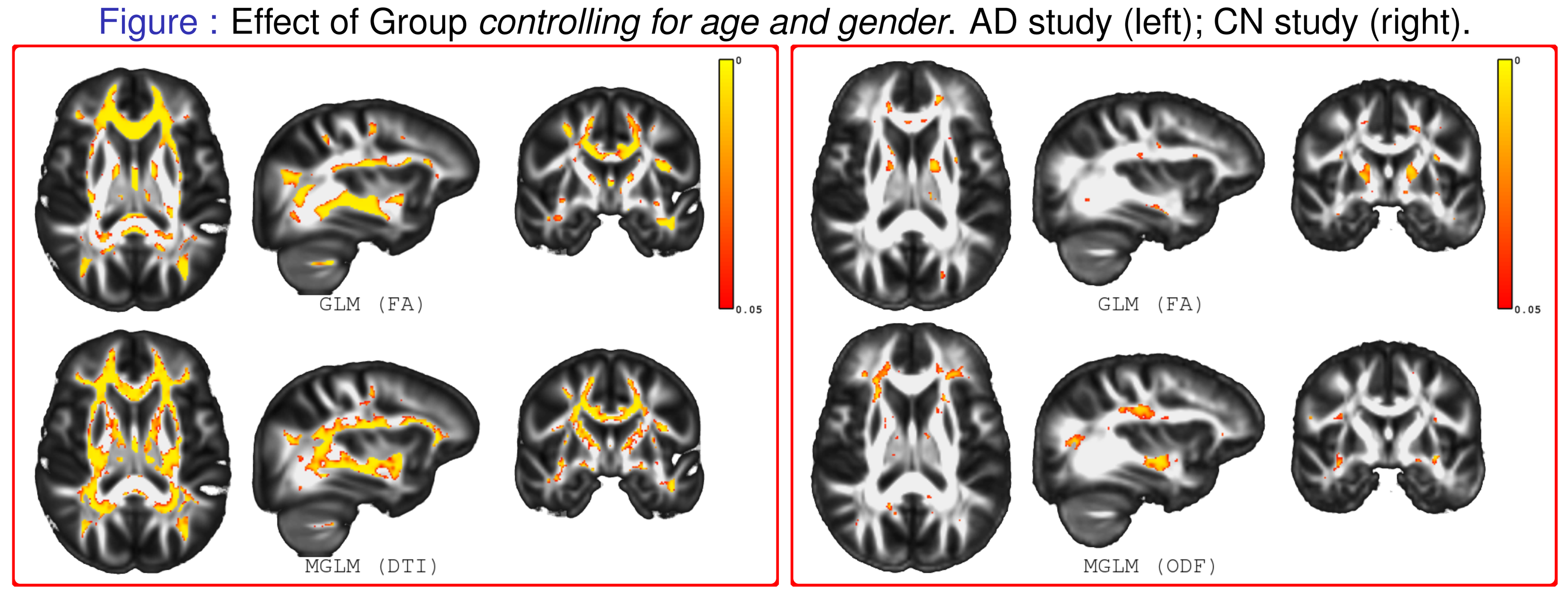


Figure : Effect of Age *controlling for group and gender.* AD study (left). CN study (right).

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