Canonical Correlation Analysis in high dimensions with structured regularization

Elena Tuzhilina

(joint work with Trevor Hastie and Leonardo Tozzi)

Stanford University, Department of Statistics

elenatuz@stanford.edu

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Data

1. brain activations during a task designed to probe working memory
2. behavioral performance measures of cognitive tests assessing memory, executive function, language and processing speed
   (flanker, picture sequence, list sorting, picture vocabulary, oral reading, card sorting, pattern comparison)

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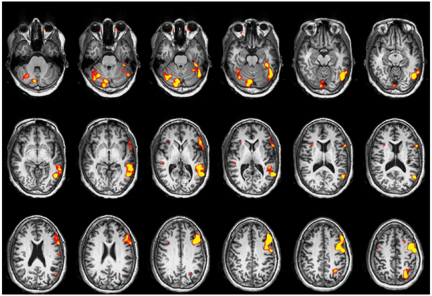

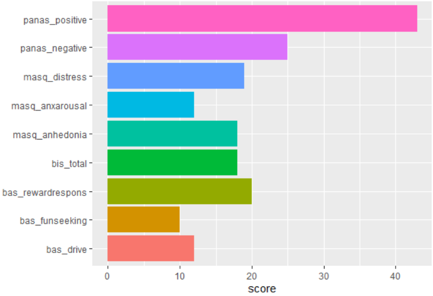

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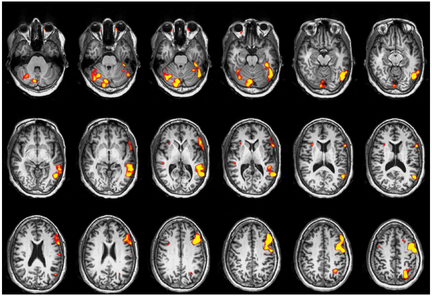
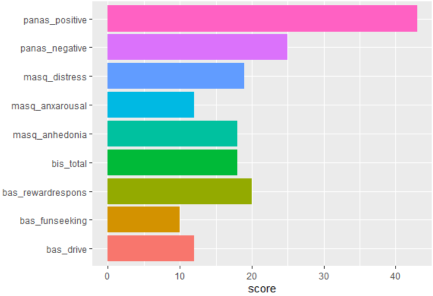
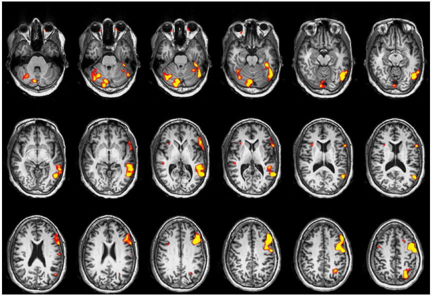


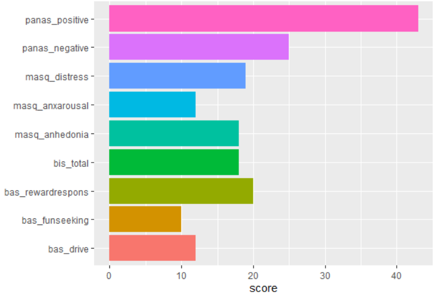


Question: is there any correlation between brain activity and behavioral measures of performance during the cognitive tasks?

Notations



$X \in \mathbb{R}^{n \times p}$ – brain activations



$Y \in \mathbb{R}^{n \times q}$ – behavior test scores

Dimensions:

- $n = 696$ participants
- $p = 91,282$ greyordinates
- $q = 7$ scores

Canonical Correlation Analysis

Goal: given two random vectors $x = (x_1, \ldots, x_p)$ and $y = (y_1, \ldots, y_q)$

$$\text{maximize } \operatorname{cor}(\alpha^T x, \beta^T y) \text{ w.r.t. } \alpha \in \mathbb{R}^p, \beta \in \mathbb{R}^q$$

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- canonical coefficients α and β
- canonical variates $u = \alpha^T x$ and $v = \beta^T y$
- canonical correlation $\rho(\alpha, \beta) = \operatorname{cor}(u, v)$

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Correlation coefficient

$$\rho(\alpha, \beta) = \operatorname{cor}(\alpha^T x, \beta^T y) = \frac{\alpha^T \operatorname{cov}(x, y)\beta}{\sqrt{\alpha^T \operatorname{var}(x)\alpha}\,\sqrt{\beta^T \operatorname{var}(y)\beta}},$$

Canonical Correlation Analysis

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Correlation coefficient

$$\rho(\alpha, \beta) = \frac{\alpha^T \Sigma_{XY} \beta}{\sqrt{\alpha^T \Sigma_{XX} \alpha} \sqrt{\beta^T \Sigma_{YY} \beta}}$$

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CCA optimization problem:

$$\text{maximize } \alpha^T \Sigma_{XY} \beta \text{ w.r.t. } \alpha \in \mathbb{R}^p \text{ and } \beta \in \mathbb{R}^q$$
$$\text{s.t. } \alpha^T \Sigma_{XX} \alpha = 1 \text{ and } \beta^T \Sigma_{YY} \beta = 1$$

Correlation coefficient

$$\rho(\alpha, \beta) = \frac{\alpha^T \Sigma_{XY} \beta}{\sqrt{\alpha^T \Sigma_{XX} \alpha} \sqrt{\beta^T \Sigma_{YY} \beta}}$$

CCA optimization problem:

$$\text{maximize } \widetilde{\alpha}^T \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-\frac{1}{2}} \widetilde{\beta} \text{ w.r.t. } \widetilde{\alpha} \in \mathbb{R}^p \text{ and } \widetilde{\beta} \in \mathbb{R}^q$$
$$\text{s.t. } \|\widetilde{\alpha}\| = 1 \text{ and } \|\widetilde{\beta}\| = 1$$

Correlation coefficient

$$\rho(\alpha, \beta) = \frac{\alpha^T \Sigma_{XY} \beta}{\sqrt{\alpha^T \Sigma_{XX} \alpha} \sqrt{\beta^T \Sigma_{YY} \beta}}$$

CCA optimization problem:

$$\begin{aligned} &\text{maximize } \widetilde{\alpha}^T \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-\frac{1}{2}} \widetilde{\beta} \text{ w.r.t. } \widetilde{\alpha} \in \mathbb{R}^p \text{ and } \widetilde{\beta} \in \mathbb{R}^q \\ &\text{s.t. } \|\widetilde{\alpha}\| = 1 \text{ and } \|\widetilde{\beta}\| = 1 \end{aligned}$$

Solution: via Singular Value Decomposition of $\Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-\frac{1}{2}}$

Correlation Coefficient

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Solution: via Singular Value Decomposition of $\Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-\frac{1}{2}}$

Problem: does not work for $p > n$!

Modified correlation coefficient

$$\rho(\alpha, \beta) = \frac{\alpha^T \Sigma_{XY} \beta}{\sqrt{\alpha^T (\Sigma_{XX} + \lambda_1 I) \alpha} \sqrt{\beta^T \Sigma_{YY} \beta}}$$

RCCA optimization problem:

$$\text{maximize } \alpha^T \Sigma_{XY} \beta \text{ w.r.t. } \alpha \in \mathbb{R}^p \text{ and } \beta \in \mathbb{R}^q$$
$$\text{s.t. } \alpha^T \Sigma_{XX} \alpha = 1,\ \beta^T \Sigma_{YY} \beta = 1 \text{ and } \|\alpha\| \leq t_1$$

Solution: via Singular Value Decomposition of $(\Sigma_{XX} + \lambda I)^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-\frac{1}{2}}$

CCA package

rcc {CCA} R Documentation

Regularized Canonical Correlation Analysis

Description

The function performs the Regularized extension of the Canonical Correlation Analysis to seek correlations between two data matrices when the number of columns (variables) exceeds the number of rows (observations)

Usage

```
rcc(X, Y, lambda1, lambda2)
```

Arguments

`X`	numeric matrix (n * p), containing the X coordinates.
`Y`	numeric matrix (n * q), containing the Y coordinates.
`lambda1`	Regularization parameter for X
`lambda2`	Regularization parameter for Y

Details

When the number of columns is greater than the number of rows, the matrice X'X (and/or Y'Y) may be ill-conditioned. The regularization allows the inversion by adding a term on the diagonal.

Value

A list containing the following components:

`corr`	canonical correlations
`names`	a list containing the names to be used for individuals and variables for graphical outputs
`xcoef`	estimated coefficients for the 'X' variables as returned by `cancor()`
`ycoef`	estimated coefficients for the 'Y' variables as returned by `cancor()`
`scores`	a list returned by the internal function comput() containing individuals and variables coordinates on the canonical variates basis.

Author(s)

Sébastien Déjean, Ignacio González

CCA package

```
library(CCA)
rcc(X = activation, Y = behavior, lambda1 = 10, lambda2 = 0)
```

```
Error: cannot allocate vector of size 62.1 Gb
Traceback:

1. rcc(X = activation, Y = behavior, lambda1 = 10, lambda2 = 0)
2. var(X, na.rm = TRUE, use = "pairwise")
```

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Traceback:

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2. var(X, na.rm = TRUE, use = "pairwise")
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```
"rcc" <-
function (X, Y, lambda1, lambda2)
{
    Xnames <- dimnames(X)[[2]]
    Ynames <- dimnames(Y)[[2]]
    ind.names <- dimnames(X)[[1]]
    Cxx <- var(X, na.rm = TRUE, use = "pairwise") + diag(lambda1,
        ncol(X))
    Cyy <- var(Y, na.rm = TRUE, use = "pairwise") + diag(lambda2,
        ncol(Y))
    Cxy <- cov(X, Y, use = "pairwise")
    res <- geigen(Cxy, Cxx, Cyy)
    names(res) <- c("cor", "xcoef", "ycoef")
    scores <- comput(X, Y, res)
    return(list(cor = res$cor, names = list(Xnames = Xnames,
        Ynames = Ynames, ind.names = ind.names), xcoef = res$xcoef,
        ycoef = res$ycoef, scores = scores))
}
```

CCA package

```r
library(CCA)
rcc(X = activation, Y = behavior, lambda1 = 10, lambda2 = 0)
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"rcc" <-
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}
```

$$C_{XX} = \boxed{p \times p}$$

$$C_{YY} = \boxed{q \times q}$$

$$C_{XY} = \boxed{p \times q}$$

Problem: C_{XX}, C_{XY} are large for $p \gg n$

Kernel trick

Goal: find a linear transformation such that RCCA for (X, Y) is equivalent to RCCA for (R, Y) and

$$V = \boxed{p \times n} \qquad R = XV = \boxed{n \times p}\ \boxed{p \times n} = \boxed{n \times n}$$

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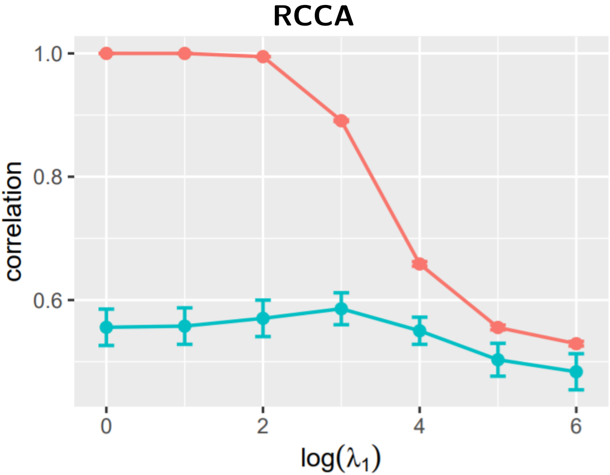
$$V = \boxed{p \times n} \qquad R = XV = \boxed{n \times p}\,\boxed{p \times n} = \boxed{n \times n}$$

Solution:

1. $X = UDV^T = \boxed{n \times n}\,\boxed{n \times n}\,\boxed{n \times p}$
2. set $R = XV = UD$ and solve RCCA problem for $(R, Y) \Longrightarrow$ canonical coefficients α_R, β_R
3. apply inverse transformation $\alpha_X = V\alpha_R$ and $\beta_X = \beta_R$
4. the variates stay the same $v_R = R\alpha_R = X\alpha_X = v_X$ and $u_R = u_X$

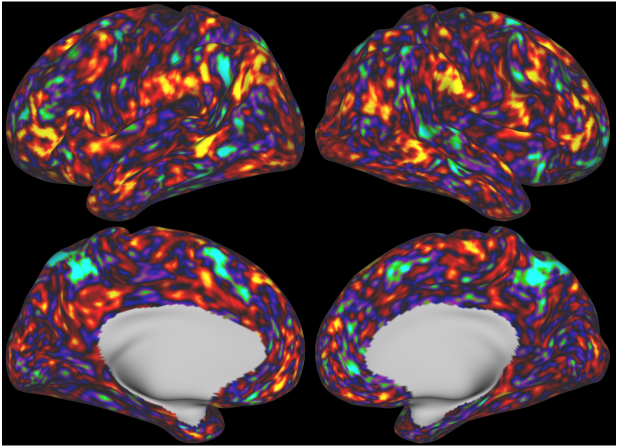
Brain data: RCCA best model



Best:
$\lambda_1 = 1000$
$\rho = 0.59$

Brain data: RCCA best model

RCCA



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Brain regions

Motivation: brain features come in groups (aka brain regions). How to take into account the group structure?

Grouped structure

Notations:

- $K = 379$ groups
- $p_k = \#$ features in group k
- X_k – set of features in group k
- α_k – set of coefficients in group k

$$\alpha = (\underbrace{\alpha_1}_{p_1}, \dots, \underbrace{\alpha_K}_{p_K}) \text{ and } X = (\underbrace{X_1}_{p_1}, \dots, \underbrace{X_K}_{p_K})$$

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Assumptions:

1. group homogeneity
$$\alpha_k \approx \bar{\alpha}_k$$
2. sparsity on a group level
$$\bar{\alpha}_k \approx 0$$

$$\alpha = (\underbrace{\alpha_1}_{p_1}, \dots, \underbrace{\alpha_K}_{p_K}) \text{ and } X = (\underbrace{X_1}_{p_1}, \dots, \underbrace{X_K}_{p_K})$$

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GRCCA optimization problem:

$$\text{maximize } \alpha^T \Sigma_{XY} \beta \text{ w.r.t. } \alpha \in \mathbb{R}^p \text{ and } \beta \in \mathbb{R}^q$$
$$\text{s.t } \alpha^T \Sigma_{XX} \alpha = 1, \ \beta^T \Sigma_{YY} \beta = 1,$$
$$\sum_{k=1}^{K} \|\alpha_k - \bar{\alpha}_k\|^2 \leq t_1 \ \textit{and} \ \sum_{k=1}^{K} p_k \bar{\alpha}_k^2 \leq s_1$$

GRCCA

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$$\sum_{k=1}^{K} \|\alpha_k - \bar{\alpha}_k\|^2 \leq t_1 \textit{ and } \sum_{k=1}^{K} p_k \bar{\alpha}_k^2 \leq s_1$$

Modified correlation coefficient

$$\rho(\alpha, \beta) = \frac{\alpha^T \Sigma_{XY} \beta}{\sqrt{\alpha^T (\Sigma_{XX} + \lambda_1 (I - C) + \mu_1 C)\alpha} \sqrt{\beta^T \Sigma_{YY} \beta}}$$

$$C = \begin{bmatrix} \frac{11^T}{p_1} & 0 & \dots & 0 \\ 0 & \frac{11^T}{p_2} & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \frac{11^T}{p_K} \end{bmatrix}$$

GRCCA vs. RCCA

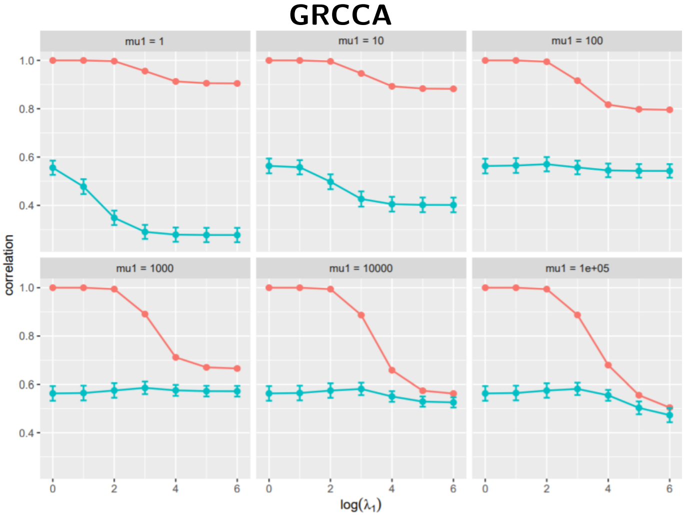
Lemma

GRCCA for (X, Y) is equivalent to RCCA for $(\widetilde{X}, Y)$ where

$$\widetilde{X} = \left(\mathrm{X}_1 - \bar{\mathrm{X}}_1, \sqrt{\frac{p_1\lambda_1}{\mu_1}}\bar{\mathrm{X}}_1, \ldots, \mathrm{X}_K - \bar{\mathrm{X}}_K, \sqrt{\frac{p_K\lambda_1}{\mu_1}}\bar{\mathrm{X}}_K\right)$$

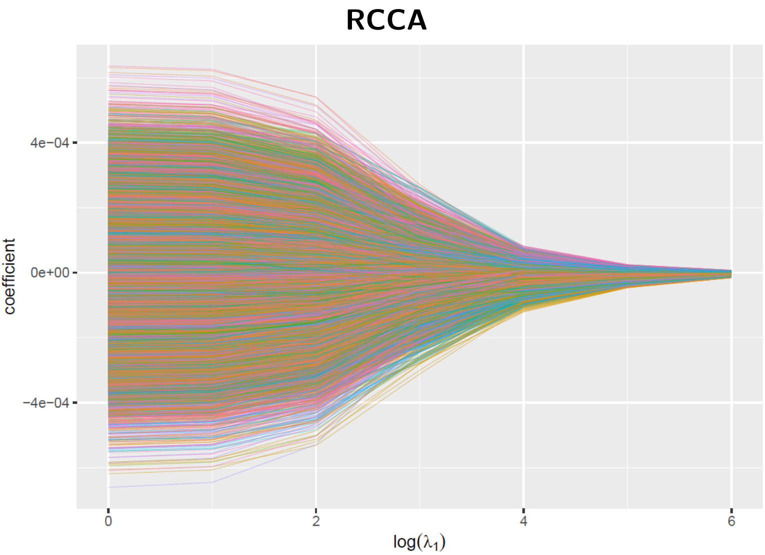
Can use Kernel trick!

Brain data: GRCCA best model



Best:
$\lambda_1 = 1000$
$\mu_1 = 1000$
$\rho = 0.59$

Brain data: coefficient paths



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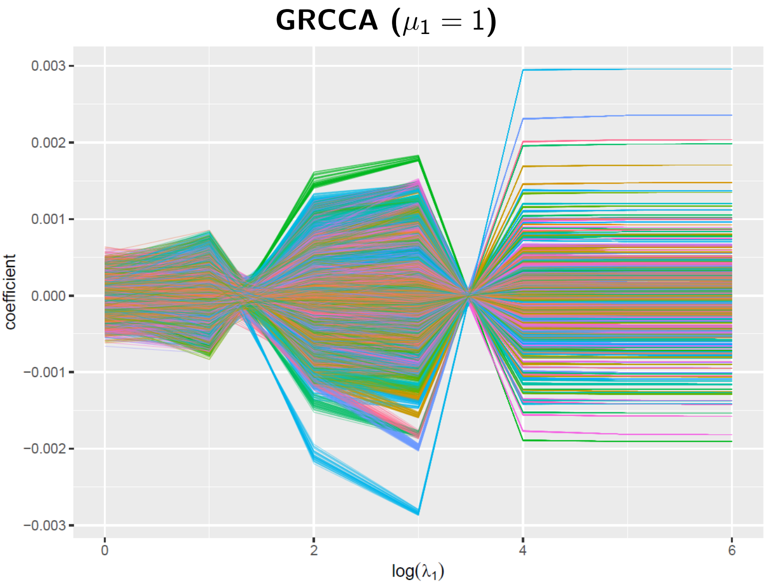

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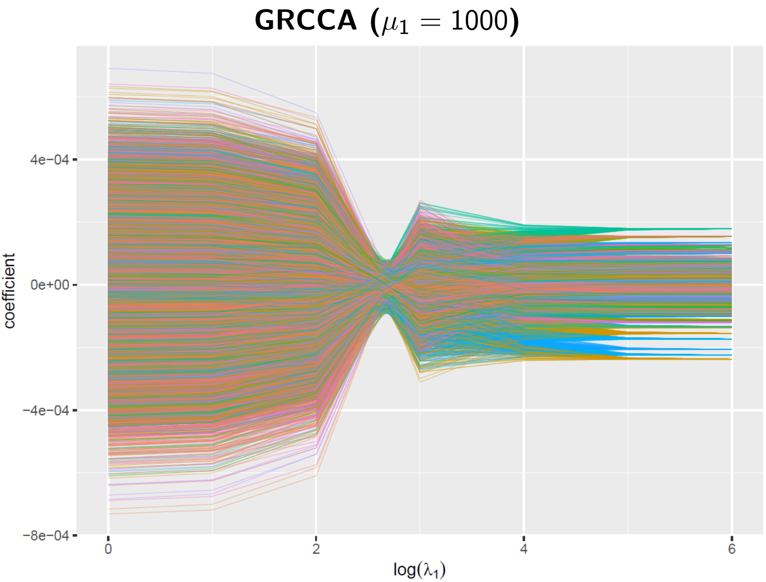

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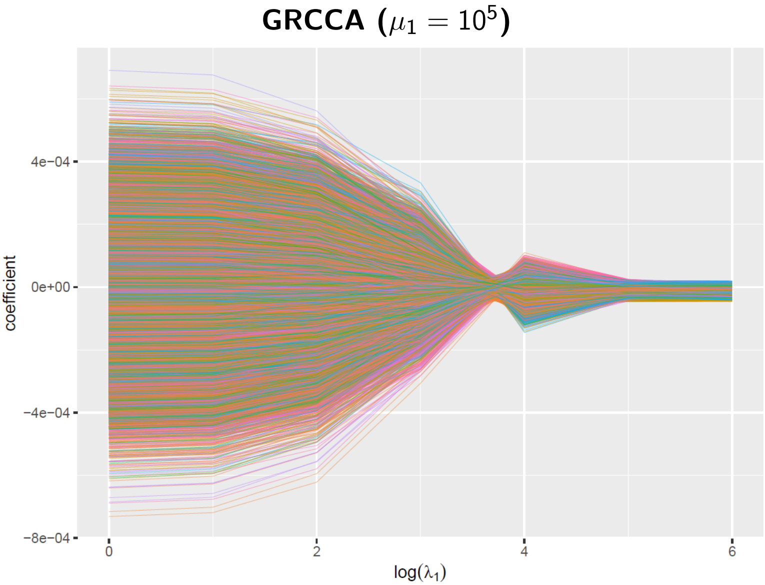
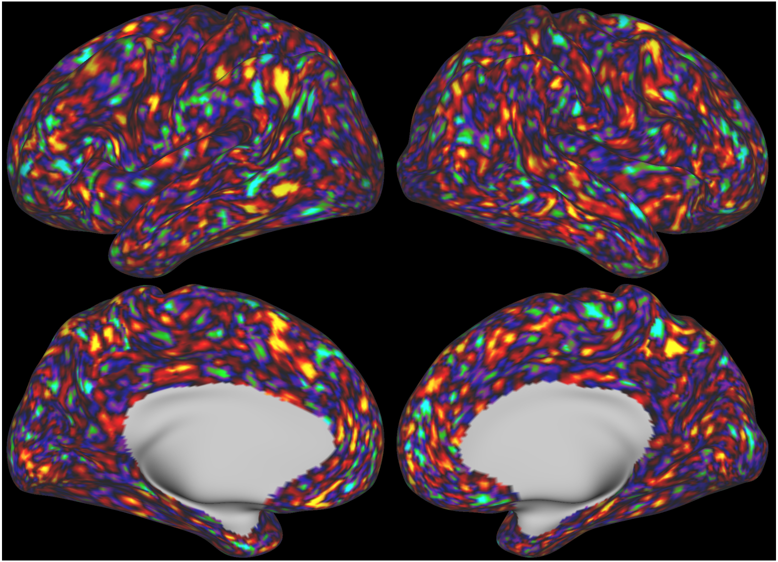


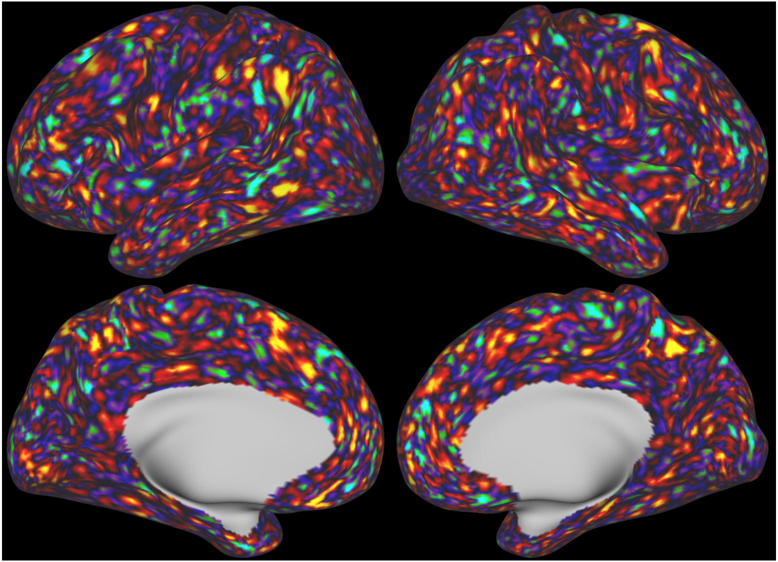
Brain data: coefficient paths

GRCCA ($\lambda_1 = 1, \mu_1 = 1000$)



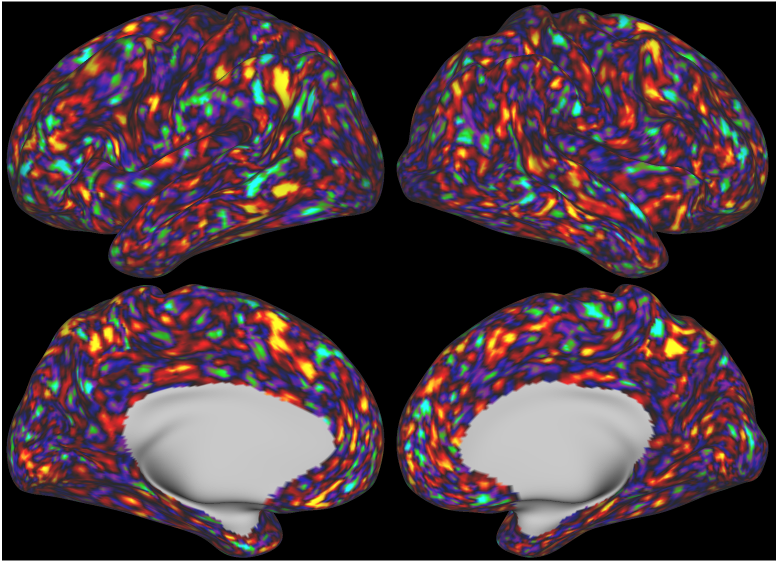
Brain data: coefficient paths

GRCCA ($\lambda_1 = 10, \mu_1 = 1000$)



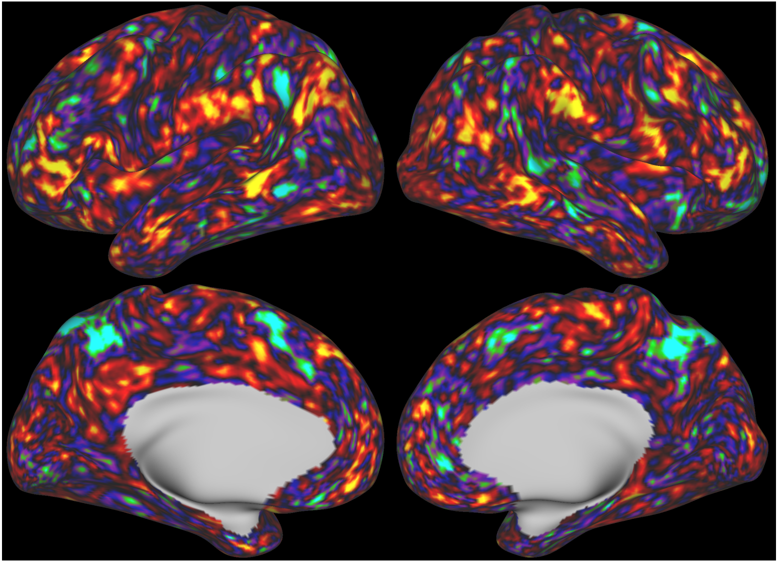
Brain data: coefficient paths

GRCCA ($\lambda_1 = 100, \mu_1 = 1000$)



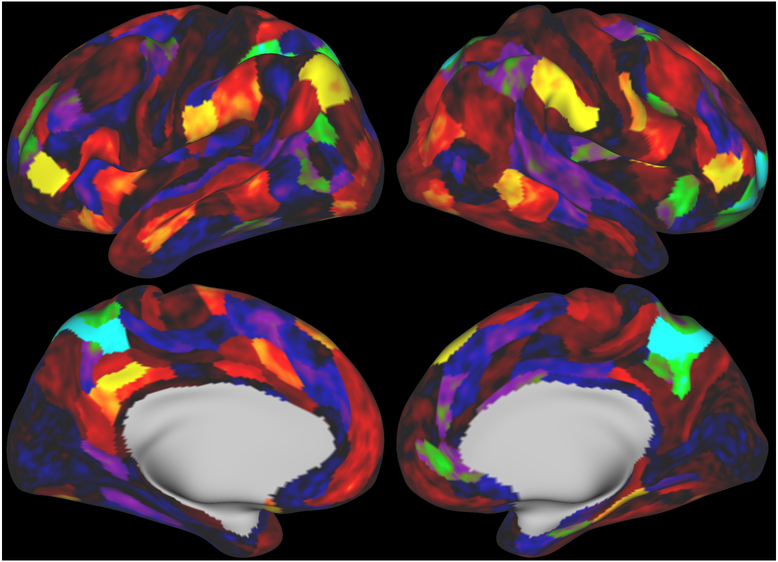
Brain data: coefficient paths

GRCCA ($\lambda_1 = 1000, \mu_1 = 1000$)



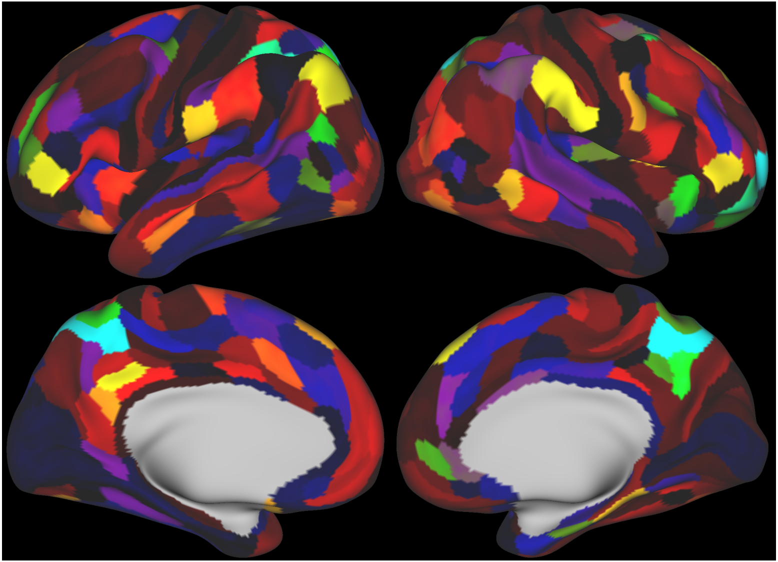
Brain data: coefficient paths

GRCCA ($\lambda_1 = 10^4, \mu_1 = 1000$)



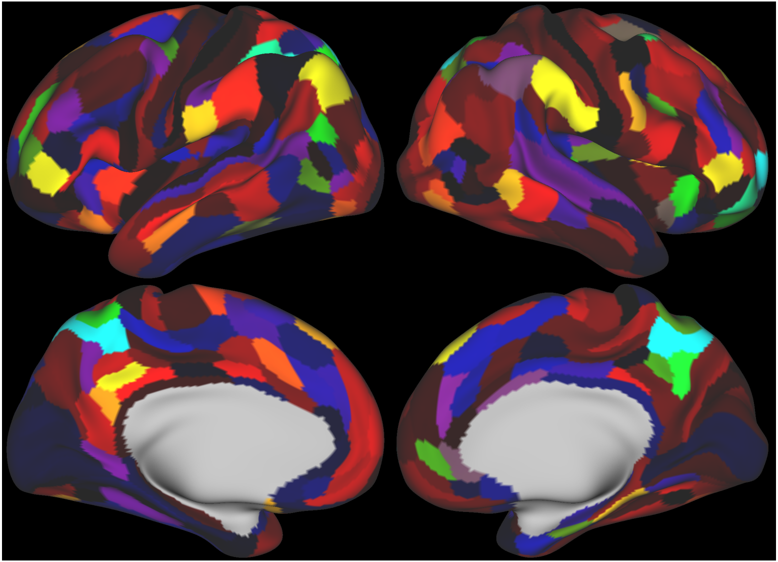
Brain data: coefficient paths

GRCCA $(\lambda_1 = 10^5, \mu_1 = 1000)$



Brain data: coefficient paths

GRCCA ($\lambda_1 = 10^6, \mu_1 = 1000$)



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Thank you for your attention!