Inversion and Canonical Analysis in Functional Neuroimaging

Finn Årup Nielsen

Section for Digital Signal Processing
Department of Mathematical Modelling
Technical University of Denmark
DK-2800 Lyngby, Denmark

Email: fn@imm.dtu.dk
WWW: http://www.imm.dtu.dk/~fn

OVERVIEW

Methods from multivariate analysis in statistics are the same as those used in numerical analysis:

- Singular Value Decomposition (SVD)
- Generalized Singular Value Decomposition (GSVD)
- Regularization

Statisticians in multivariate analysis and inversion researchers do not communicate enough.

Overview

- Multivariate analysis: Canonical Ridge Analysis as a general framework
- Link to generalized singular value decomposition
- Application to functional neuroimaging analysis

ANALYSIS OF FUNCTIONAL NEUROIMAGES

Understanding of the mental process by explorations of functional neuroimages.

Modality	Variable	Initial inversion
PET	Metabolism, ...	Radon
fMRI, fMRSI	"BOLD", ...	Fourier
MEG	Surface magnetism	MUSIC, ECD, ...
EEG	Surface potentials	MUSIC, ...
NIRS, TMS	...	...

fMRI example

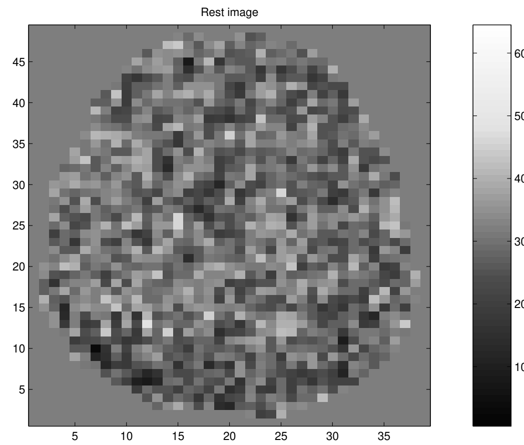


Figure 1: Rest image

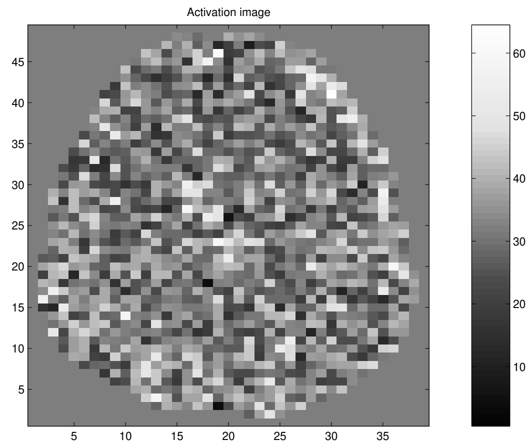


Figure 2: Activation image

DATAMATRIX AND DESIGNMATRIX

- **Datamatrix** — $\mathbf{X}$ — scans × voxels. Large rank deficient data matrix containing functional neuroimaging scans.
- **Designmatrix** — $\mathbf{G}$ — scans × design variables. Small full rank matrix containing description of the scanning protocol: the "paradigm".
  - Activation — Rest.
  - Different conditions. (Cognitive conjunction)
  - Set of basis functions (to model the hemodynamic response, e.g., a Poisson function with different delays.

SINGULAR VALUE DECOMPOSITION

Singular Value Decomposition (SVD), Principal Components Analysis (PCA), Subprofile Scaling Model (SSM).

$$\mathbf{U}\mathbf{\Lambda}\mathbf{V}^{\mathsf{T}} = \mathsf{svd}\left[\mathbf{X}\right] \tag{1}$$

- $\mathbf{V}$ — a large matrix, "right singular vectors". Neuroimaging: "Eigenimages".
- $\mathbf{U}$ — a small matrix, "left singular vectors". Neuroimaging: "Eigensequences".

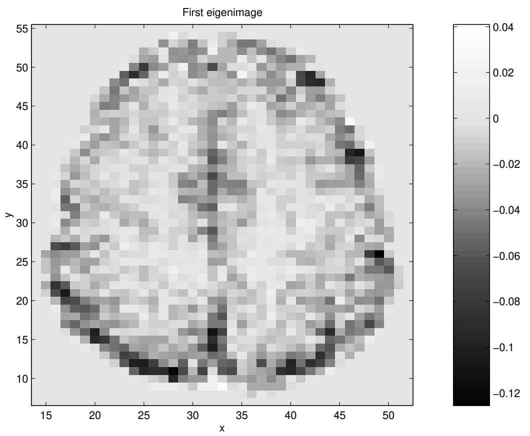


Figure 3: First eigenimage: $\mathbf{v}_1$

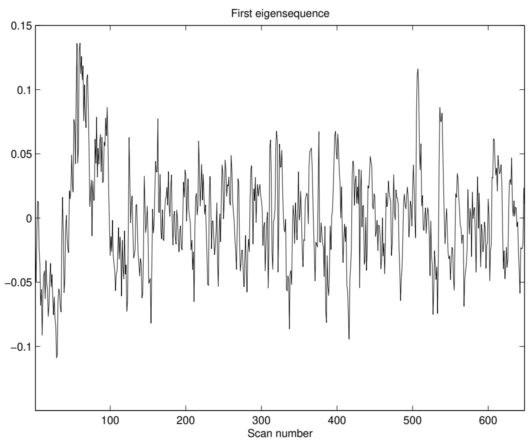


Figure 4: First eigensequence: $\mathbf{u}_1$

- The first singular value components do usually *not* correspond to the design components.
- A design component is not confined to one single singular value component.

USUAL MULTIVARIATE LINEAR ANALYSES

- PLS. Partial Least Square. [McIntosh et al., 1996]

$$\mathbf{U}\boldsymbol{\Lambda}\mathbf{V}^{\mathsf{T}} = \mathsf{svd}\left[\mathbf{G}^{\mathsf{T}}\mathbf{X}\right] \tag{2}$$

- OPLS. Orthonormalized Partial Least Square [Worsley, 1997].

$$\mathbf{U}'\boldsymbol{\Lambda}\mathbf{V}^{\mathsf{T}} = \mathsf{svd}\left[\left(\mathbf{G}^{\mathsf{T}}\mathbf{G}\right)^{-1/2}\mathbf{G}^{\mathsf{T}}\mathbf{X}\right] \tag{3}$$

$$\mathbf{U} = \left(\mathbf{G}^{\mathsf{T}}\mathbf{G}\right)^{-1/2}\mathbf{U}' \tag{4}$$

- CCA. Canonical Correlation Analysis (Canonical Variate Analysis. [Mardia et al., 1979]

$$\mathbf{U}'\boldsymbol{\Lambda}\mathbf{V}'^{\mathsf{T}} = \mathsf{svd}\left[\left(\mathbf{G}^{\mathsf{T}}\mathbf{G}\right)^{-1/2}\mathbf{G}^{\mathsf{T}}\mathbf{X}\left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)^{-1/2}\right] \tag{5}$$

$$\mathbf{U} = \left(\mathbf{G}^{\mathsf{T}}\mathbf{G}\right)^{-1/2}\mathbf{U}' \tag{6}$$

$$\mathbf{V} = \left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)^{-1/2}\mathbf{V}' \tag{7}$$

Problem: $\mathbf{X}$ is rank deficient. It is not possible to invert the covariance matrix $\mathbf{X}^{\mathsf{T}}\mathbf{X}$.

REGULARIZED CANONICAL CORRELATION ANALYSIS

- Perform an initial SVD (or other transformation, e.g., ICA) and truncate (Inversion: TSVD), subset select (statistics) or prune (connectionistics) the singular components and, lastly, pipe the remaining components to CCA: SVD-CCA
- Ridge regularize: Canonical Ridge Analysis
- LASSO, Shrunken, Tikhonov, Total Least Square, ...

- SVD-CCA. Canonical Correlation Analysis with initial Singular Value Decomposition

$$\mathbf{U}^{*}\boldsymbol{\Lambda}^{*}\mathbf{V}^{*\mathsf{T}} = \mathsf{svd}\left[\mathbf{X}\right] \tag{8}$$

$$\mathbf{X}^{*} = \mathbf{U}^{*}_{11}\boldsymbol{\Lambda}^{*} = \mathbf{X}\mathbf{V}^{*}_{11} \tag{9}$$

$$\mathbf{U}'\boldsymbol{\Lambda}\mathbf{V}'^{\mathsf{T}} = \mathsf{svd}\left[\left(\mathbf{G}^{\mathsf{T}}\mathbf{G}\right)^{-1/2}\mathbf{G}^{\mathsf{T}}\mathbf{X}^{*}\left(\mathbf{X}^{*\mathsf{T}}\mathbf{X}^{*}\right)^{-1/2}\right] \tag{10}$$

$$\mathbf{U} = \left(\mathbf{G}^{\mathsf{T}}\mathbf{G}\right)^{-1/2}\mathbf{U}' \tag{11}$$

$$\mathbf{V}^{\#} = \left(\mathbf{X}^{*\mathsf{T}}\mathbf{X}^{*}\right)^{-1/2}\mathbf{V}' \tag{12}$$

$$\mathbf{V} = \mathbf{V}^{*}_{11}\mathbf{V}^{\#} \tag{13}$$

CANONICAL RIDGE ANALYSIS

- CRA. Canonical Ridge Analysis. [Vinod, 1976] [Mardia et al., 1979]

$$\mathbf{U}'\mathbf{\Lambda}\mathbf{V}'^{\mathsf{T}} = \text{svd}\left[\left[\mathbf{G}^{\mathsf{T}}\mathbf{G}\right]^{-1/2}\mathbf{G}^{\mathsf{T}} \ldots \right. \\ \left. \mathbf{X}\left[(1-k_X)\,\mathbf{X}^{\mathsf{T}}\mathbf{X} + k_X\mathbf{I}\right]^{-1/2}\right] \quad (14)$$

$$\mathbf{U} = \left[\mathbf{G}^{\mathsf{T}}\mathbf{G}\right]^{-1/2}\mathbf{U}' \quad (15)$$

$$\mathbf{V} = \left[(1-k_X)\,\mathbf{X}^{\mathsf{T}}\mathbf{X} + k_X\mathbf{I}\right]^{-1/2}\mathbf{V}' \quad (16)$$

  - Extension of ridge regression to CCA.
  - $k_X = 0$ gives ordinary CCA and $k_X = 1$ gives PLS (OPLS). Interpolation between PLS and CCA.
  - $\mathbf{X}^{\mathsf{T}}\mathbf{X}$ invertible.
  - $k_X\mathbf{I}$ could be exchanged with $k_X\mathbf{R}$ with $\mathbf{R}$ as a positive semi-definit matrix: Shrunken estimator (statistics), Tikhonov regularization (inverse).
  - $\mathbf{X}^{\mathsf{T}}\mathbf{X}$ is still a huge matrix.

CRA WITH INITIAL SVD

- SVD-CRA. Canonical Ridge Analysis with Singular Value Decomposition. [Nielsen et al., 1998]

$$\mathbf{U}^* \mathbf{\Lambda}^* \mathbf{V}^{*\mathsf{T}} = \mathsf{svd}\left[\mathbf{X}\right] \tag{17}$$

$$\mathbf{X}^* = \mathbf{U}^* \mathbf{\Lambda}^* = \mathbf{X}\mathbf{V}^* \tag{18}$$

$$\begin{aligned}\mathbf{U}' \mathbf{\Lambda} \mathbf{V}'^{\mathsf{T}} = \quad & \mathsf{svd}\left[\left[\mathbf{G}^{\mathsf{T}}\mathbf{G}\right]^{-1/2} \mathbf{G}^{\mathsf{T}} \ldots \right. \\ & \left. \mathbf{X}^* \left[\left(1 - k_X\right) \mathbf{X}^{*\mathsf{T}} \mathbf{X}^* + k_X \mathbf{I}\right]^{-1/2}\right]\end{aligned} \tag{19}$$

$$\mathbf{U} = \left[\mathbf{G}^{\mathsf{T}}\mathbf{G}\right]^{-1/2} \mathbf{U}' \tag{20}$$

$$\mathbf{V}^{\#} = \left[\left(1 - k_X\right) \mathbf{X}^{*\mathsf{T}} \mathbf{X}^* + k_X \mathbf{I}\right]^{-1/2} \mathbf{V}' \tag{21}$$

$$\mathbf{V} = \mathbf{V}^* \mathbf{V}^{\#} \tag{22}$$

  – Overcoming the memory problem while still stabilizing the solution.

CONNECTION TO GSVD

Population	Sample
$\boldsymbol{\Sigma}_{\mathbf{gg}}$	$\mathbf{G}^{\mathsf{T}}\mathbf{G}$
$\boldsymbol{\Sigma}_{\mathbf{gx}}$	$\mathbf{G}^{\mathsf{T}}\mathbf{X}$
$\boldsymbol{\Sigma}_{\mathbf{xx}}$	$\mathbf{X}^{\mathsf{T}}\mathbf{X} = \mathbf{T}$ (Total)
$\boldsymbol{\Sigma}_{\mathbf{xg}}\boldsymbol{\Sigma}_{\mathbf{gg}}^{-1}\boldsymbol{\Sigma}_{\mathbf{gx}}$	$\mathbf{X}^{\mathsf{T}}\mathbf{G}\left[\mathbf{G}^{\mathsf{T}}\mathbf{G}\right]^{-1}\mathbf{G}^{\mathsf{T}}\mathbf{X} = \mathbf{B}$ (Between)
$\boldsymbol{\Sigma}_{\mathbf{xx}\vert\mathbf{g}} = \boldsymbol{\Sigma}_{\mathbf{xx}} - \boldsymbol{\Sigma}_{\mathbf{xg}}\boldsymbol{\Sigma}_{\mathbf{gg}}^{-1}\boldsymbol{\Sigma}_{\mathbf{gx}}$	$\mathbf{X}^{\mathsf{T}}\left[\mathbf{I} - \mathbf{G}\left[\mathbf{G}^{\mathsf{T}}\mathbf{G}\right]^{-1}\mathbf{G}^{\mathsf{T}}\right]\mathbf{X} = \mathbf{W}$ (Within)

- $\mathbf{T}$, $\mathbf{B}$ and $\mathbf{W}$ symmetric and positive semi-definite — rank-deficient. Canonical Correlation Analysis with respect to the columns in $\mathbf{X}$:

  $$\mathbf{V} \propto \text{eigvec}\left[\mathbf{T}^{-1}\mathbf{B}\right] \qquad \text{(Problem!!!)} \tag{23}$$

  Rank-deficient symmetric generalized eigenvalue problem.

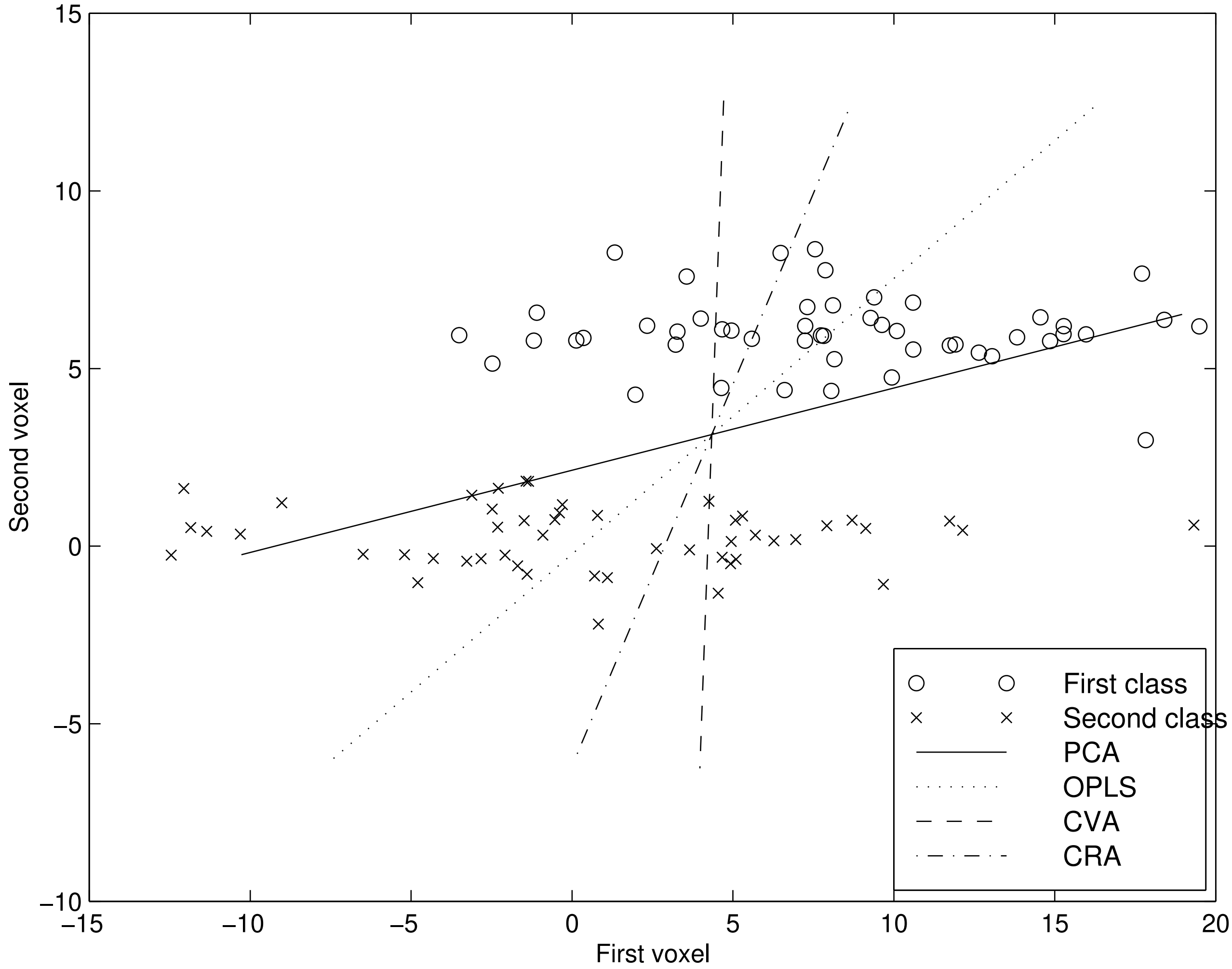
- Solution: initial SVD of $\mathbf{X}$, i.e.(?), generalized singular value decomposition.

- SVD-CRA solution: initial SVD of $\mathbf{X}$ and ridge regularization of $\mathbf{T}^*$ (The SVD version of $\mathbf{T}^*$):

  $$\mathbf{T}' = (1 - k_X)\mathbf{T}^* + k_X\mathbf{I} \tag{24}$$

  $$\mathbf{V} \propto \text{eigvec}\left[\mathbf{T}'^{-1}\mathbf{B}\right] \tag{25}$$

EXAMPLE



- A two-voxel brain
- Both voxels activated
- One voxel with much noise

EXAMPLE: FMRI, SINGLE-SUBJECT, SEQUENTIAL FINGER OPPOSITION

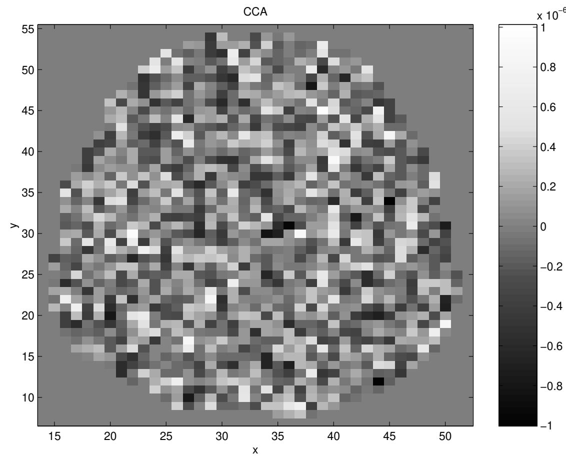


Figure 5: First CCA image.

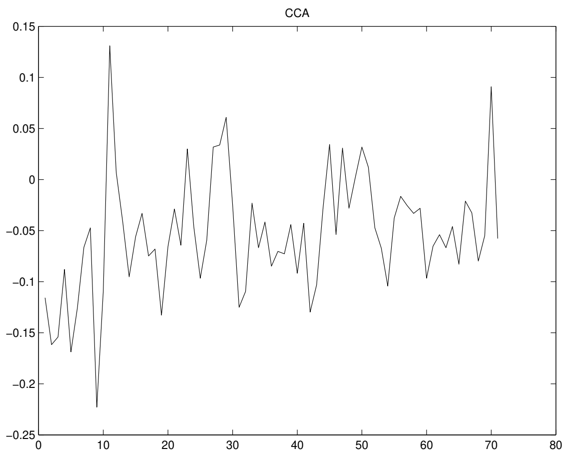


Figure 6: First CCA sequence.

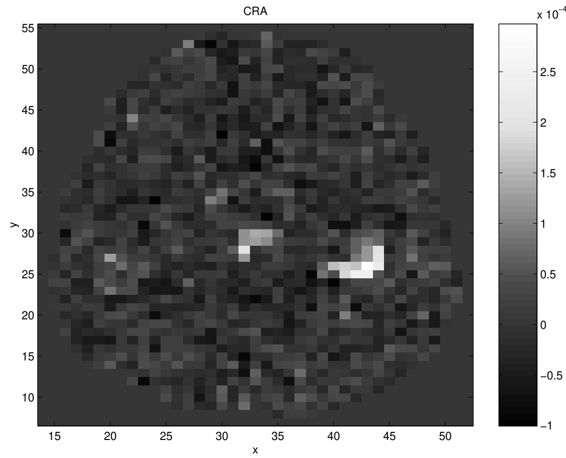


Figure 7: First CRA image.

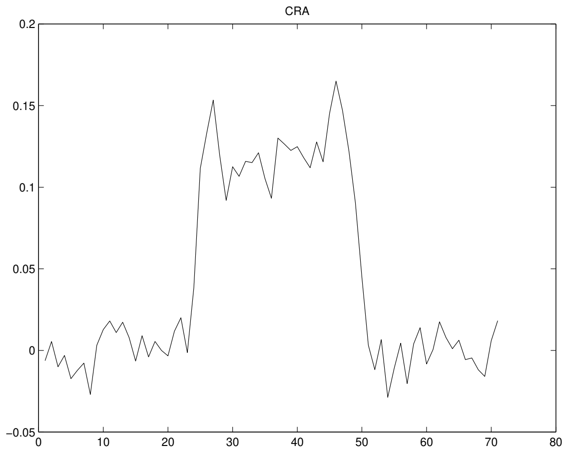


Figure 8: First CRA sequence.

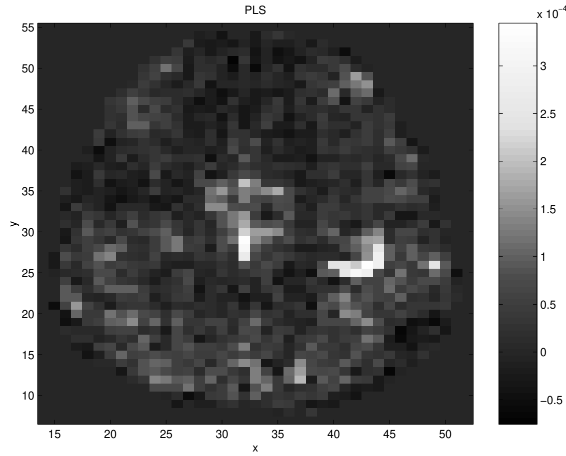


Figure 9: First PLS image.

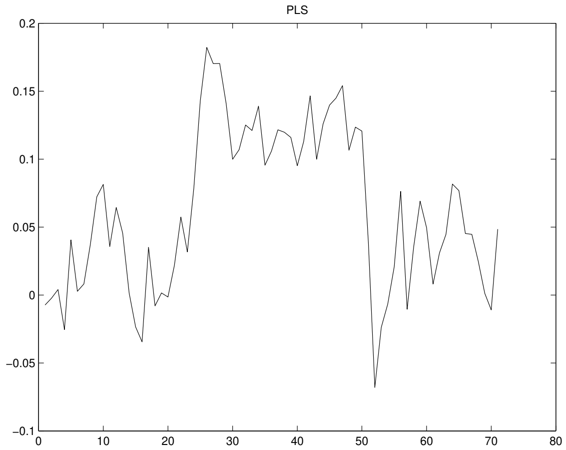


Figure 10: First PLS sequence.

. . . EXAMPLE

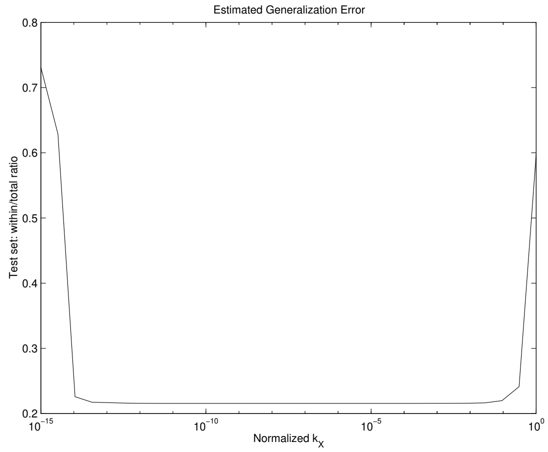


Figure 11: Generalization error.

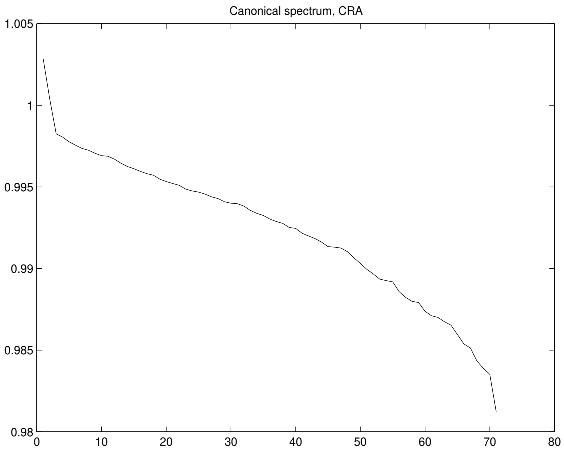


Figure 12: CCA Spectrum.

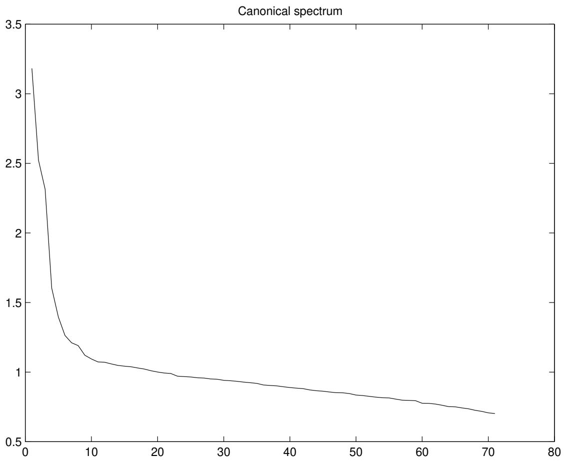


Figure 13: PLS Spectrum.

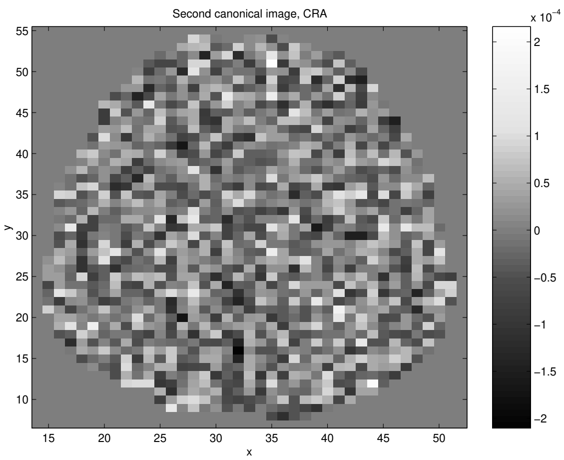


Figure 14: Second CRA image.

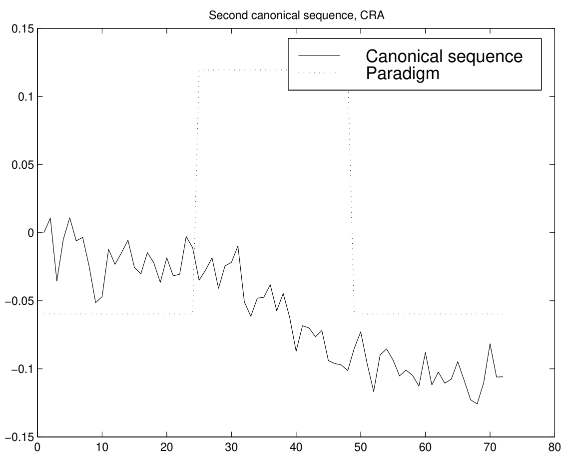


Figure 15: Second CRA sequence.

SUMMARY

- Two different inversion in functional imaging: initial scanner-specific inversion and "analysis" inversion.
- Functional neuroimage data rank-deficient.
- Interesting features not necessarily in the first SVD components.
- Supervised analysis needed: generalized SVD.
- Canonical Correlation Analysis: Generalized symmetric eigenvalue decomposition.
- SVD-CRA: A "regularized generalized singular value decomposition".
- Ridge regularization: Optimization needed.
- Generalization error as a function of the ridge parameter: The setting of the ridge parameter is not critical (with this specific measure).

REFERENCES

References

[Mardia et al., 1979] Mardia, K. V., Kent, J. T., and Bibby, J. M. (1979). *Multivariate Analysis*. Academic Press, London.

[McIntosh et al., 1996] McIntosh, A. R., Bookstein, F. L., Haxby, J. V., and Grady, C. L. (1996). Spatial pattern analysis of functional brain images using Partial Least Square. *NeuroImage*, 3:143–157.

[Nielsen et al., 1998] Nielsen, F. Å., Hansen, L. K., and Strother, S. C. (1998). Canonical ridge analysis with ridge parameter optimization. NeuroImage, page S758. Academic Press.

[Vinod, 1976] Vinod, H. D. (1976). Canonical ridge and econometrics of joint production. *J. Econometrics*, 4:147–166.

[Worsley, 1997] Worsley, K. J. (1997). An overview and some new developments in the statistical analysis of PET and fMRI data. *Human Brain Mapping*, 5(4):254–258.