Multivariate Linear Analyses

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DATAMATRIX AND DESIGNMATRIX

- **Datamatrix** — $\mathbf{X}$ — voxels $\times$ scans

$$\mathbf{X} = \begin{array}{cc} \text{Voxels} & \\ \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1j} & \cdots & x_{1p} \\ x_{21} & x_{12} & & \vdots & & \\ \vdots & & & \vdots & & \\ x_{i1} & \cdots & \cdots & x_{ij} & & \\ \vdots & & & & & \\ x_{n1} & & & & & x_{np} \end{bmatrix} & \text{Scans} \end{array} \tag{1}$$

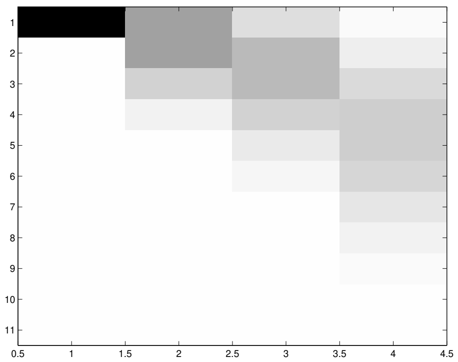
- **Designmatrix** — $\mathbf{G}$ — design variables $\times$ scans

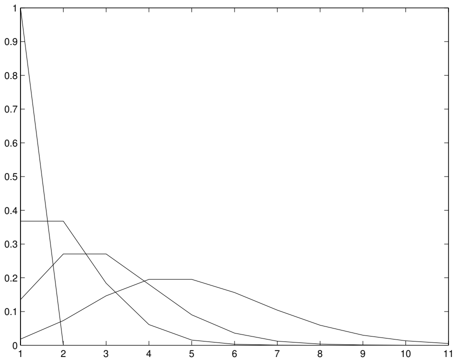
$$\mathbf{G} = \begin{array}{cc} \text{Design variables} & \\ \begin{bmatrix} x_{11} & \cdots & x_{1j} & \cdots & x_{1q} \\ \vdots & & \vdots & & \\ x_{i1} & \cdots & x_{ij} & & \\ \vdots & & & & \\ x_{n1} & & & & x_{nq} \end{bmatrix} & \text{Scans} \end{array} \tag{2}$$

DESIGNMATRICES

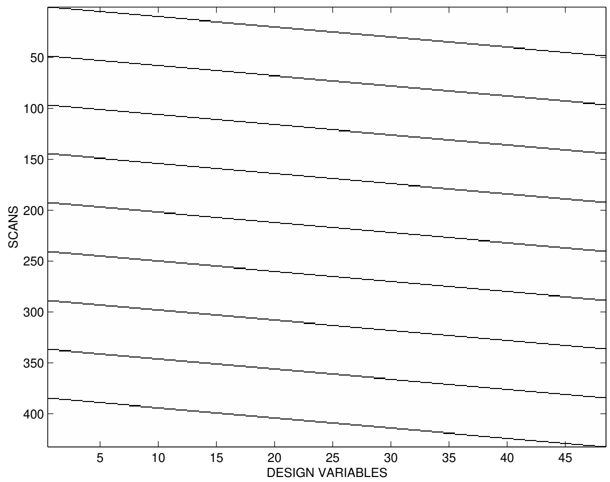
What can be put into a designmatrix:

- Activation — Rest. PLS becomes simple subtraction. CVA becomes FLD — Fisher's Linear Discriminant. Size: scans $\times$ 1.
- Different conditions. (Cognitive conjunction)
- Set of basis functions (to model the hemodynamic response, e.g., a Poisson function with different delays.





- Reproducibility across runs.



WORSLEY'S OVERVIEW OF MULTIVARIATE LINEAR ANALYSES ...

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

$$\mathbf{U}\mathbf{\Lambda}\mathbf{V}^{\mathsf{T}} = \mathbf{X} \tag{3}$$

- PLS. Partial Least Square. [3]

$$\mathbf{U}\mathbf{\Lambda}\mathbf{V}^{\mathsf{T}} = \mathbf{G}^{\mathsf{T}}\mathbf{X} \tag{4}$$

- OPLS. Orthonormalized Partial Least Square. [5]

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

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

- CVA. Canonical Variate Analysis (Canonical Correlation Analysis. [2]

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

$$\mathbf{U} = \left(\mathbf{G}^{\mathsf{T}}\mathbf{G}\right)^{-1/2}\mathbf{U}' \tag{8}$$

$$\mathbf{V} = \left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)^{-1/2}\mathbf{V}' \tag{9}$$

- CRA. Canonical Ridge Analysis. Interpolating between PLS and CVA. [2]

$$\begin{aligned}\mathbf{U}'\mathbf{\Lambda}\mathbf{V}'^{\mathsf{T}} &= \left[(1-k_G)\,\mathbf{G}^{\mathsf{T}}\mathbf{G} + k_G\mathbf{I}\right]^{-1/2}\mathbf{G}^{\mathsf{T}}\ldots \\ &\qquad \mathbf{X}\left[(1-k_X)\,\mathbf{X}^{\mathsf{T}}\mathbf{X} + k_X\mathbf{I}\right]^{-1/2}\end{aligned} \tag{10}$$

$$\mathbf{U} = \left[(1-k_G)\,\mathbf{G}^{\mathsf{T}}\mathbf{G} + k_G\mathbf{I}\right]^{-1/2}\mathbf{U}' \tag{11}$$

$$\mathbf{V} = \left[(1-k_X)\,\mathbf{X}^{*\mathsf{T}}\mathbf{X}^{*} + k_X\mathbf{I}\right]^{-1/2}\mathbf{V}' \tag{12}$$

...WORSLEY'S OVERVIEW OF MULTIVARIATE LINEAR ANALYSES

- SVD-CVA. Canonical Variate Analysis with Singular Value Decomposition

$$\mathbf{X} = \mathbf{U}^* \mathbf{\Lambda}^* \mathbf{V}^{*\mathsf{T}} \tag{13}$$

$$\mathbf{X}^* = \mathbf{U}^* \mathbf{\Lambda}^* = \mathbf{X}\mathbf{V}^* \tag{14}$$

$$\mathbf{U}' \mathbf{\Lambda} \mathbf{V}'^{\mathsf{T}} = \left(\mathbf{G}^{\mathsf{T}}\mathbf{G}\right)^{-1/2} \mathbf{G}^{\mathsf{T}}\mathbf{X}^* \left(\mathbf{X}^{*\mathsf{T}}\mathbf{X}^*\right)^{-1/2} \tag{15}$$

$$\mathbf{U} = \left(\mathbf{G}^{\mathsf{T}}\mathbf{G}\right)^{-1/2} \mathbf{U}' \tag{16}$$

$$\mathbf{V}^{\#} = \left(\mathbf{X}^{*\mathsf{T}}\mathbf{X}^*\right)^{-1/2} \mathbf{V}' \tag{17}$$

$$\mathbf{V} = \mathbf{V}^* \mathbf{V}^{\#} \tag{18}$$

However, $\mathbf{X}^* \left(\mathbf{X}^{*\mathsf{T}}\mathbf{X}^*\right)^{-1/2}$ is spherical if all components are maintained!

...WORSLEY'S OVERVIEW OF MULTIVARIATE LINEAR ANALYSES

- SVD-CRA. Canonical Ridge Analysis with Singular Value Decomposition. [4]

$$\mathbf{X} = \mathbf{U}^{*}\mathbf{\Lambda}^{*}\mathbf{V}^{*\mathsf{T}} \tag{19}$$

$$\mathbf{X}^{*} = \mathbf{U}^{*}\mathbf{\Lambda}^{*} = \mathbf{X}\mathbf{V}^{*} \tag{20}$$

$$\begin{aligned}\mathbf{U}'\mathbf{\Lambda}\mathbf{V}'^{\mathsf{T}} &= \left[(1-k_G)\,\mathbf{G}^{\mathsf{T}}\mathbf{G} + k_G\mathbf{I}\right]^{-1/2}\mathbf{G}^{\mathsf{T}}\ldots \\ &\qquad \mathbf{X}^{*}\left[(1-k_X)\,\mathbf{X}^{*\mathsf{T}}\mathbf{X}^{*} + k_X\mathbf{I}\right]^{-1/2}\end{aligned} \tag{21}$$

$$\mathbf{U} = \left[(1-k_G)\,\mathbf{G}^{\mathsf{T}}\mathbf{G} + k_G\mathbf{I}\right]^{-1/2}\mathbf{U}' \tag{22}$$

$$\mathbf{V}^{\#} = \left[(1-k_X)\,\mathbf{X}^{*\mathsf{T}}\mathbf{X}^{*} + k_X\mathbf{I}\right]^{-1/2}\mathbf{V}' \tag{23}$$

$$\mathbf{V} = \mathbf{V}^{*}\mathbf{V}^{\#} \tag{24}$$

GENERAL OBSERVATION

- SVD finds the principal axis in a hyperellipsoide
- Canonic variables analyses "impose" a model, dividing the scans (to several ellipses) and find the principal axis for the largest *between* variation among the ellipses.
- $\mathbf{U}$ has been called the eigenvectors, canonic correlation vectors, eigensequences, canonic sequences or "temporale eigenvectors"
- $\mathbf{\Lambda}$ is the eigenvalues, singular values or (the squared) canonical correlation coefficients
- $\mathbf{V}$ is the eigenvectors, canonic correlation vectors, eigenimages or canonic images
- The "activation plane" is a linear combination of the components
- The first PCA components is the ones which "explains" most of the variation (interesting, nuisance or noise).
  - Multisubject studies: First PCA components spans the intersubject space.
  - Single subject studies: Some of the first PCA components contain the paradigm.
- Eigensequences (and eigenimages) are not necessary in phase with the paradigm. However, the sign of the inner cross-product between the paradigm and the eigensequence can mend that.

SUPERVISED/UNSUPERVISED

Unsupervised, Exploratory

PCA

Cluster analysis

PLS, CVA, CRA

General Linear Model

Neural network

Supervised, Inferential

MANCOVA

MANCOVA: Split the designmatrix $\mathbf{G}$ in two set:

- Interesting effects $\mathbf{H}$.
- Nuisance effects $\mathbf{D}$. "Confounding effects", "Effects of no interest". Indicator variable for subject, block effects

$$\mathbf{G} = [\mathbf{HD}] \tag{25}$$

Multivariate Regression Analysis (General Linear Model) [1]

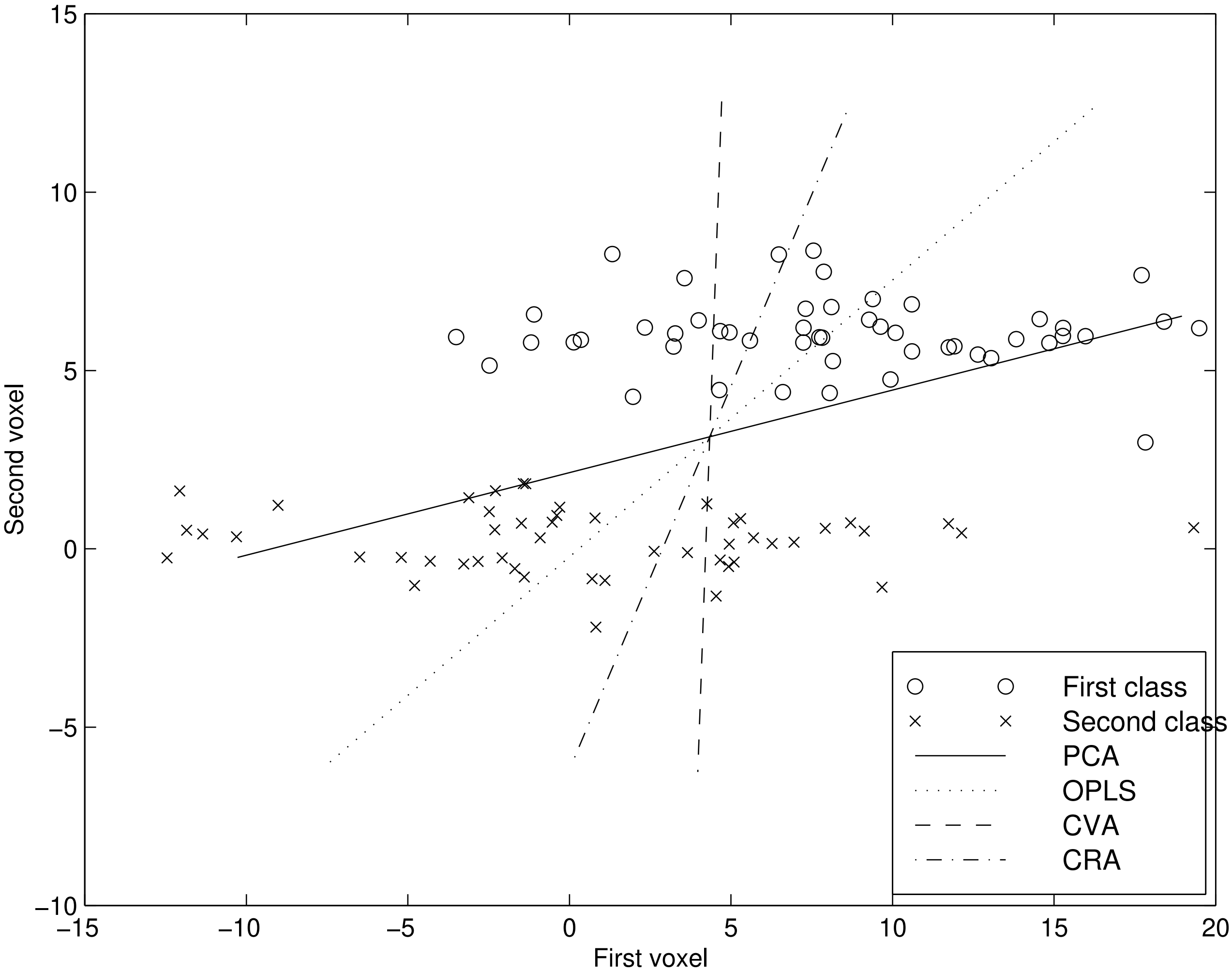
$$\mathbf{X} = \mathbf{GB} + \mathbf{E} \tag{26}$$

$$\hat{\mathbf{B}} = \left(\mathbf{G}^\top \mathbf{G}\right)^{-1} \mathbf{G}^\top \mathbf{X} \tag{27}$$

Multivariate Linear Models [6]

$$\mathbf{U}' \mathbf{\Lambda} \mathbf{V}'^\top = \left(\mathbf{G}^\top \mathbf{\Sigma} \mathbf{G}\right)^{-1/2} \mathbf{G}^\top \mathbf{X} \tag{28}$$

EXAMPLE



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

LYNGBY MATLAB TOOLBOX EXAMPLE

```
% Two clusters
A = ones(50,1) * [8 6] + randn(50,2) .* (ones(50,1) * [6 1]);
B = ones(50,1) * [0 0] + randn(50,2) .* (ones(50,1) * [6 1]);

% The datamatrix
X = [ A ; B ];
Xmean = mean(X);
XMean = ones(size(X,1),1) * Xmean;
XN = X - XMean;

% The designmatrix
G = [ones(size(A,1),1) ; -ones(size(B,1),1)];

% Analysis
[PCA_U, PCA_S, PCA_V] = lyngby_svd(XN);
[PLS_U, PLS_S, PLS_V] = lyngby_opls(XN, G);
[CVA_U, CVA_S, CVA_V] = lyngby_cva(XN, G);
[CRA_U, CRA_S, CRA_V] = lyngby_cva(XN, G, 'RidgeX', 0.9995);

% Plot
plot(A(:,1), A(:,2), 'o', B(:,1), B(:,2), 'x')

hold on
  f = 15;
  p = [Xmean + f * PCA_V(:,1)' ; Xmean - f * PCA_V(:,1)'];
  plot(p(:,1), p(:,2), '-')
  p = [Xmean + f * PLS_V(:,1)' ; Xmean - f * PLS_V(:,1)'];
  plot(p(:,1), p(:,2), ':')
  p = [Xmean + f * CVA_V(:,1)' ; Xmean - f * CVA_V(:,1)'];
  plot(p(:,1), p(:,2), '--')
  p = [Xmean + f * CRA_V(:,1)' ; Xmean - f * CRA_V(:,1)'];
  plot(p(:,1), p(:,2), '-.')
hold off

xlabel('First voxel')
ylabel('Second voxel')
legend('First class', 'Second class', 'PCA', 'OPLS', 'CVA', 'CRA');
```

EXAMPLE: SINGLE-SUBJECT, SEQUENTIAL FINGER OPPOSITION, "SOP"-MODEL . . .

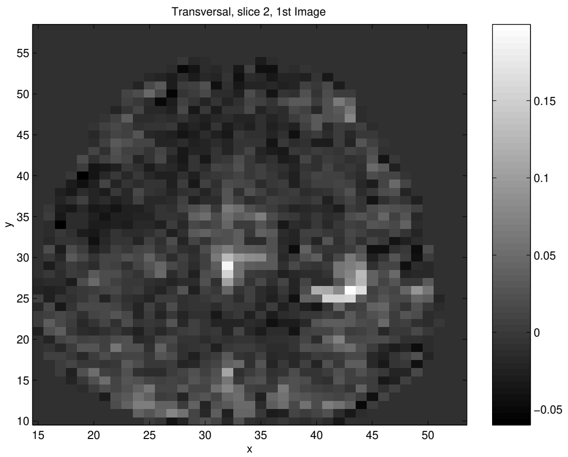


Figure 1: First canonic image.

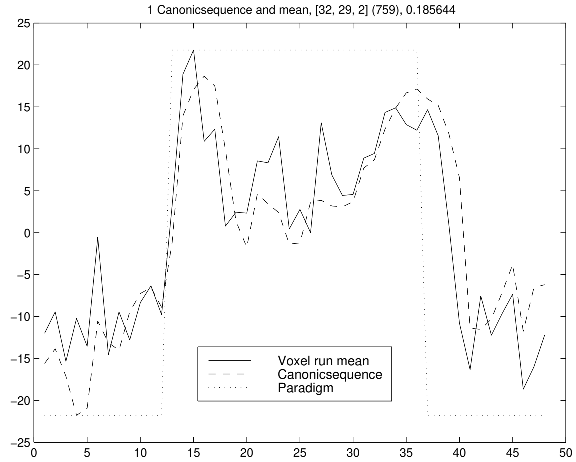


Figure 2: First canonic sequence.

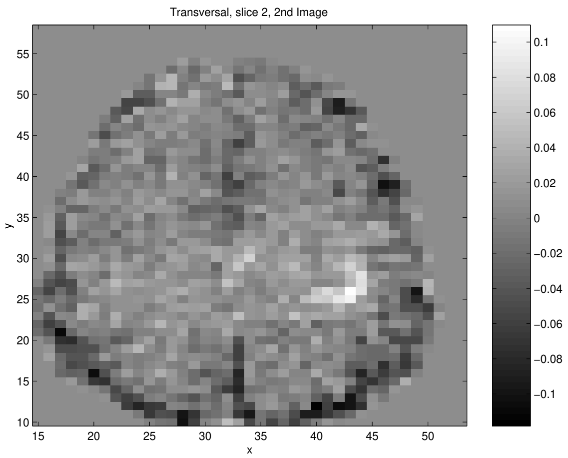


Figure 3: Second canonic image.

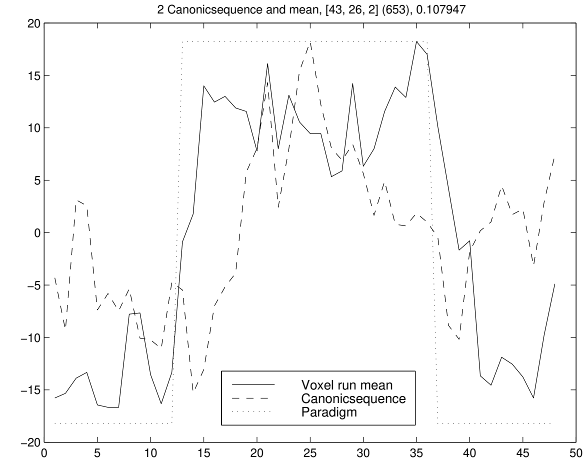


Figure 4: Second canonic sequence.

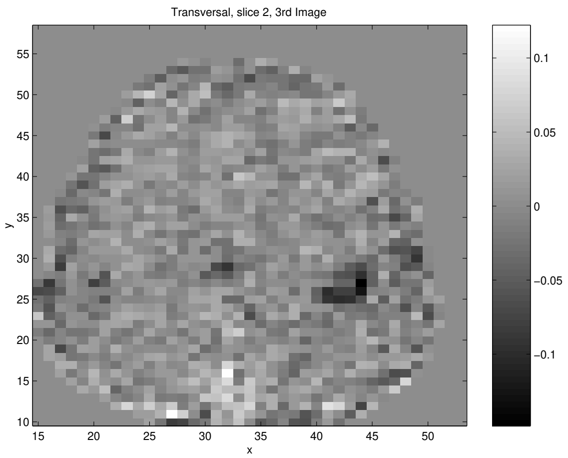


Figure 5: Third canonic image.

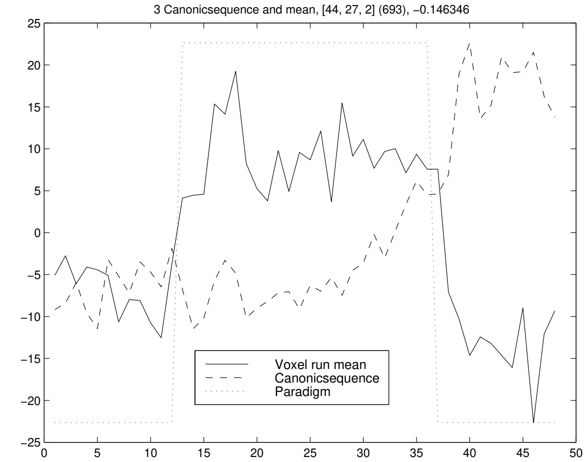


Figure 6: Third canonic sequence.

... EXAMPLE: SINGLE-SUBJECT, SEQUENTIAL FINGER OPPOSITION, "SOP"-MODEL

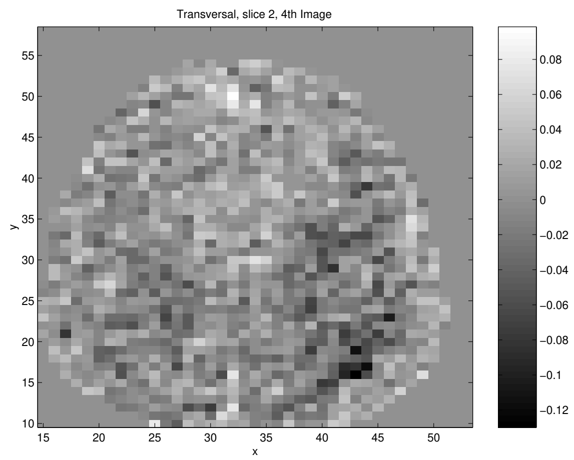


Figure 7: Fourth canonic image.

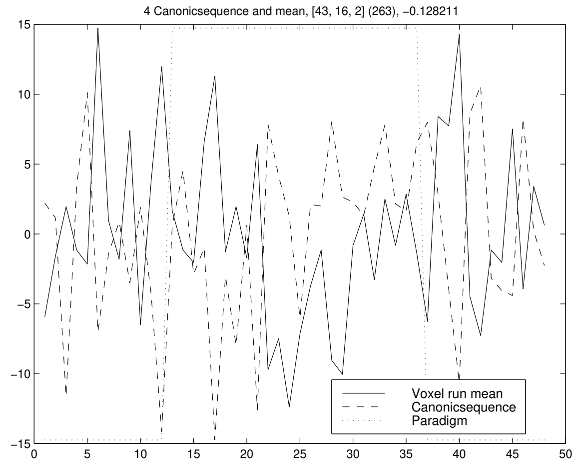


Figure 8: Fourth canonic sequence.

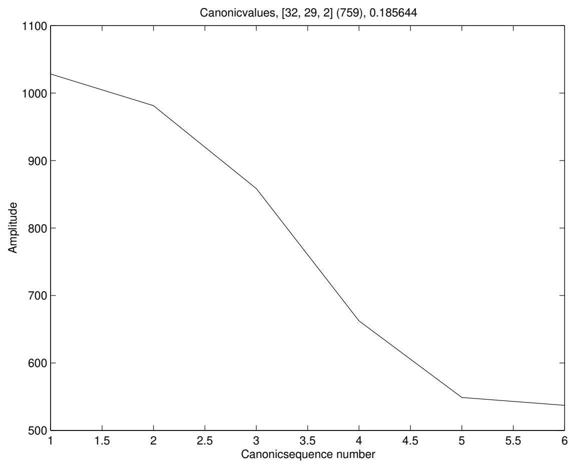


Figure 9: Spectrum.

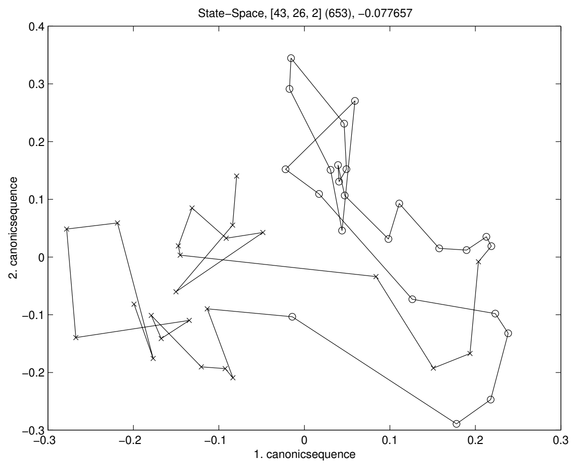


Figure 10: State space.

- State space: Activation a linear combination of the canonic components.
- "SOP"-model: First components usually contain the paradigm. Higher components nuisance.

REFERENCES

References

[1] Karl J. Friston, J.-P. Poline, A. P. Holmes, C. D. Frith, and R. S. J. Frackowiak. A multivariate analysis of pet activation studies. *Human Brain Mapping*, 1996.

[2] Kantilal Varichand Mardia, J. T. Kent, and J. M. Bibby. *Multivariate Analysis*. Academic Press, 1979.

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

[4] Finn Årup Nielsen, Lars Kai Hansen, and Stephen C. Strother. Canonical ridge analysis with ridge parameter optimization. Submitted to HBM'98.

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

[6] Keith J. Worsley, Jean-Baptiste Poline, Karl J. Friston, and A. C. Evans. Characterizing the response of fMRI data using multivariate linear models. In Press, 1997.