Canonical Correlation Analysis (CCA) and extensions for high-dimensional data with non-instantaneous couplings

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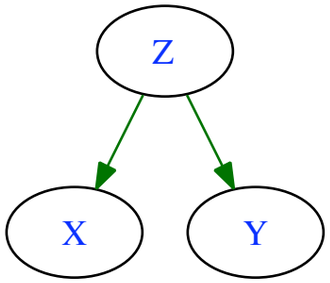
Outline

- **Canonical Correlation Analysis (CCA)**
  - Standard CCA Solution using Covariance Matrices
  - Example: Unsupervised categorisation of car types
- **Kernel Canonical Correlation Analysis (kCCA)**
  - For high-dimensional data and non-linear dependencies
  - Example: Cross-Language Topic detection on news websites
- **Temporal Kernel CCA (tkCCA)**
  - For data with non-instantaneous couplings
  - Example: Multi-modal neuronal signals (invasive vs. non-invasive)
  - tkCCA estimates convolution linking non-invasive to invasive signals

Canonical Correlation Analysis (CCA)

Canonical Correlation Analysis (CCA)

Latent variable Z is measured at multivariate variables X and Y



Which dimensions of X and Y are important to describe Z?

Canonical Correlation Analysis (CCA)

Given two (or more) multivariate variables

$$X \in \mathbb{R}^M, Y \in \mathbb{R}^N$$

CCA finds projections

$$w_x \in \mathbb{R}^M, w_y \in \mathbb{R}^N$$

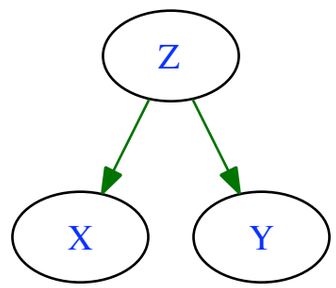
that maximise the covariance between the variables

$$\underset{w_x, w_y}{\operatorname{argmax}} \left(w_x^\top X Y^\top w_y \right) \quad \text{s.t.} \quad \begin{aligned} w_x^\top X X^\top w_x &= 1 \\ w_y^\top Y Y^\top w_y &= 1 \end{aligned}$$

[Hotelling, Biometrika, 1936]

Canonical Correlation Analysis (CCA)

- Latent Variable **Z: Car Types**
- Measurements
  - **X**: Displacement, Horsepower, Weight
  - **Y**: Acceleration, Miles/Gallon



X =

Dimensions

Car models

Displacement	Horsepower	Weight
307	130	3504
350	165	3693
318	150	3436
	...	

Y =

Acceleration	Miles/Gallon
12.0000	18.0000
11.5000	15.0000
11.0000	18.0000
...	

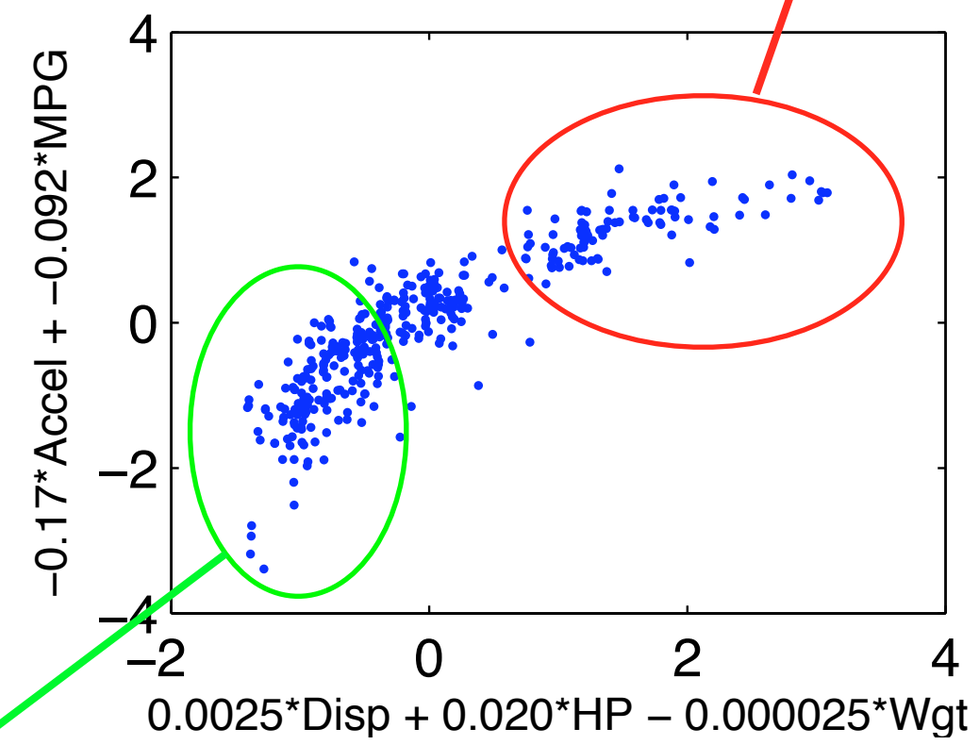
Canonical Correlation Analysis (CCA)

- Latent Variable **Z: Car Types**
- Measurements
  - **X**: Displacement, Horsepower, Weight
  - **Y**: Acceleration, Miles/Gallon

$$w_x = \begin{bmatrix} 0.0025 \\ 0.0202 \\ -0.000025 \end{bmatrix}$$

$$w_y = \begin{bmatrix} -0.17 \\ -0.092 \end{bmatrix}$$

Sport Cars
(big engine, strong, thirsty)



$Y w_y$

$X w_x$

Commercial Cars
(small engine, low consumption)

Canonical Correlation Analysis (CCA)

Assuming centered data

$$\sum_i x_i = \sum_i y_i = 0$$

We can compute empirical *cross*-covariance matrices and *auto*-covariance matrices

$$C_{xy} = \frac{1}{N} X Y^\top$$

$$C_{xx} = \frac{1}{N} X X^\top$$

Canonical Correlation Analysis (CCA)

CCA objective

$$\underset{w_x, w_y}{\operatorname{argmax}} \left(w_x^\top X Y^\top w_y \right) \quad \text{s.t.} \quad \begin{aligned} w_x^\top X X^\top w_x &= 1 \\ w_y^\top Y Y^\top w_y &= 1 \end{aligned}$$

Lagrangian

$$\mathcal{L} = w_x^\top C_{xy} w_y - \frac{1}{2}\alpha(w_x^\top C_{xx} w_x - 1) - \frac{1}{2}\beta(w_y^\top C_{yy} w_y - 1)$$

Partial Derivatives

$$\frac{\partial \mathcal{L}}{\partial w_x^\top} = C_{xy} w_y - \alpha C_{xx} w_x \qquad \frac{\partial \mathcal{L}}{\partial w_y^\top} = C_{yx} w_x - \beta C_{yy} w_y$$

Canonical Correlation Analysis (CCA)

We set the partial derivatives to 0 and multiply with $w_x^\top,\ w_y^\top$

$$w_x^\top C_{xy} w_y = \alpha w_x^\top C_{xx} w_x$$

$$w_x^\top C_{xy} w_y = \beta w_y^\top C_{yy} w_y$$

Thus from the auto-covariance constraints

$$1 = w_x^\top C_{xx} w_x = w_y^\top C_{yy} w_y$$

follows

$$\alpha = \beta$$

Canonical Correlation Analysis (CCA)

Given $\alpha = \beta$

the partial derivatives become

$$C_{xy} w_y = \alpha \; C_{xx} w_x$$
$$C_{yx} w_x = \alpha \; C_{yy} w_y$$

We can now reformulate these equations in block matrix form

$$\begin{bmatrix} 0 & C_{xy} \\ C_{yx} & 0 \end{bmatrix} \begin{bmatrix} w_x \\ w_y \end{bmatrix} = \alpha \begin{bmatrix} C_{xx} & 0 \\ 0 & C_{yy} \end{bmatrix} \begin{bmatrix} w_x \\ w_y \end{bmatrix}$$

which is just a *generalised eigenvalue equation*

A short history of CCA

- **Extensions of CCA**
  - more than two variables [Kettenring 1971]
  - Kernel CCA (kCCA) [Akaho 2001]
    - finds **non-linear** dependencies
    - applicable to **high-dimensional** data

- **Recently CCA became popular in**
  - Machine Learning
    - Objective function for **kernel ICA** [Bach 2002]
    - **Mutual information** estimation [Gretton 2005]
  - Neuroscience
    - *Receptive fields* without spike triggering [Macke 2008]
    - Analysis of *fMRI and multivariate stimuli* [Hardoon 2007]
    - Analysis of *multi-modal recordings* [Bießmann 2009]

Shortcomings of CCA computed on Covariances

- Sometimes covariance matrices too big to compute
  - Example: Bag-of-Words feature space (potentially infinite dimensional)
- CCA does not capture *non-linear dependencies*
- Solution:
  - Kernel Canonical Correlation Analysis (kCCA)
  - Operates on kernels of the data (not covariance matrices)

Kernel Canonical Correlation Analysis (kCCA)

Solving CCA on the Data Kernels

Intuition behind the Kernel Trick:

Any solution found by CCA has to lie
in the subspace spanned by the data points

A sufficient representation of this subspace can be obtained by the inner products of all data points (linear kernels)

$$K_x = X^\top X$$

$$K_y = Y^\top Y$$

No need to compute big covariance matrices!

Solving CCA on the Data Kernels

The solution of CCA in kernel space is obtained by solving the generalised eigenvalue problem

$$\begin{bmatrix} 0 & K_x K_y \\ K_y K_x & 0 \end{bmatrix} \begin{bmatrix} \alpha_x \\ \alpha_y \end{bmatrix} = \rho \begin{bmatrix} K_x^2 & 0 \\ 0 & K_y^2 \end{bmatrix} \begin{bmatrix} \alpha_x \\ \alpha_y \end{bmatrix}$$

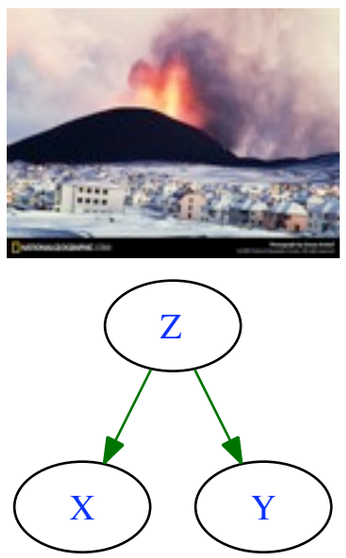
The solutions in the input space can be recovered by

$$w_x = X\alpha_x$$

$$w_y = Y\alpha_y$$

Kernel Canonical Correlation Analysis (kCCA)

- **Example for high-dimensional data**
  - Two news websites (e.g. English and German)
  - **huge feature spaces** (as many dimensions per variable as words on each website)



kCCA finds **hot topics** present on both sites (without translations)

Kernel Canonical Correlation Analysis (kCCA)

U.K.

Germany

Time [Days]

Words

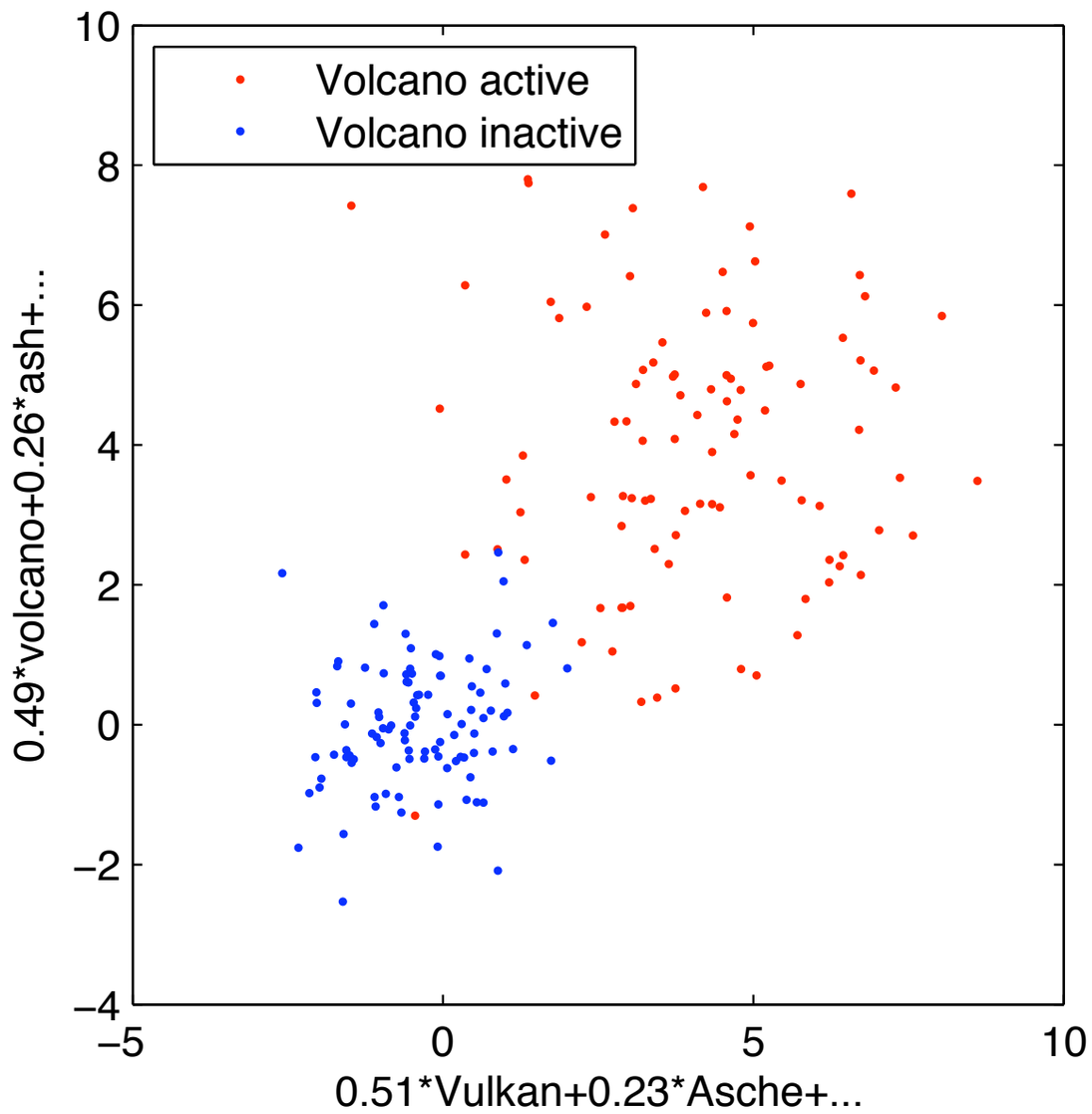
Extracted Word Counts

Volcano	0	4	3	…
ash	0	3	2	
flights	1	5	2	
	⋮			

Vulkan	0	3	2	
Asche	0	1	2	…
Flüge	2	4	3	
	⋮			

Kernel Canonical Correlation Analysis (kCCA)

U.K.



Germany

Temporal kernel CCA (tkCCA)

Non-instantaneous Couplings

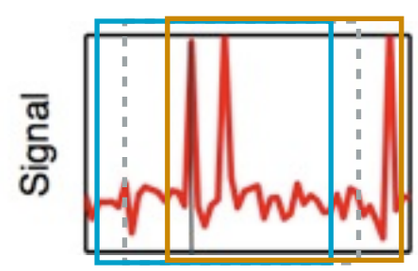
- If variables are coupled with **delays**
  - simultaneous samples *will not be correlated*
  - Standard (k)CCA will not find the right solution
- **Solution**
  - Shift one variable relative to the other
  - Maximise correlation for **all relative time lags**

$$\underset{w_x(\tau), w_y}{\operatorname{argmax}} \operatorname{Corr}\left(\sum_{\tau} w_x(\tau)^\top x(t-\tau),\ w_y^\top y(t)\right)$$

Temporal kernel CCA

$$\underset{w_x(\tau), w_y}{\operatorname{argmax}} \operatorname{Corr}\left(\sum_{\tau} w_x(\tau)^\top x(t-\tau),\ w_y^\top y(t) \right)$$

$$\tilde{X} = \begin{bmatrix} X_{\tau_1} \\ X_{\tau_2} \\ \vdots \\ X_{\tau_T} \end{bmatrix}$$



Data is *embedded in its temporal context* by appending time shifted copies to each data point

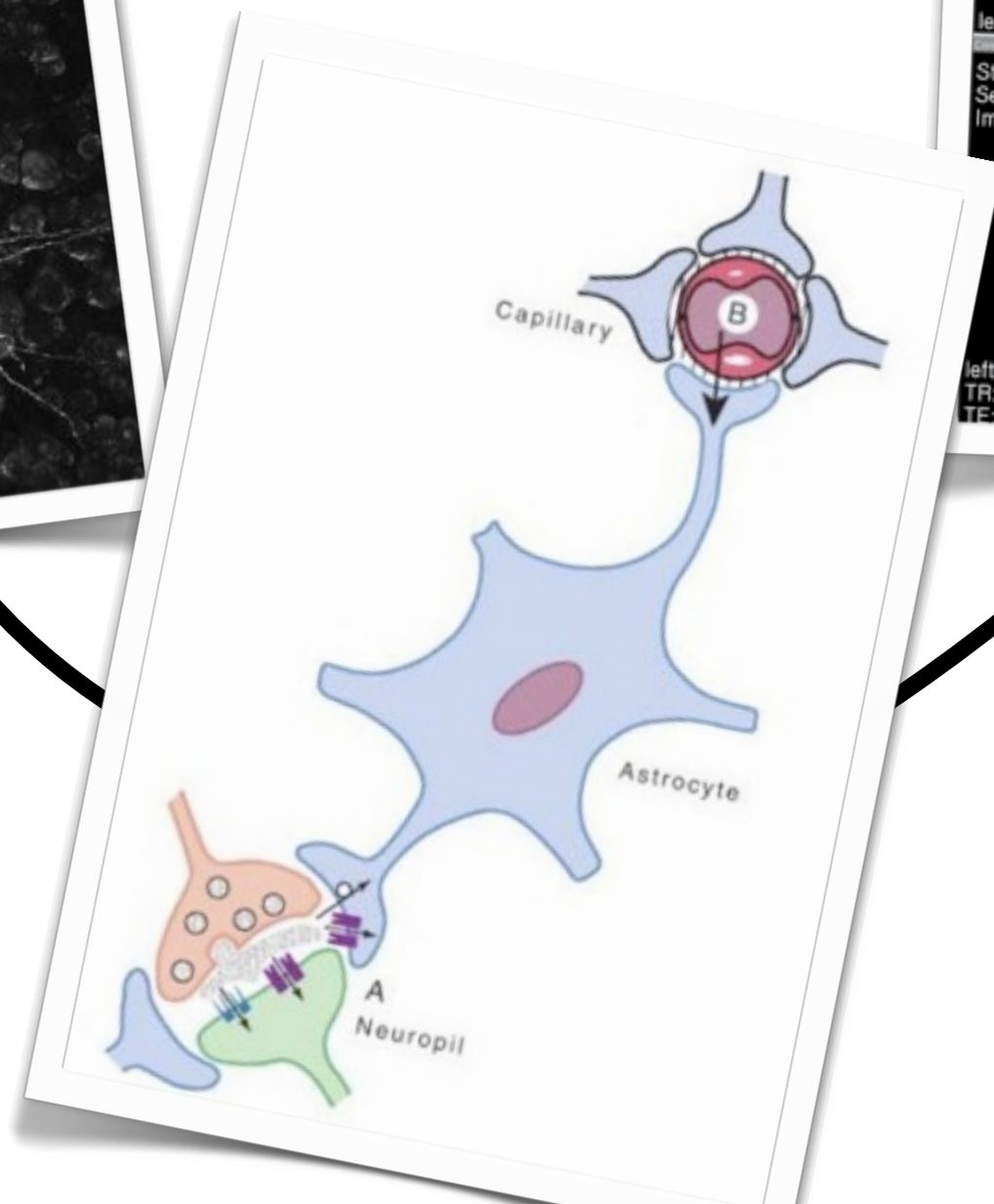
Temporal kernel CCA

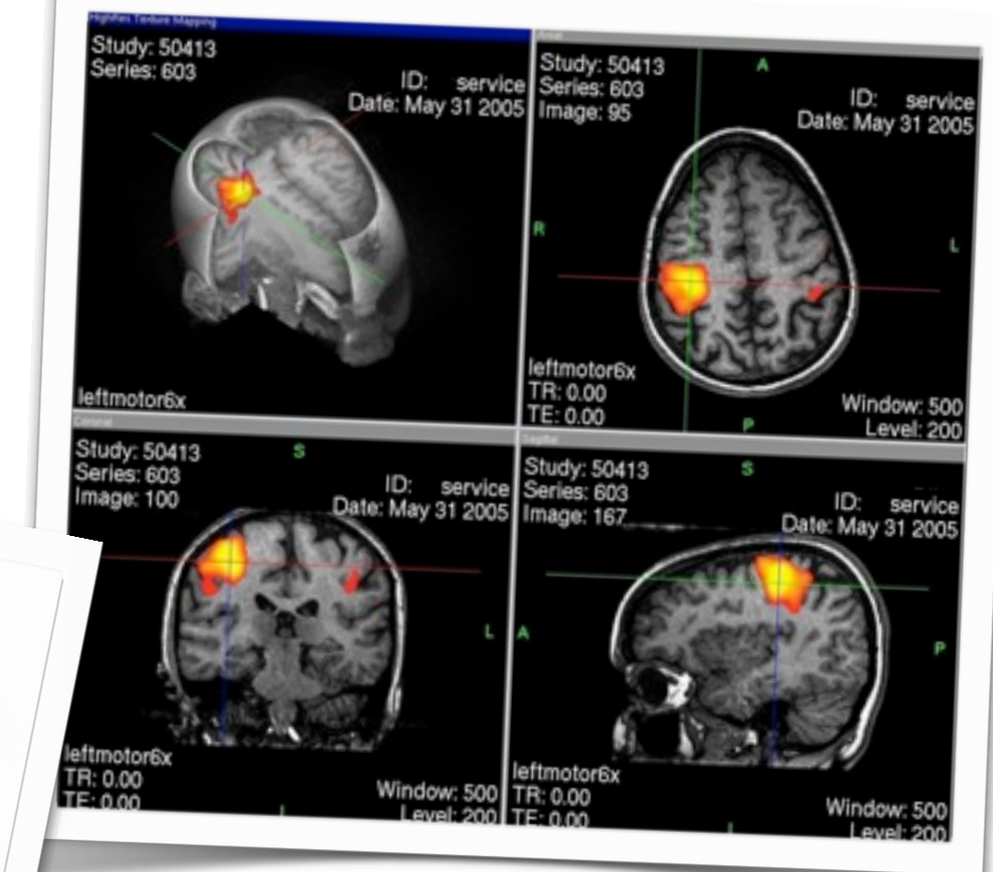
$$\underset{w_x(\tau), w_y}{\operatorname{argmax}} \operatorname{Corr}\left(\sum_{\tau} w_x(\tau)^\top x(t-\tau),\ w_y^\top y(t)\right)$$

$$\tilde{X} = \begin{bmatrix} X_{\tau_1} \\ X_{\tau_2} \\ \vdots \\ X_{\tau_T} \end{bmatrix} \qquad \tilde{w}_x = \begin{bmatrix} w_x(\tau_1) \\ w_x(\tau_2) \\ \vdots \\ w_x(\tau_T) \end{bmatrix}$$

$$\underset{w_{\tilde{x}}, w_y}{\operatorname{argmax}} \operatorname{Corr}\left(\tilde{w}_x^\top \tilde{X}, w_y^\top Y\right)$$

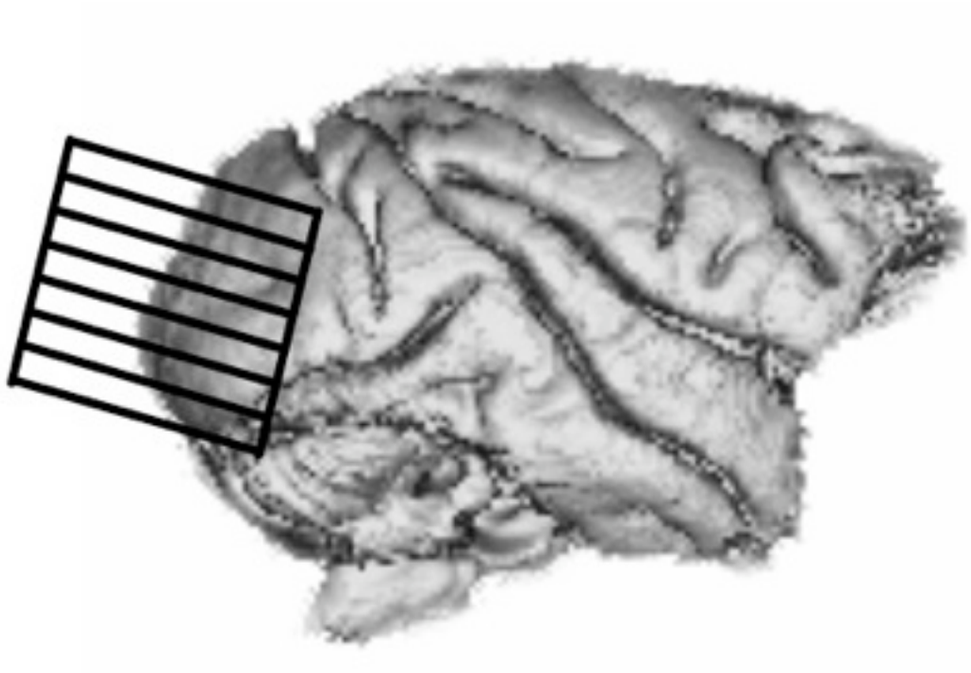
Application: Neuro-Vascular Coupling

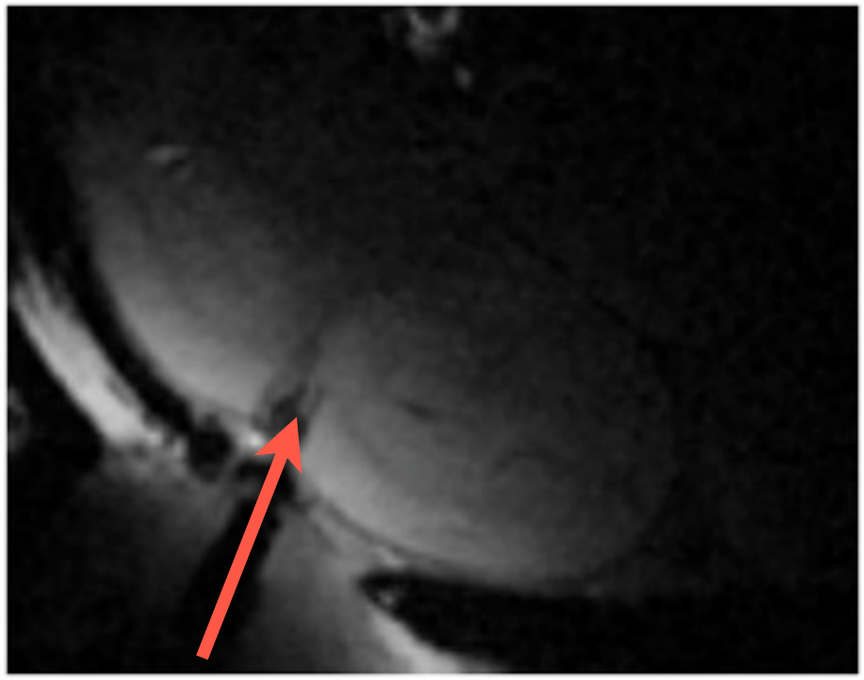




Experimental Setup

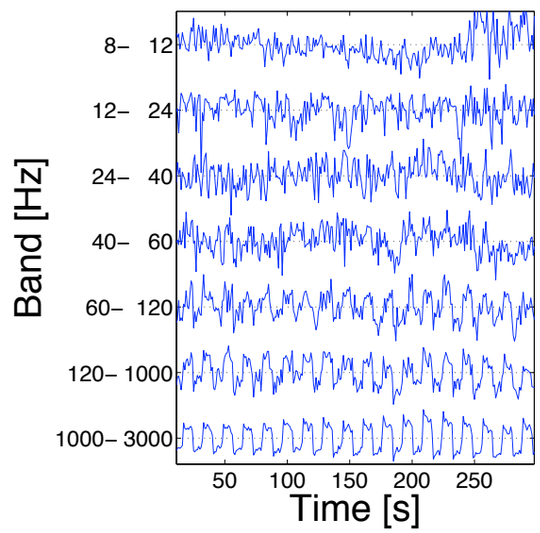
- **Simultaneous measurements of**
  - fMRI/ BOLD signal
  - Intracortical neural activity



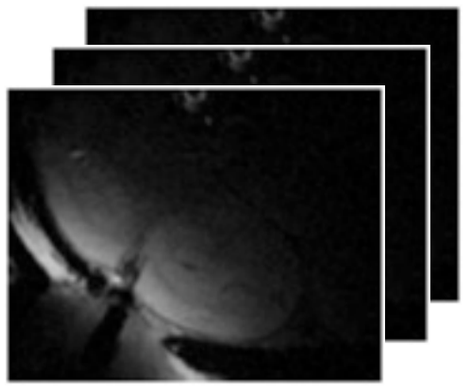


Analysis of Simultaneous Recordings

Spectrogram of neural activity



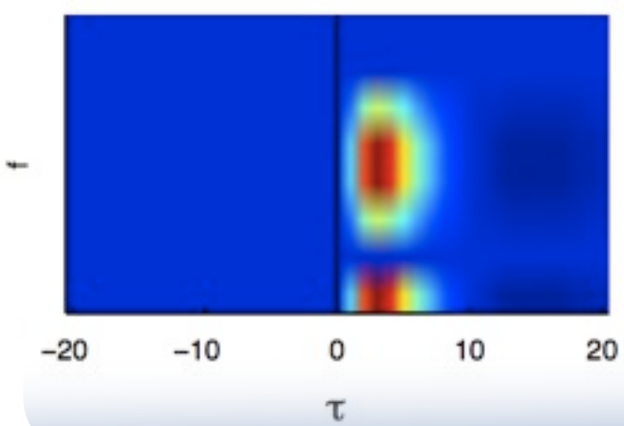
fMRI
Time series



- **Mass-univariate approach?**
  - correlate each voxel with each frequency band
  - Problem: *Multivariate dependencies* neglected [Lange 1999]
- **Unsupervised Methods?**
  - ICA/PCA can only be applied to *one data source*
- **Pattern Classifiers?**
  - SVMs not designed for "*multivariate labels*" (i.e. neural data)

Temporal kernel CCA

$w_x(\tau)$ $\quad$ $x(t)$ $\quad$ w_y $\quad$ $y(t)$



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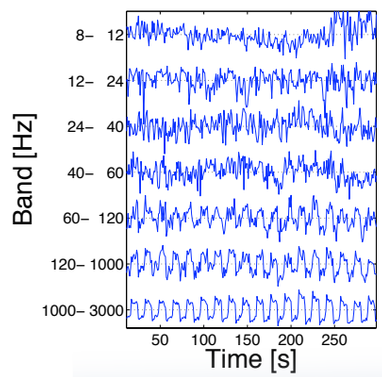
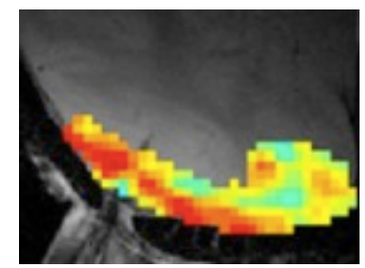
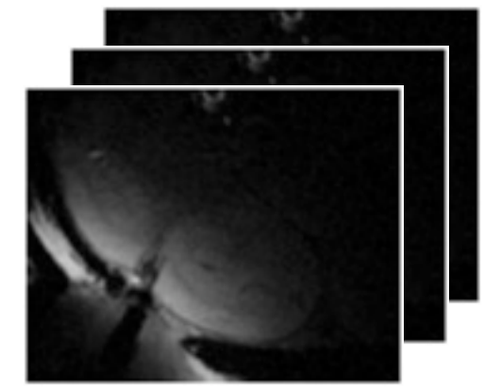




$\times$



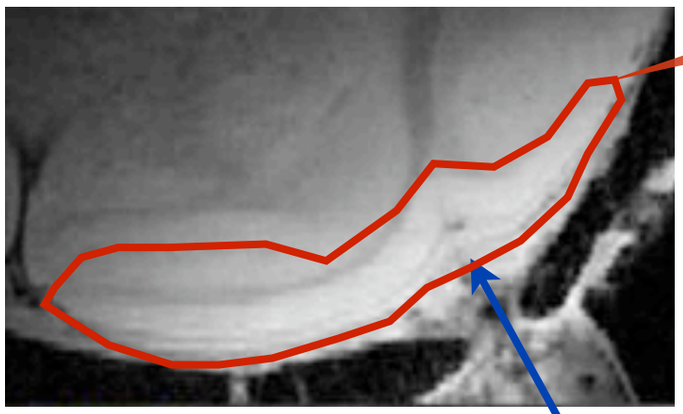
$$\underset{w_x(\tau), w_y}{\operatorname{argmax}} \operatorname{Corr}\left(\sum_{\tau} w_x(\tau)^\top x(t-\tau),\ w_y^\top y(t) \right)$$

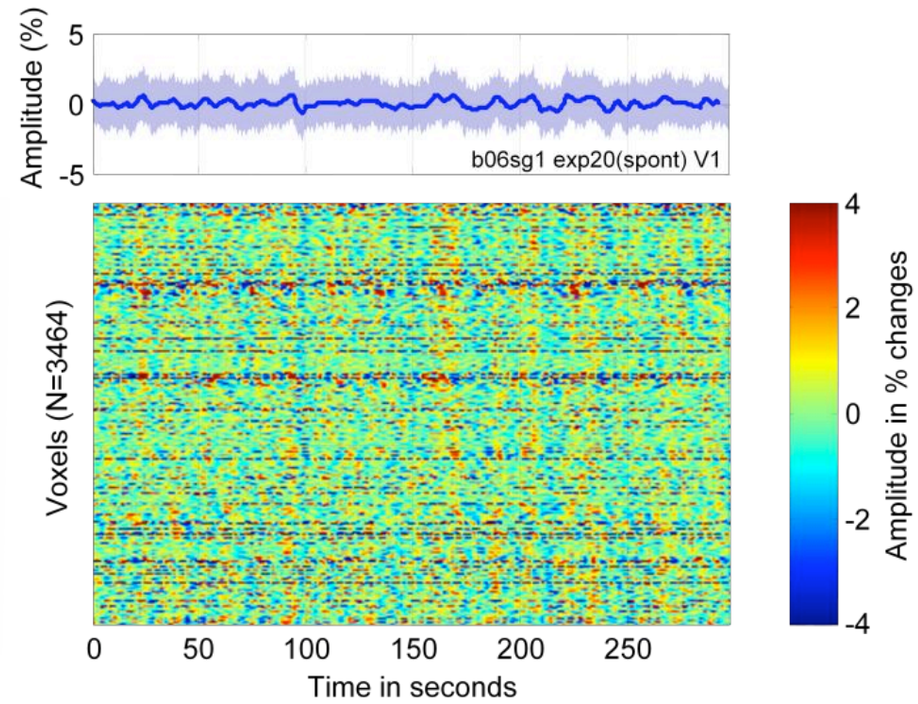
multivariate convolution of the neurophysiological signal with frequency dependent HRF

spatial weighting of voxels with activation pattern.

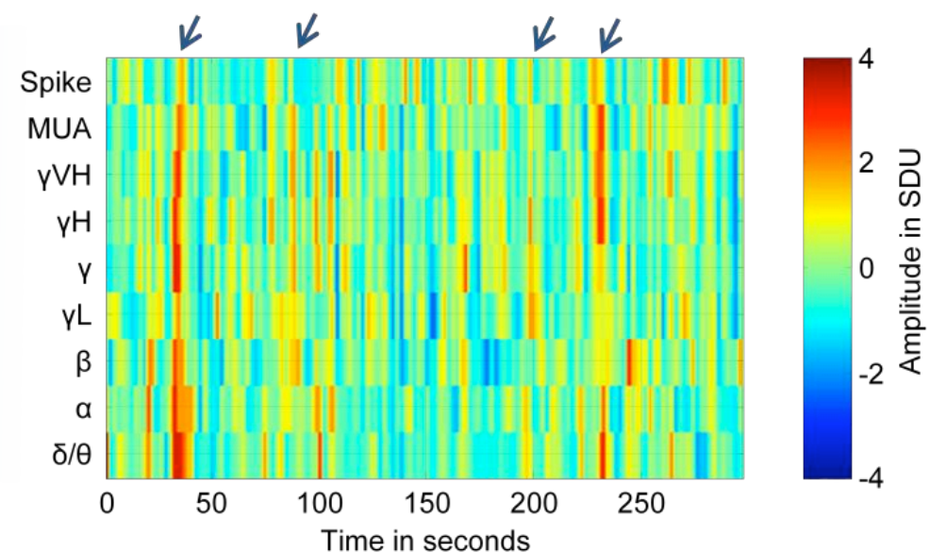
Raw Data During Spontaneous Activity

BOLD signal

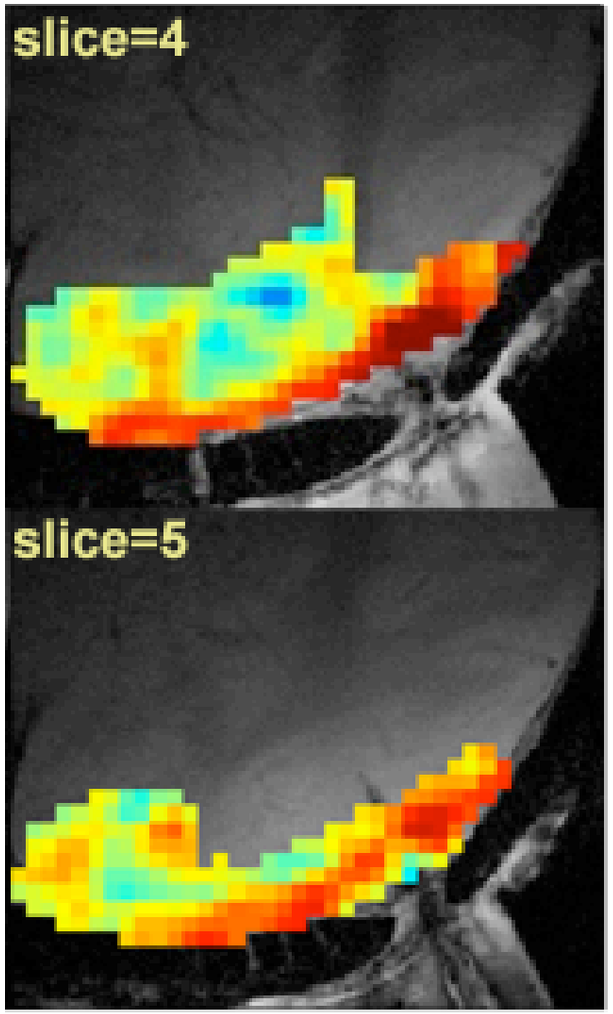




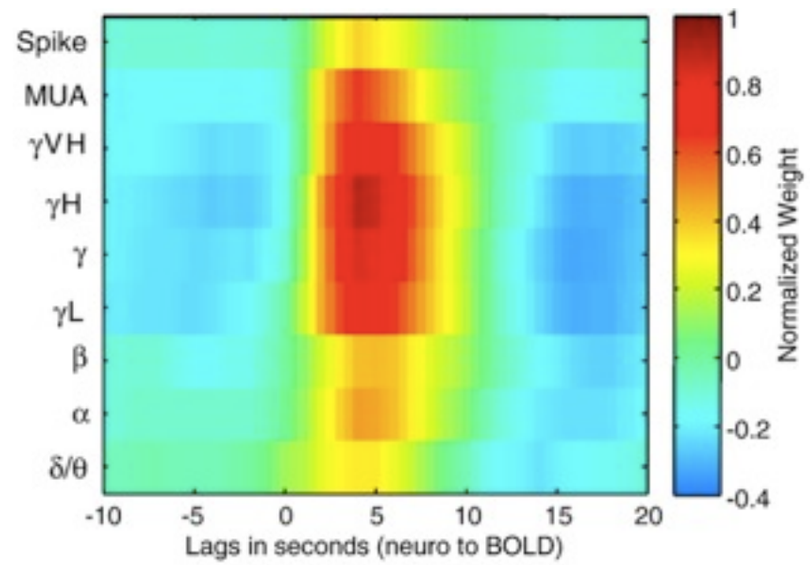
Neural signal



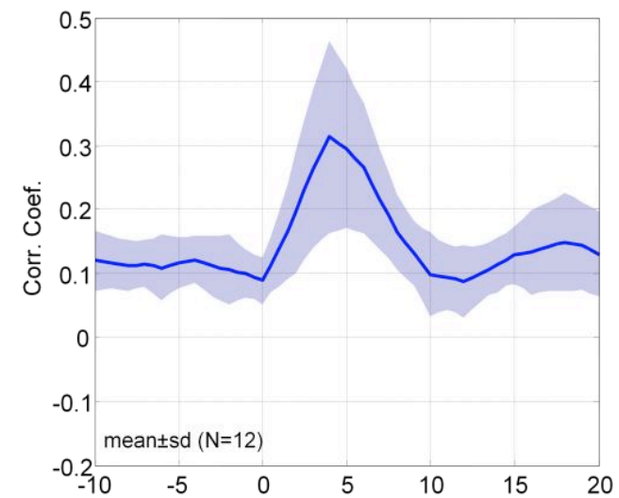
tkCCA Results: Spatial dependencies and HRF



Spatial Dependencies



Haemodynamic Response Function



Canonical Correlogram

Murayama et al., "*Relationship between neural and haemodynamic signals during spontaneous activity studied with temporal kernel CCA*", Magnetic Resonance Imaging, 2010

Summary

- **CCA**
  - finds projections for sets of variables that maximise correlation
- **kernel CCA**
  - extends CCA to non-linear dependencies
  - applicable to high dimensional data
- **Temporal kernel CCA**
  - extends kCCA to data with non-instantaneous correlations
  - computes multivariate convolution from one modality to another

References

H. Hotelling, *"Relations between two sets of variates"*, Biometrika 1936

T.W. Anderson, "*An Introduction to Multivariate Statistical Analysis*", 1958

F. Bießmann, F.C. Meinecke, A. Gretton, A. Rauch, G. Rainer, N.K. Logothetis, K.-R. Müller
"Temporal Kernel CCA and its Application in Multimodal Neuronal Data Analysis"
Machine Learning Journal, 2009

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"Relationship between neural and haemodynamic signals during spontaneous activity studied with tkCCA",
Magnetic Resonance Imaging, 2010