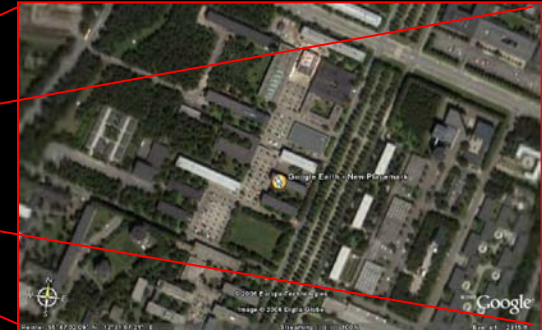
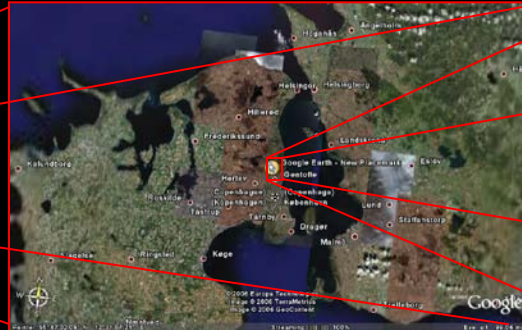
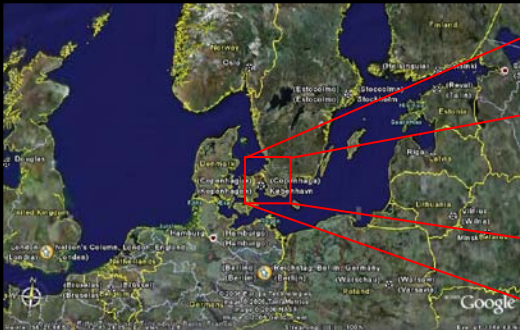




Shift Invariant Data Decomposition

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University Hospital of Copenhagen

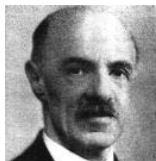


Outline

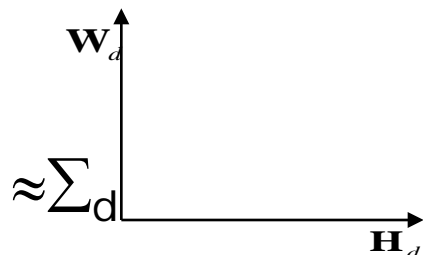
- Shifted Non-negative Matrix Factorization
- Shifted Independent Component analysis
- Generalization to tensors (i.e., the PARAFAC model)
- Shift Invariant Sparse Coding



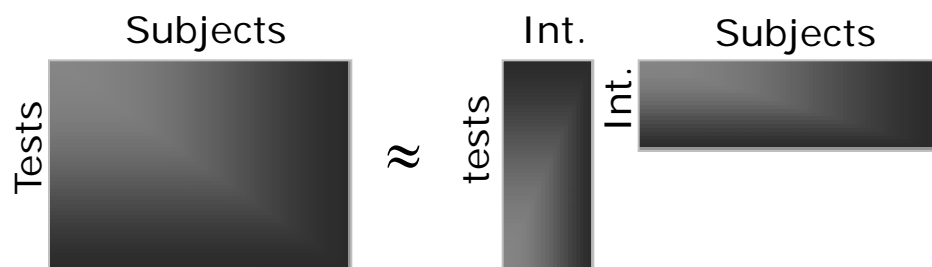
Factor Analysis



Spearman ~ 1900



$$\mathbf{V} \approx \mathbf{W}\mathbf{H}$$



$$\mathbf{V}^{\text{tests} \times \text{subjects}} \approx \mathbf{W}^{\text{tests} \times \text{intelligences}} \mathbf{H}^{\text{intelligences} \times \text{subject}}$$

Independent Component Analysis (ICA)
rows of \mathbf{H} statistically independent

(P. Common, Bell & Sejnowski ~1995)

Non-negative Matrix Factorization (NMF):

$$\mathbf{V}_{n,m}, \mathbf{W}_{n,d}, \mathbf{H}_{d,m} \geq 0$$

(~1970 Lawson, ~1995 Paatero,
~2000 Lee & Seung)



Multiplicative updates

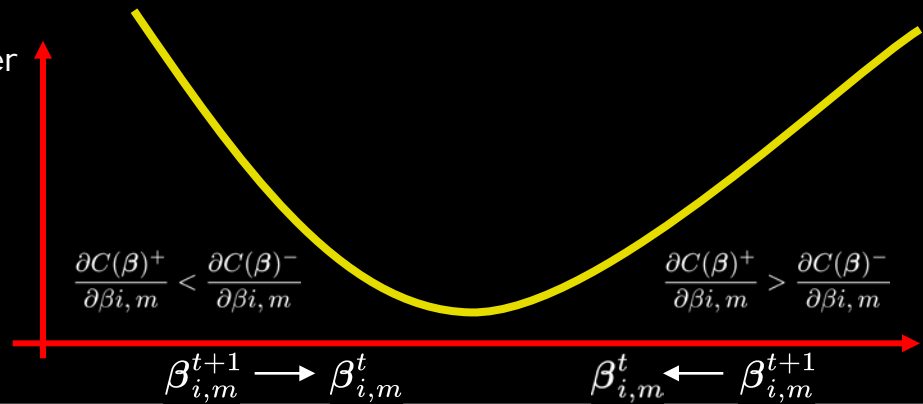
$$\frac{\partial C(\beta)}{\partial \beta_{i,m}} = \frac{\partial C(\beta)^+}{\partial \beta_{i,m}} - \frac{\partial C(\beta)^-}{\partial \beta_{i,m}}$$

$$\beta_{i,m} = \beta_{i,m} - \mu_{i,m} \frac{\partial C(\beta)}{\partial \beta_{i,m}}, \mu_{i,m} = \frac{\beta_{i,m}}{\frac{\partial C(\beta)^+}{\partial \beta_{i,m}}}$$

$$\beta_{i,m} = \beta_{i,m} - \frac{\beta_{i,m}}{\frac{\partial C(\beta)^+}{\partial \beta_{i,m}}} \left(\frac{\partial C(\beta)^+}{\partial \beta_{i,m}} - \frac{\partial C(\beta)^-}{\partial \beta_{i,m}} \right) = \beta_{i,m} \frac{\frac{\partial C(\beta)^-}{\partial \beta_{i,m}}}{\frac{\partial C(\beta)^+}{\partial \beta_{i,m}}}$$

Step size parameter α

$$\beta_{i,m}^{t+1} \leftarrow \beta_{i,m}^t \left(\frac{\frac{\partial C(\beta)^-}{\partial \beta_{i,m}^t}}{\frac{\partial C(\beta)^+}{\partial \beta_{i,m}^t}} \right)^\alpha$$





Non-negative matrix factorization

$$\mathbf{V}_{i,j} \geq 0, \quad \mathbf{W}_{i,d} \geq 0 \quad \text{and} \quad \mathbf{H}_{d,j} \geq 0$$

$$C_{LS} = \frac{1}{2} \|\mathbf{V} - \mathbf{WH}\|_F^2 = \frac{1}{2} \sum_{i,j} (\mathbf{V}_{i,j} - (\mathbf{WH})_{i,j})^2$$

$$\mathbf{W}_{i,d} \leftarrow \mathbf{W}_{i,d} \frac{(\mathbf{VH}^T)_{i,d}}{(\mathbf{WHH}^T)_{i,d}}$$

$$\mathbf{H}_{d,j} \leftarrow \mathbf{H}_{d,j} \frac{(\mathbf{W}^T \mathbf{V})_{d,j}}{(\mathbf{W}^T \mathbf{WH})_{d,j}}$$

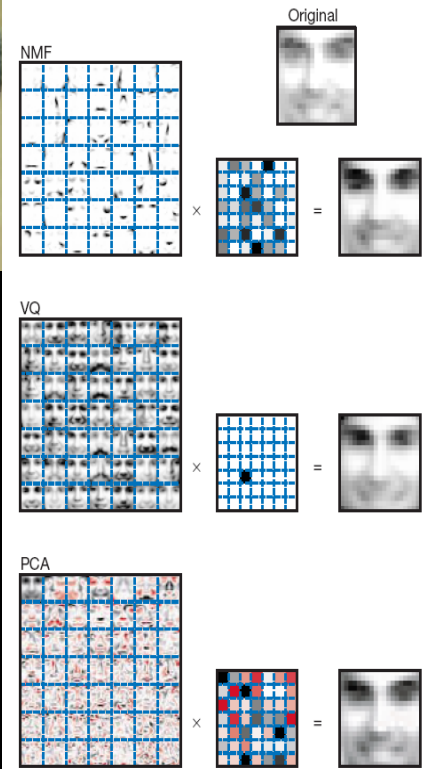
$$C_{KL} = \sum_{i,j} \mathbf{V}_{i,j} \log \frac{\mathbf{V}_{i,j}}{(\mathbf{WH})_{i,j}} - \mathbf{V}_{i,j} + (\mathbf{WH})_{i,j}$$

$$\mathbf{W}_{i,d} \leftarrow \mathbf{W}_{i,d} \frac{\sum_j \frac{\mathbf{V}_{i,j}}{(\mathbf{WH})_{i,j}} \mathbf{H}_{d,j}}{\sum_j \mathbf{H}_{d,j}}$$

$$\mathbf{H}_{d,j} \leftarrow \mathbf{H}_{d,j} \frac{\sum_i \mathbf{W}_{i,d} \frac{\mathbf{V}_{i,j}}{(\mathbf{WH})_{i,j}}}{\sum_i \mathbf{W}_{i,d}}$$



(Lee & Seung - 2001)



(Some other approaches:
Active Set, projected gradient,
barrier functions, exponentiation)

NMF gives Part based representation
(Lee & Seung – Nature 1999)



Maximum likelihood (ML) ICA approach

$$[\mathbf{A}', \mathbf{S}', \mathbf{H}'] = \text{SVD}(\mathbf{X})$$

$$\mathbf{W}' = \mathbf{A}'\mathbf{S}'$$

Notice decomposition then ambiguous since

$$\mathbf{W}\mathbf{H} = (\mathbf{W}'\mathbf{Q}^{-1})(\mathbf{Q}\mathbf{H}') = \mathbf{W}'\mathbf{H}'$$

Thus ICA forms objective for ambiguity \mathbf{Q} that minimizes:

Equivalently we derive two step procedure
 Shift Invariant Subspace Analysis (SISA)

Shifted Independent Component Analysis (SICA)

ICA-ML

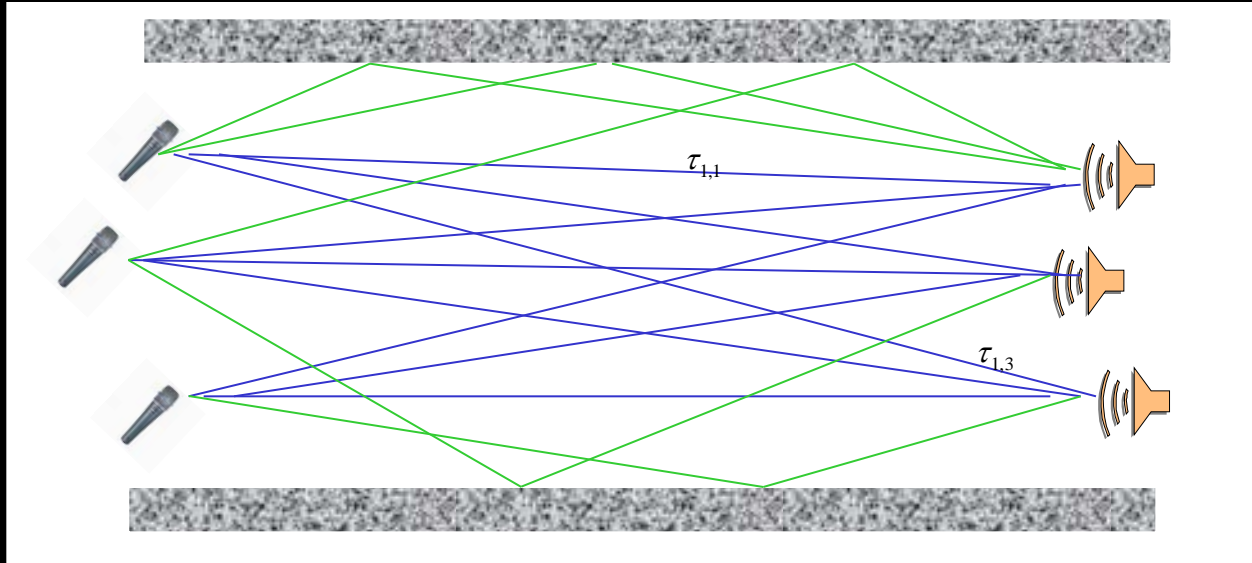
$$p(\mathbf{H}|\mathbf{Q}) = \prod_m p(\mathbf{H}_m|\mathbf{Q}) = \prod_m |\det(\mathbf{Q})| p(\mathbf{Q}\mathbf{H}_m)$$

Assume Independence

Change of variable principle



The shift problem



Convolutional ICA/NMF
(echo effects, Smaragdis 2003)

Shifted ICA/NMF
(One specific delay between each sensor and source)

$$\mathbf{V}_{n,m} = \sum_{d,\tau} \mathbf{W}_{n,d}^\tau \mathbf{H}_{d,m-\tau} + \mathbf{E}_{n,m}$$

$$\mathbf{V}_{n,m} = \sum_d \mathbf{W}_{n,d} \mathbf{H}_{d,m-\tau_{n,d}} + \mathbf{E}_{n,m}$$



History of shift

- Bell & Sejnowski 1995
(Sketched how to handle time delays in networks)
- Torkkola 1996
(Further developed Bell and Sejnowski's work)
- Emile & Comon 1998
(delay in model based on equally mixed sources formed by moving averages)
- Hong and Harshman 2003 – shifted factor analysis
(a procedure based on exhaustive search over integer shifts – model conjectured unique)
- Yeredor 2003 (Solved the ICA model with shifts by joint diagonalization (sources=sensors) of the source cross spectra based on the AC-DC algorithm with non-integer shifts for the 2x2 system)
- Yeredor 2005 (extension to complex signals)





Why shifted ICA/NMF

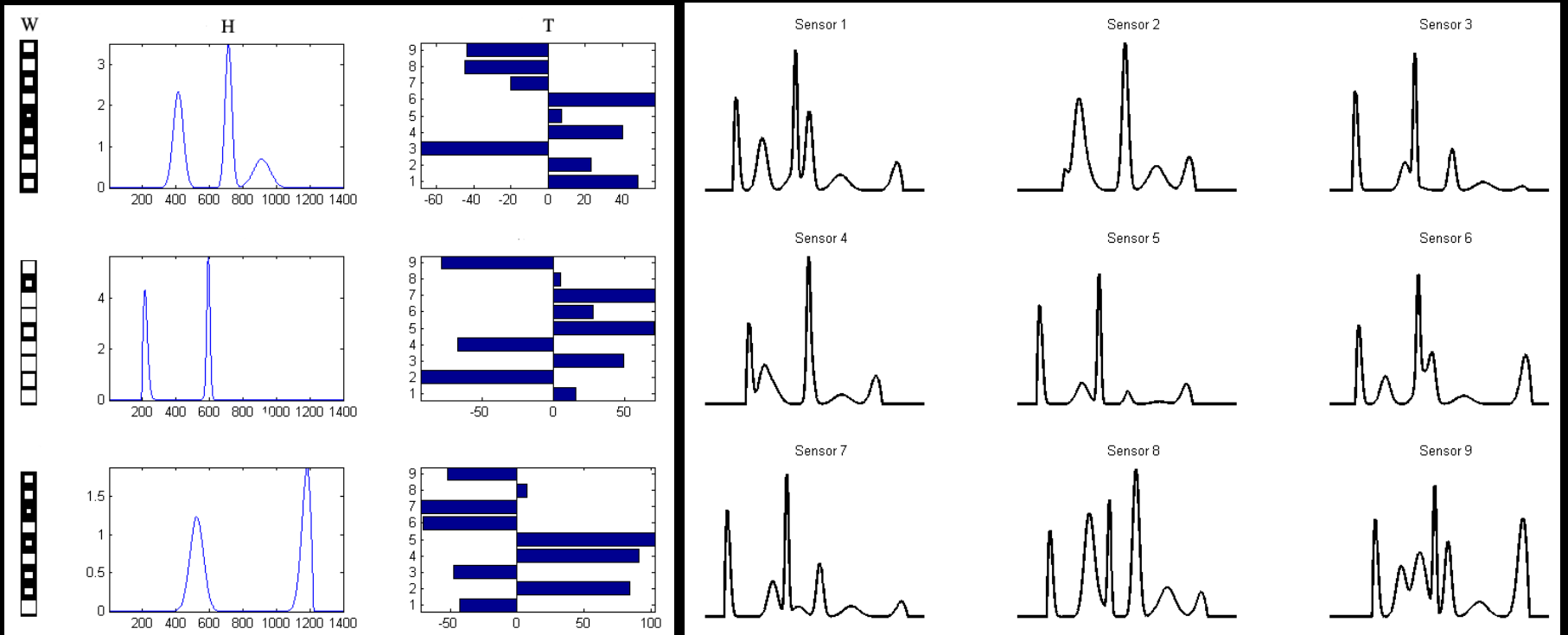
Causes of shifts for instance

Doppler effect, Time of arrival differences

- Magnetic resonance spectra
(Du et al, 2005)
- Astronomical spectrometers (red shift)
(Pauca et al. 2006)
- Fluorescence spectra
(Gobinet et al. 2004)
- PET imaging
(Kim et al. 2001, Lee et al., 2001,
Bödvarsson et al. 2007)
- Sound recording (delays between source and sensor
due to propagation delay)



Generative model





Notation and LS-objective

- \mathbf{U} and $\tilde{\mathbf{U}}$ denotes same matrix in time and frequency domain respectively.
- $\tilde{\mathbf{U}}^H$ denotes the conjugate transpose of $\tilde{\mathbf{U}}$
- $\mathbf{U}_{d,m-\tau} \sim \tilde{\mathbf{U}}_{d,f} e^{-i2\pi \frac{f-1}{M} \tau}$
- $\mathbf{U} \bullet \mathbf{V}$ denotes the direct product, i.e. element-wise multiplication.
- $(e^{-i2\pi \frac{f-1}{M} \tau})_{n,d} = e^{-i2\pi \frac{f-1}{M} \tau_{n,d}}$.
- $\tilde{\mathbf{U}}(f) = \mathbf{U} \bullet e^{-i2\pi \frac{f-1}{M} \tau}$
- \mathbf{U}_d d^{th} column, \mathbf{U}_n , n^{th} row and $\mathbf{U}_{n,d}$ a given element of \mathbf{U} .

$$\begin{aligned}
 C_{LS}(W, H) &= \frac{1}{2} \sum_{n,m} (\mathbf{V}_{n,m} - \sum_d \mathbf{W}_{n,d} \mathbf{H}_{d,m-\tau_{n,d}})^2 \\
 &= \frac{1}{2M} \|\tilde{\mathbf{V}}_f - (\mathbf{W} \bullet e^{-i2\pi \frac{f-1}{M} \tau}) \tilde{\mathbf{H}}_f\|_F^2 = \frac{1}{2M} \|\tilde{\mathbf{V}}_f - \mathbf{W}^{(f)} \tilde{\mathbf{H}}_f\|_F^2
 \end{aligned}$$

Follows from Parsevals identity with the above notation



W update

Let $\tilde{\mathbf{H}}_{d,f}^{(n)} = \tilde{\mathbf{H}}_{d,f} e^{-i2\pi \frac{f-1}{M} \tau_{n,d}}$ denote the delayed version of the source signal $\tilde{\mathbf{H}}_{d,f}$ to the n^{th} channel. The shift ICA/NMF model can then be stated as

$$\mathbf{V}_{n,:} = \mathbf{W}_{n,:} \mathbf{H}^{(n)} + \mathbf{E}_{n,:}.$$

This is the regular ICA/NMF problem which can be solved by the least squares ICA/NMF-update

$$\begin{aligned} \text{SISA} : \mathbf{W}_{n,:} &= \mathbf{V}_{n,:} / (\mathbf{H}^{(n)} \mathbf{H}^{(n)T}), \\ \text{NMF} : \mathbf{W}_{n,d} &= \mathbf{W}_{n,d} \frac{\mathbf{V}_{n,:} \mathbf{H}_{d,:}^{(n)T}}{\mathbf{W}_{n,:} \mathbf{H}^{(n)} \mathbf{H}_{d,:}^{(n)T}}. \end{aligned}$$



H update

$$C_{LS} = \frac{1}{2M} \|\tilde{\mathbf{V}}_f - \tilde{\mathbf{W}}^{(f)} \tilde{\mathbf{H}}_f\|_F^2$$

$$\mathbf{G}_f = \frac{\partial C_{LS}}{\partial \tilde{\mathbf{H}}_f} = -\frac{1}{M} \tilde{\mathbf{W}}^{(f)H} (\tilde{\mathbf{X}}_f - \tilde{\mathbf{W}}^{(f)} \tilde{\mathbf{H}}_f)$$

ShiftNMF

$$\tilde{\mathbf{G}}_f^+ = \frac{1}{M} \tilde{\mathbf{W}}^{(f)H} \tilde{\mathbf{W}}^{(f)} \tilde{\mathbf{H}}_f$$

$$\tilde{\mathbf{G}}_f^- = \frac{1}{M} \tilde{\mathbf{W}}^{(f)H} \tilde{\mathbf{X}}_f$$

$$\mathbf{H}_{d,n} = \mathbf{H}_{d,n} \left(\frac{\mathbf{G}_{d,n}^-}{\mathbf{G}_{d,n}^+} \right)^\alpha$$

SISA

$$\mathbf{G}_f = (\tilde{\mathbf{W}}^{(f)\top} \tilde{\mathbf{W}}^{(f)}) \setminus \tilde{\mathbf{X}}_f$$



Update of the shifts (τ)

$$C_{LS} = \frac{1}{2M} \sum_f (\tilde{\mathbf{v}}_f - (\mathbf{W} \bullet e^{-i2\pi \frac{f-1}{M} \tau}) \tilde{\mathbf{H}}_f)$$

Warning!
Prone to
local minima

where τ is the time delay to be estimated
 by the NLS algorithm



Update of shifts (τ) based on Cross-correlation

$$\mathbf{R}_{n,m} = \mathbf{V}_{n,m} - \sum_{d \neq d'} \mathbf{W}_{n,d} \mathbf{H}_{d,m-\tau_{n,d}}$$

$$C_{LS} = \frac{1}{2} \sum_{n,m} (\mathbf{V}_{n,m} - \sum_d \mathbf{W}_{n,d} \mathbf{H}_{d,m-\tau_{n,d}})^2$$

$$= \frac{1}{2} \sum_{n,m} (\mathbf{R}_{n,m} - \mathbf{W}_{n,d'} \mathbf{H}_{d',m-\tau_{n,d'}})^2$$

$$= \frac{1}{2} \|\mathbf{R}\|^2 - \sum_n \mathbf{W}_{n,d'} \sum_m \mathbf{R}_{n,m} \mathbf{H}_{d',m-\tau_{n,d'}} + \frac{1}{2} \|\mathbf{W}\mathbf{H}\|^2$$

Independent of τ

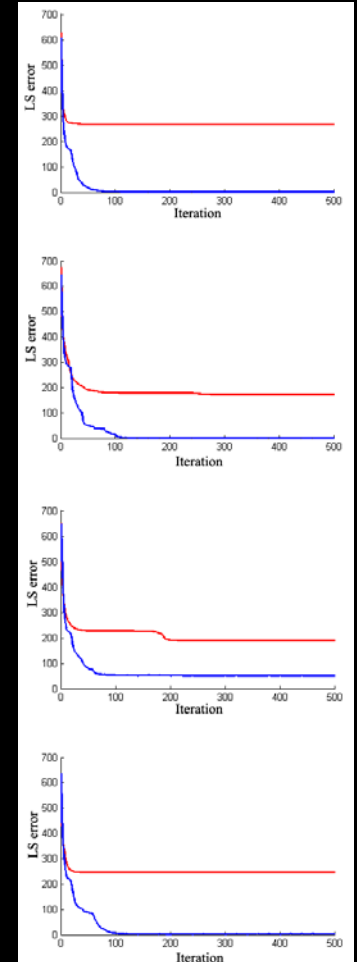
Cross correlation R and H

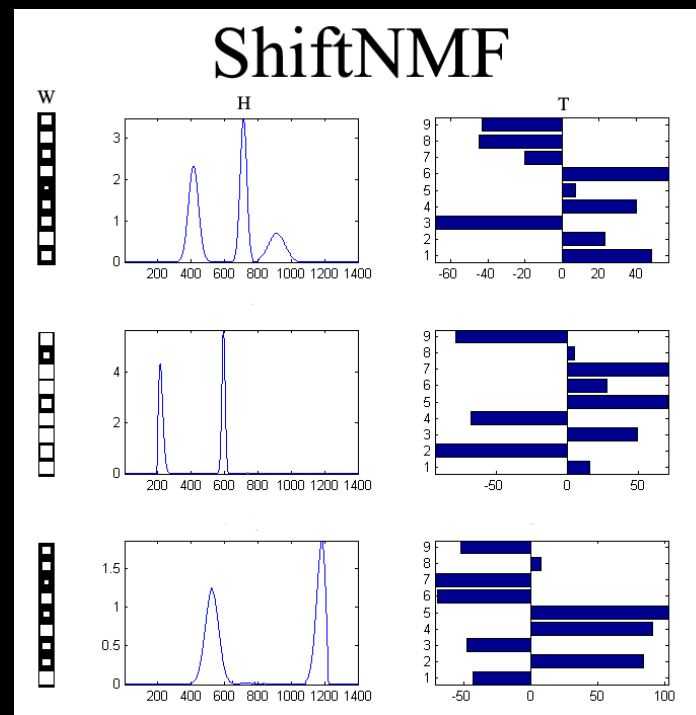
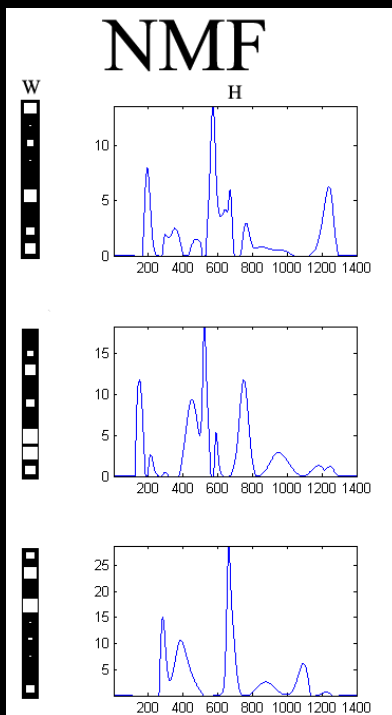
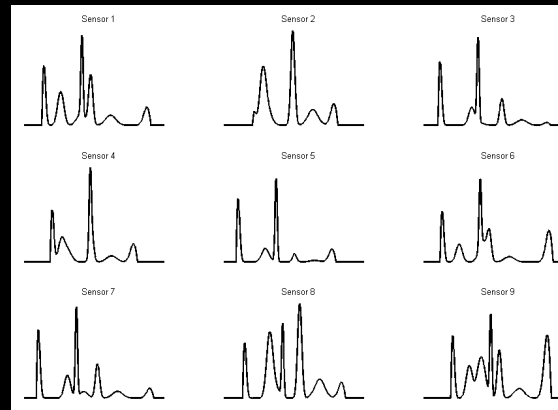
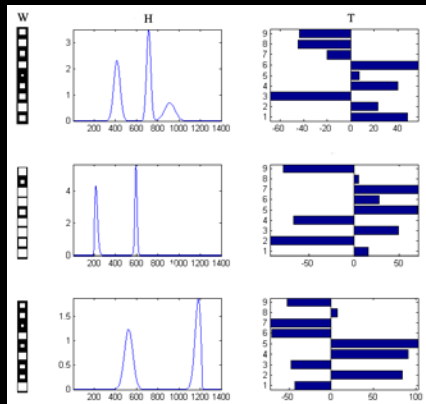
Independent of τ

$$\tilde{\mathbf{c}}_f = \tilde{\mathbf{R}}_{n,f}^* \tilde{\mathbf{H}}_{d',f} \quad t = \arg \max_m \mathbf{c}_m, \quad \tau_{n,d'} = t - (M + 1).$$

The value of $\mathbf{W}_{n,d'}$ corresponding to this delay is given by

$$\mathbf{W}_{n,d'} = \frac{\mathbf{c}_t}{\mathbf{H}_{d',:} \mathbf{H}_{d',:}^T}$$

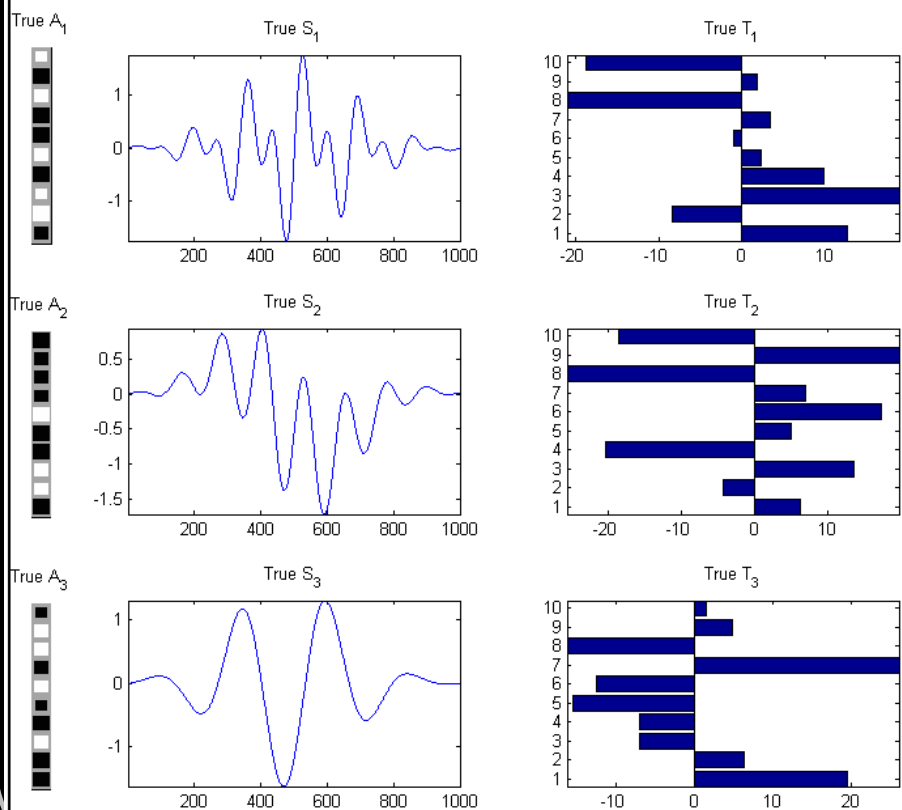




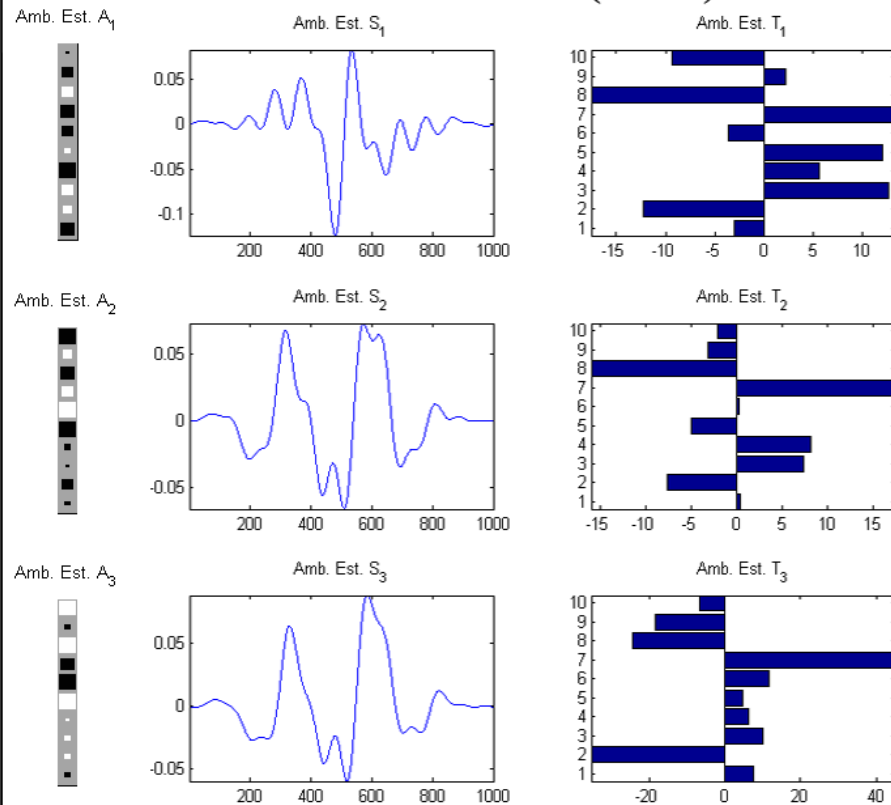


Shift Invariant Subspace Analysis

Simulated Factors



Estimated Factors (SISA)





Shifted Independent Component Analysis

Define, $\tilde{\mathbf{U}}_f = \tilde{\mathbf{Q}}^{(f)} \tilde{\mathbf{H}}_f$, i.e. the sources at frequency f when transformed according to the rotation and shift ambiguity described in the previous section. The ambiguity can be resolved by maximizing the log-likelihood assuming the (non-gaussian) Laplace distribution $p(\tilde{\mathbf{U}}_f) \propto e^{-|\tilde{\mathbf{U}}_{d,f}|}$, i.e.

$$p(\tilde{\mathbf{H}}_f | \mathbf{Q}, \hat{\boldsymbol{\tau}}) = \prod_f p(\tilde{\mathbf{H}}_f | \mathbf{Q}, \hat{\boldsymbol{\tau}}) = \prod_f |\det(\tilde{\mathbf{Q}}^{(f)})| p(\tilde{\mathbf{Q}}^{(f)} \tilde{\mathbf{H}}_f) \quad (1)$$

Such that the log-likelihood as a function of \mathbf{Q} and $\hat{\boldsymbol{\tau}}$ becomes

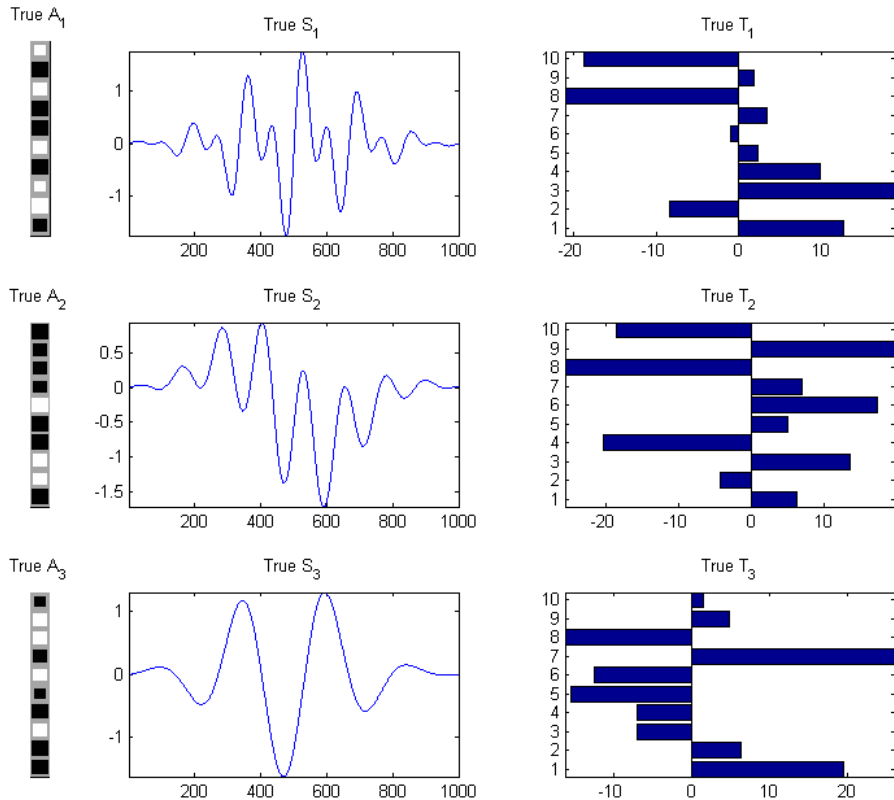
$$\mathcal{L}(\mathbf{Q}, \hat{\boldsymbol{\tau}}) = \sum_f \ln |\det(\tilde{\mathbf{Q}}^{(f)})| - \sum_d |\tilde{\mathbf{Q}}^{(f)} \tilde{\mathbf{H}}_f|_d \quad (2)$$

By maximizing $\mathcal{L}(\mathbf{W}, \hat{\boldsymbol{\tau}})$ \mathbf{W} and $\hat{\boldsymbol{\tau}}$ is estimated and a new unambiguous \mathbf{H} solution found by $\tilde{\mathbf{H}}_f = \tilde{\mathbf{Q}}^{(f)} \tilde{\mathbf{H}}_f$. The corresponding mixing and delays can be estimated alternating between the \mathbf{W} and $\boldsymbol{\tau}$ update. We initialized \mathbf{W} as $\mathbf{W} = \mathbf{W}\mathbf{Q}^{-1}$ and $\tau_{i,d}$ by the cross-correlation procedure.

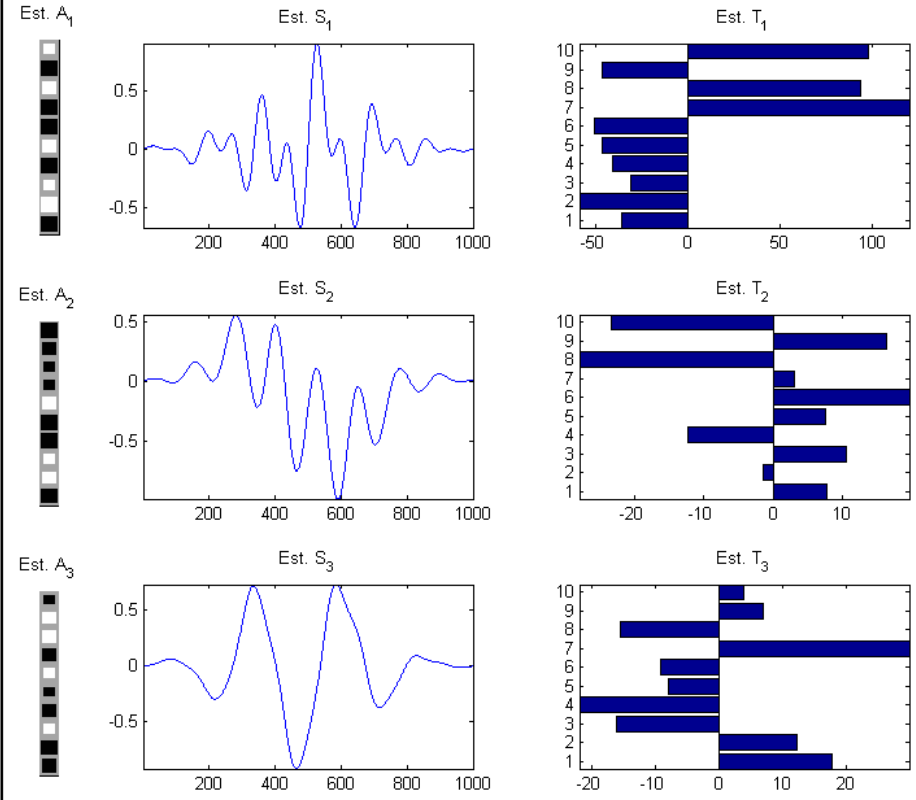


Shifted Independent Component Analysis

Simulated Factors



Estimated Factors (SICA)





Algorithm assumptions

- Sources \mathbf{H} and measured signal \mathbf{V} have to be periodic

If signals are not periodic a window function can be employed. However this is not trivial to implement in the τ -update and slows down the algorithm significantly. Zero padding is simple and fast but introduces a bias towards small delays.

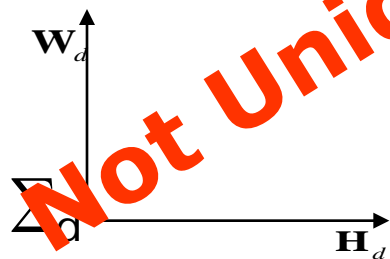
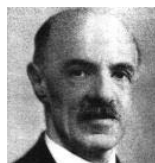
- Noise \mathbf{E} assumed homoscedatic (normal) iid.

If non-homoscedatic use weighted least squares. Algorithm works for Least squares due to Parseval's identity. No such identity exists for other types than the least squares objective.



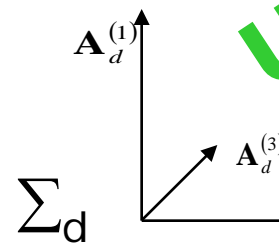
Extensions to tensors

Factor Analysis



$$\mathbf{V}_{i_1 i_2} \approx \sum_{d=1}^D \mathbf{W}_{i_1 d} \mathbf{H}_{i_2 d}$$

PARAFAC decomposition



$$\mathcal{V}_{i_1 i_2 i_3} \approx \sum_{d=1}^D \mathbf{A}_{i_1 d}^{(1)} \mathbf{A}_{i_2 d}^{(2)} \mathbf{A}_{i_3 d}^{(3)}$$



Unique



The Candecomp/PARAFAC (CP) model

$$\mathcal{X}_{i,j,k} = \sum_d^D \mathbf{A}_{i,d} \mathbf{B}_{j,d} \mathbf{C}_{k,d} + \mathcal{E}_{i,j,k}$$

$$\mathbf{X}_{(1)} = \mathbf{A}(\mathbf{C} \odot \mathbf{B})^T + \mathbf{E}_{(1)} \Rightarrow \mathbf{A} \leftarrow \mathbf{X}_{(1)}(\mathbf{C} \odot \mathbf{B})^{T\dagger}$$

$$\mathbf{X}_{(2)} = \mathbf{B}(\mathbf{C} \odot \mathbf{A})^T + \mathbf{E}_{(2)} \Rightarrow \mathbf{B} \leftarrow \mathbf{X}_{(2)}(\mathbf{C} \odot \mathbf{A})^{T\dagger}$$

$$\mathbf{X}_{(3)} = \mathbf{C}(\mathbf{B} \odot \mathbf{A})^T + \mathbf{E}_{(3)} \Rightarrow \mathbf{C} \leftarrow \mathbf{X}_{(3)}(\mathbf{B} \odot \mathbf{A})^{T\dagger}$$

$$(\mathbf{C} \odot \mathbf{B}) = (\mathbf{C}_1 \otimes \mathbf{B}_1 \ \mathbf{C}_2 \otimes \mathbf{B}_2 \ \dots \ \mathbf{C}_D \otimes \mathbf{B}_D) \quad X_{(1)} = X^{I \times JK}, \quad X_{(2)} = X^{J \times IK}, \quad X_{(3)} = X^{K \times IJ}$$

The CP model is unique if

$$k_{\mathbf{A}} + k_{\mathbf{B}} + k_{\mathbf{C}} \geq 2D + 2$$

where $k_{\mathbf{A}}$ is the k-rank denoting the smallest subset of columns of \mathbf{A} that is guaranteed to be linearly independent. Thus, $k_{\mathbf{A}} \leq \text{rank}(\mathbf{A})$.



Shifted CP model

$$\mathcal{X}_{i,j,k} = \sum_d^D \mathbf{A}_{i,d} \mathbf{B}_{j-\tau_{k,d},d} \mathbf{C}_{k,d} + \mathcal{E}_{i,j,k}$$

$$\begin{aligned} \mathbf{X}_{(1)} &= \mathbf{AZ}^T + \mathbf{E}_{(1)} & \Rightarrow & \mathbf{A} \leftarrow \mathbf{X}_{(1)} \mathbf{Z}^{T\dagger} \\ \tilde{\mathbf{X}}_{(2)f,:} &= \tilde{\mathbf{B}}_{f,:} (\tilde{\mathbf{C}}^{(f)} \odot \mathbf{A})^T + \tilde{\mathbf{E}}_{(2)f,:} & \Rightarrow & \tilde{\mathbf{B}}_{f,:} \leftarrow \tilde{\mathbf{X}}_{(2)f,:} (\tilde{\mathbf{C}}^{(f)} \odot \mathbf{A})^{T\dagger} \\ \mathbf{X}_{(3)k,:} &= \mathbf{C}_{k,:} (\mathbf{B}^{(k)} \odot \mathbf{A})^T + \mathbf{E}_{(3)k,:} & \Rightarrow & \mathbf{C}_{k,:} \leftarrow \mathbf{X}_{(3)k,:} (\mathbf{B}^{(k)} \odot \mathbf{A})^{T\dagger} \end{aligned}$$

$$\mathbf{r}_j^{(k,d')} = \sum_i \mathcal{R}_{i,j,k}^{d'} \mathbf{A}_{i,d'} \quad \tilde{\mathbf{c}}_{k,d'}(f) = \tilde{\mathbf{r}}_f^{(k,d')*} \tilde{\mathbf{B}}_{f,d'}$$

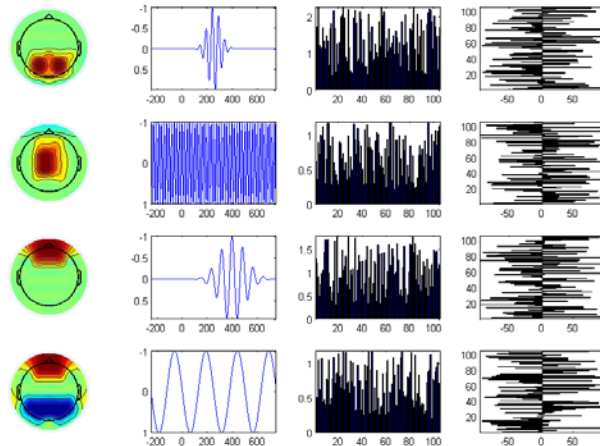
$$t_{k,d'} = \arg \max_t |\mathbf{c}_{k,d'}(t)| \quad \tau_{k,d'} = t_{k,d'} - (J + 1).$$

$$\mathbf{C}_{k,d'} = \frac{\mathbf{c}_{k,d'}(t_{k,d'})}{\mathbf{B}_{d'}^T \mathbf{B}_{d'}}.$$

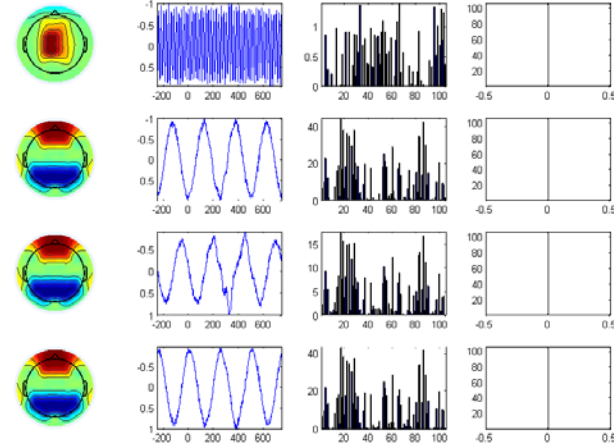


Synthetic EEG data

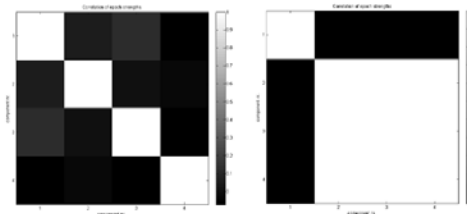
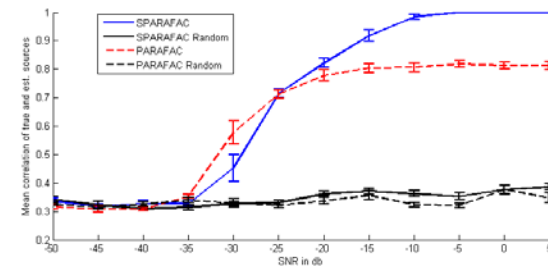
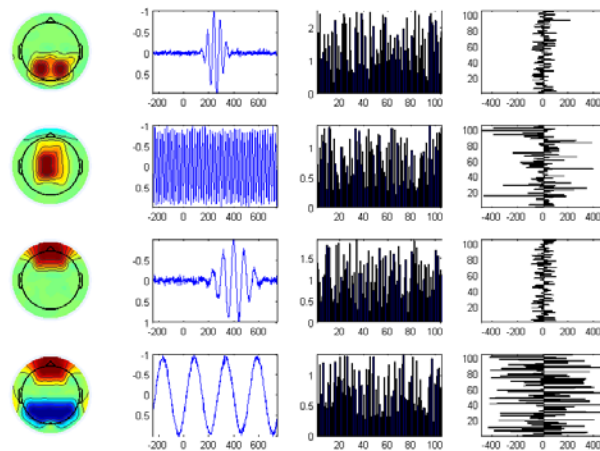
True components



Est. comp. PARAFAC



Est. comp. SPARAFAC

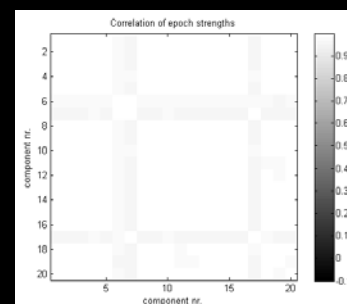
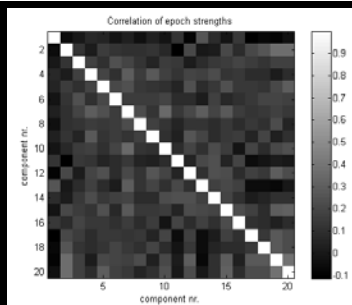
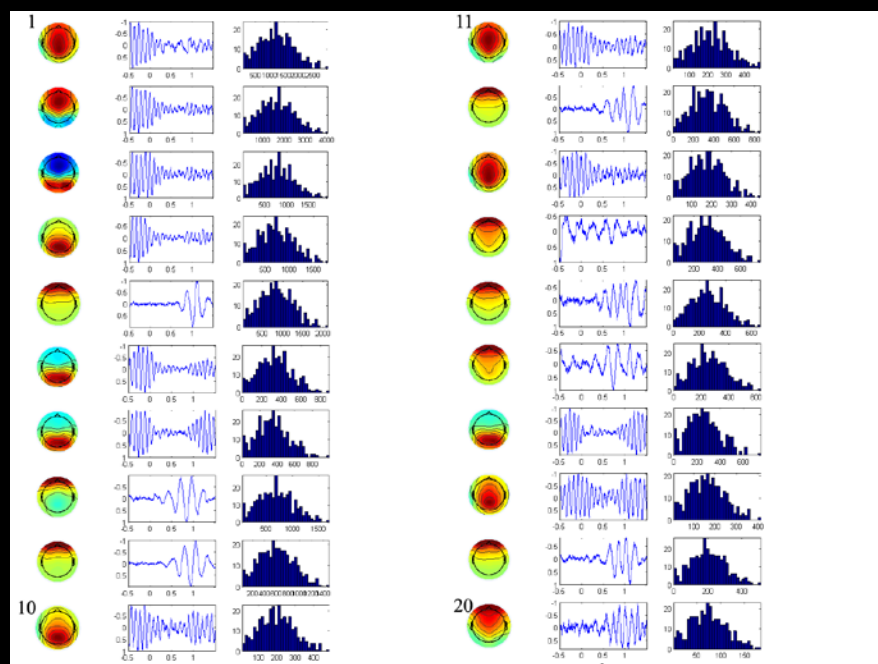
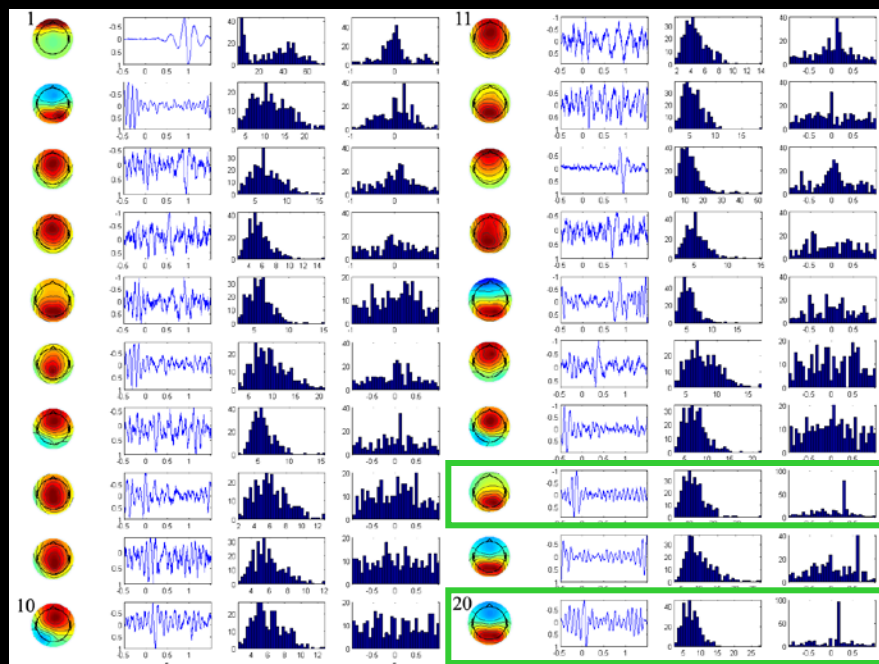




EEG data from Visual Paradigm

Shifted CP

CP



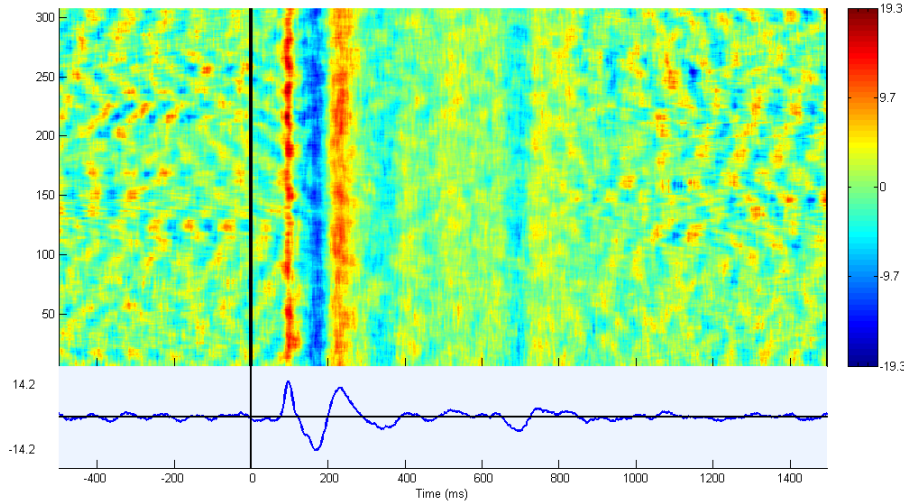


True Evoked Potential (EP)

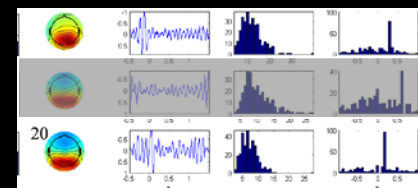
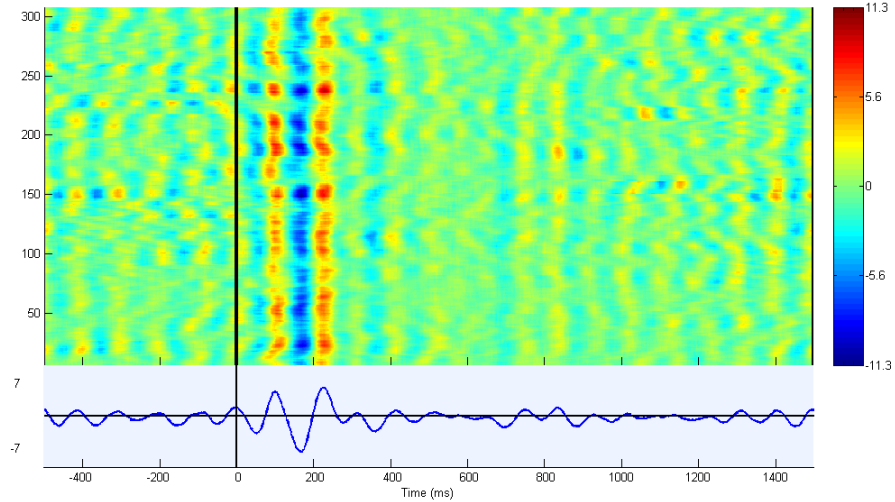
Reconstructed EP component 18 and 20



PO4



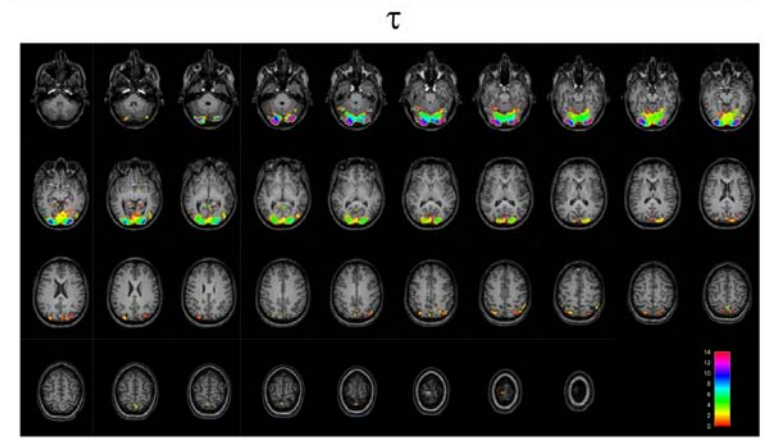
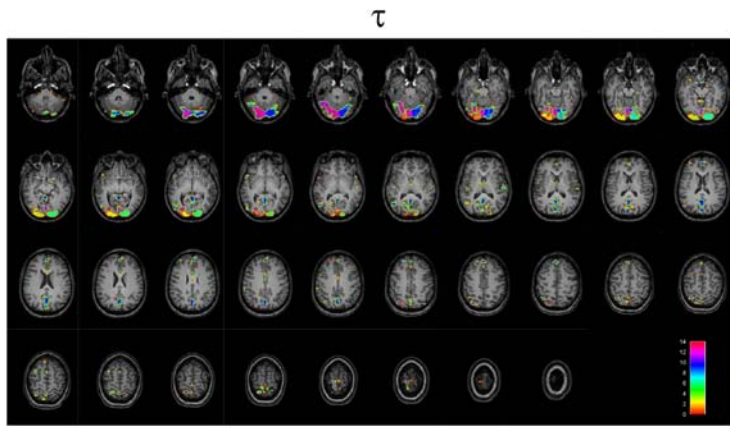
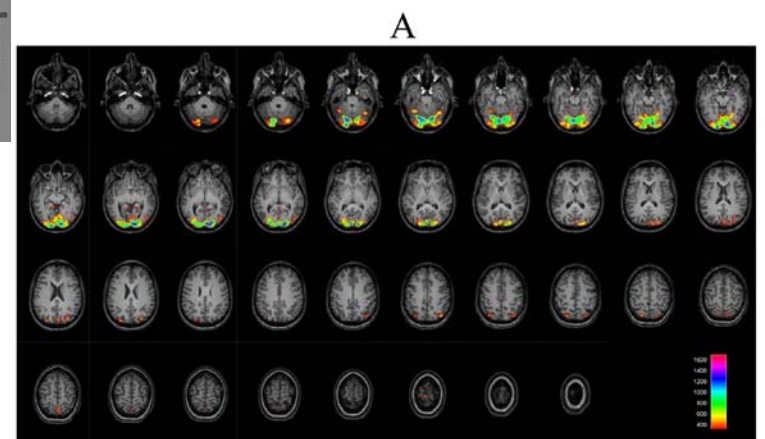
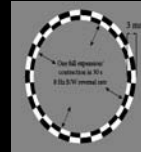
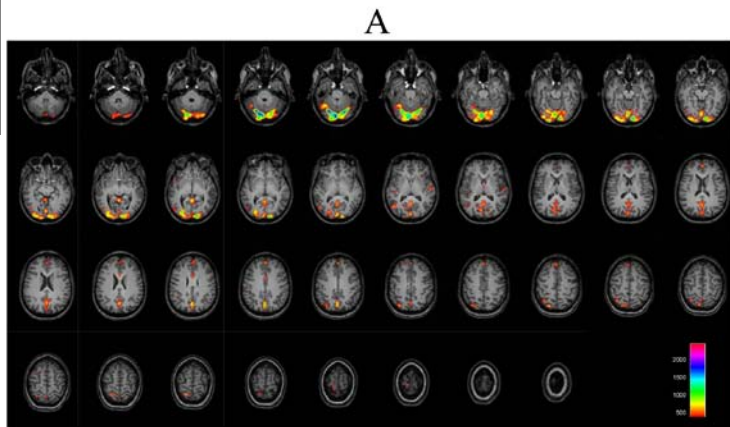
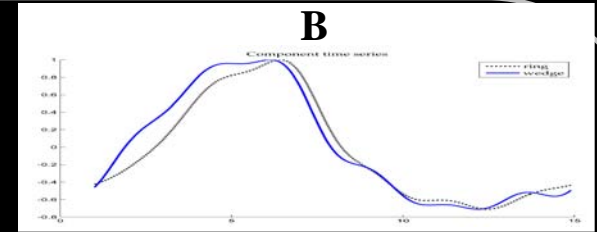
PO4





fMRI data visual paradigm

$$\mathcal{X}_{i,j,k} = \sum_d^D \mathbf{A}_{i,d} \mathbf{B}_{j-\tau_{k,d},d} \mathbf{C}_{k,d} + \mathcal{E}_{i,j,k}$$



(Kristoffer Hougaard Madsen)

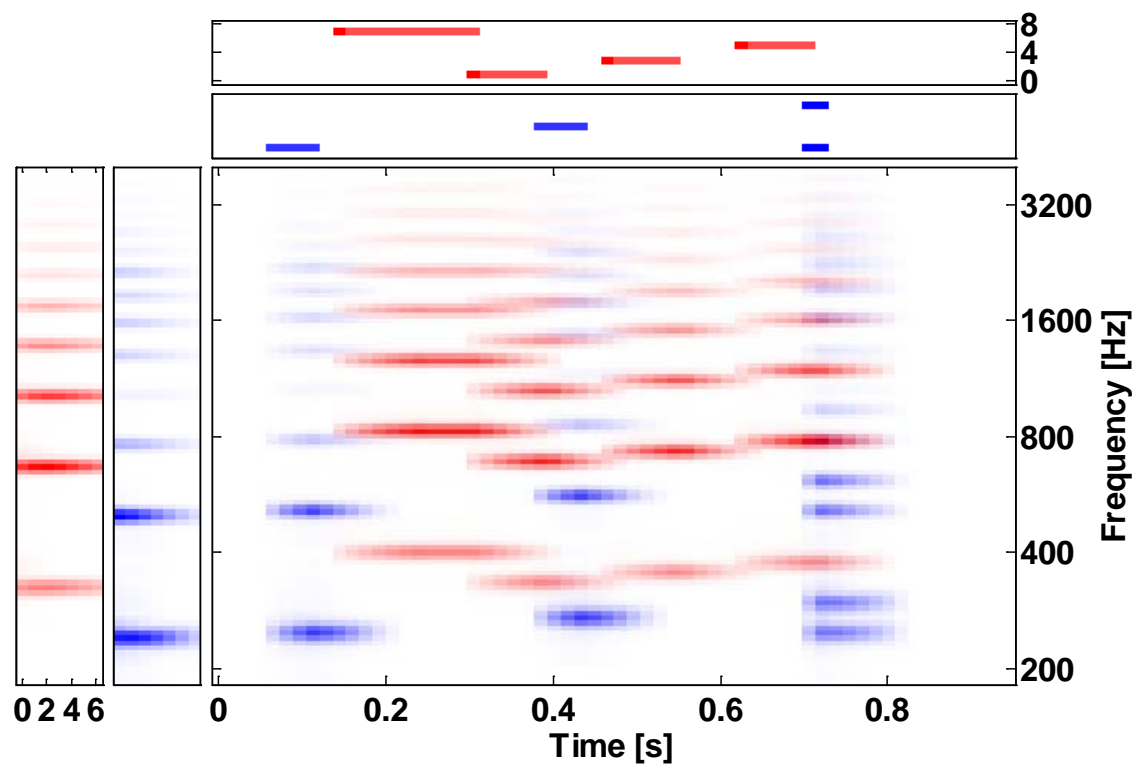


Shift invariant sparse coding

(Solving the shift problem using sparse coding)

$$X(x, y) \approx \sum_d \sum_{u, v} \alpha_d(u, v) \Phi_d(x - u, y - v)$$

Non-negative matrix 2D
de-convolution introduced in:
Schmidt and Mørup, 2006d
Extended to Sparse coding
Mørup et al. 2007b



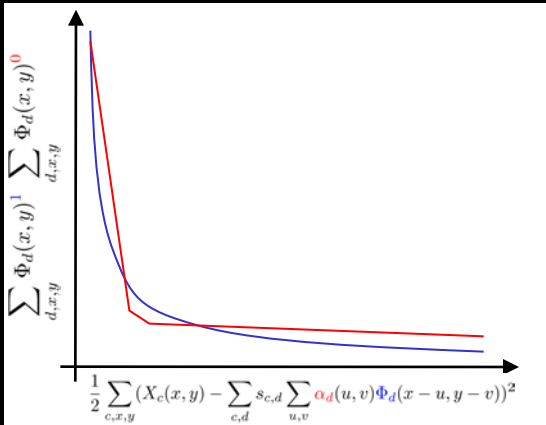


Objective function: **Reconstruction**

L₁ norm

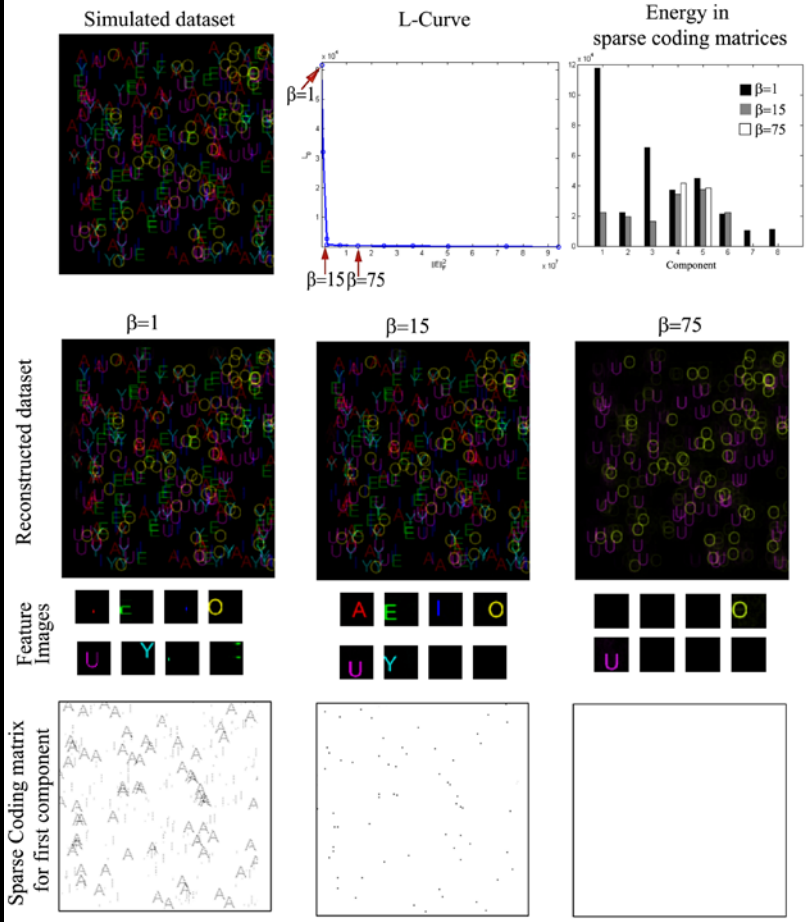
$$\frac{1}{2} \sum_{c,x,y} (X_c(x,y) - \sum_{c,d} s_{c,d} \sum_{u,v} \alpha_d(u,v) \Phi_d(x-u, y-v))^2 + \beta \sum_{d,x,y} \Phi_d(x,y)$$

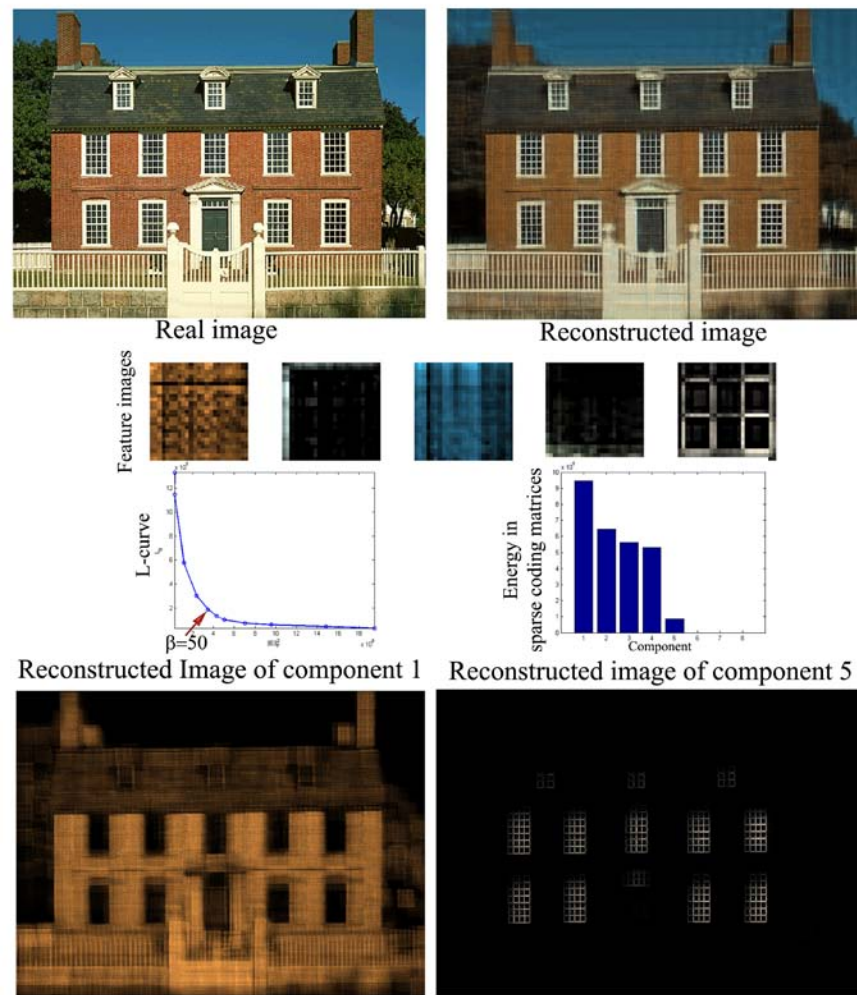
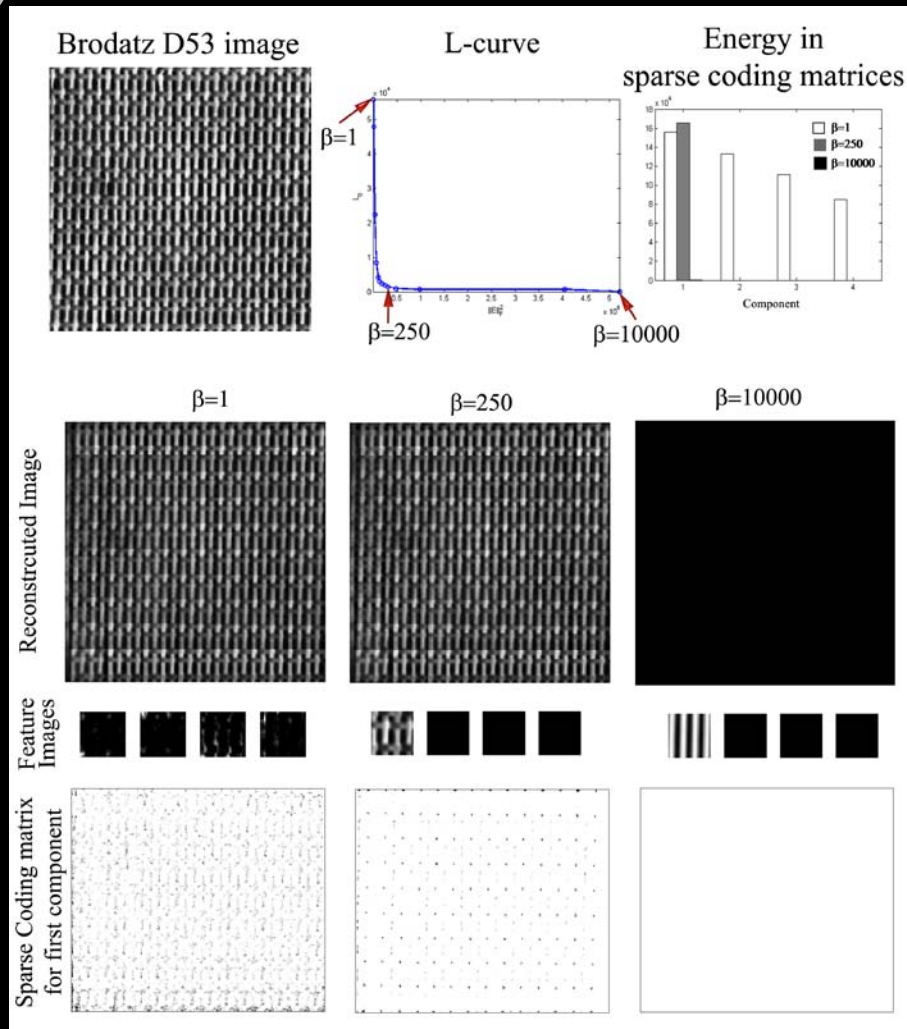
Solved by multiplicative updates (i.e., $X, s, \alpha, \Phi \geq 0$)



$$I_c(u,v) = s_{c,d} \alpha_d(u,v) \rightarrow$$

$$\Phi_d(x-u, y-v) \rightarrow$$





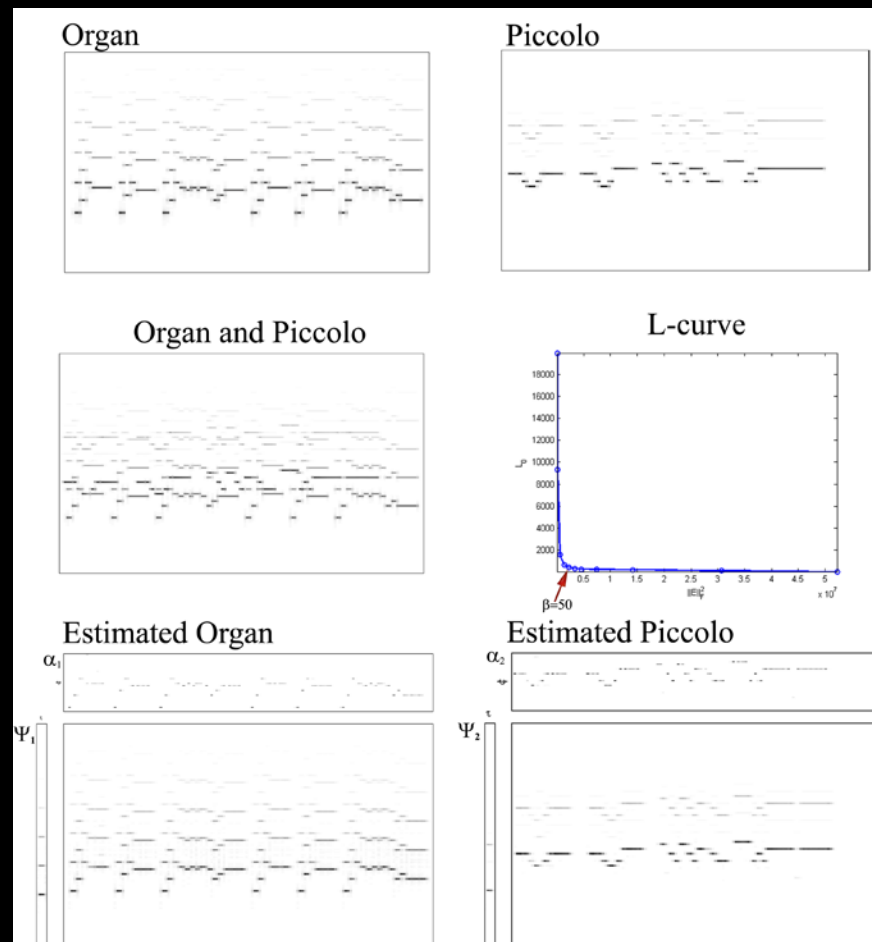
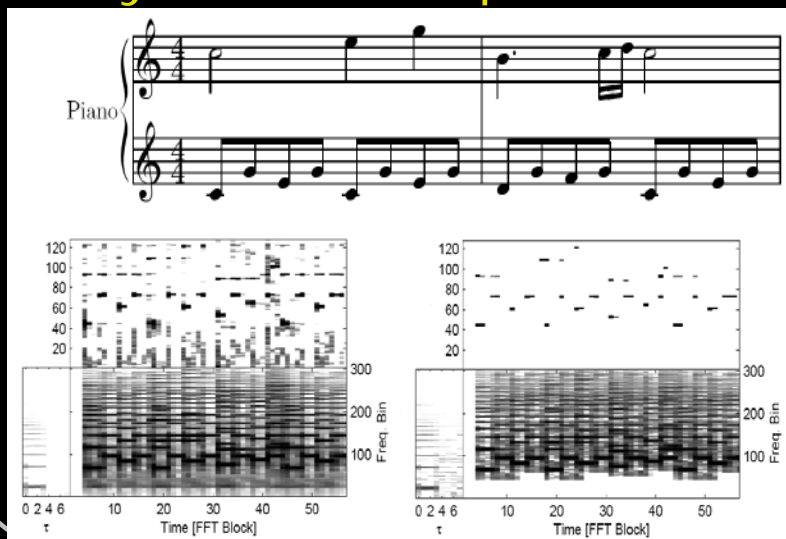


Analysis of mono signal of mixed Organ and Piccolo

(Music data taken from Y.-G. Zhang, 2005)

$$X(x, y) \approx \sum_{d, u, v} \alpha_d(u, v) \Psi_d(x - u, y - v)$$

Analysis of mono piano music





Conclusion:

Modelling data using shift invariance seems highly relevant for a wide range of data types.

Two approaches presented: 1) estimation of specific shift in the frequency domain 2) Estimation of shifts using sparse coding.

Degeneracies encountered in the Candecomp/PARAFAC (CP) model appear to vanish when allowing for shifts. Thus degeneracy in CP often a result of sources of the data being shifted.

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