ℓ_1 Approaches to PCA and ICA

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Projekt: Signalverarbeitung

Tutorium: Trennung von Datenquellen in unkorrelierte und unabhängige Komponenten

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`http://math.uni-graz.at/keeling/`

Literatur:
`http://cis.legacy.ics.tkk.fi/aapo/papers/IJCNN99_tutorialweb/`

Dokumentation:
`http://math.uni-graz.at/keeling/skripten/Tutorium.pdf`

Dank an Herrn Dipl.-Ing. Dr. Gernot Reishofer
für seine Unterstützung für diese Arbeit!

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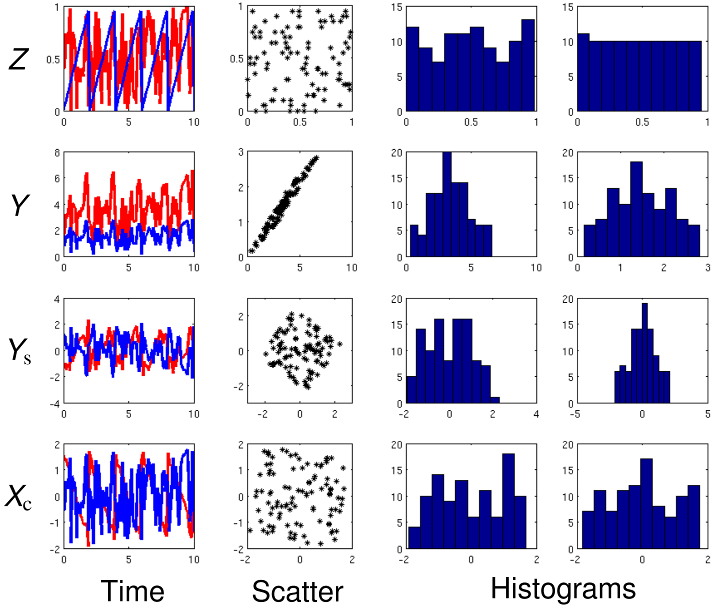
Graphical Demonstration of PCA/ICA

Sources Z, Measurements Y, sphered Y_s, separated X_c



Formulation of PCA/ICA

- Rows of Z are unknown samples of sources which are independent and not Gauß distributed.

$$Z = \begin{bmatrix} z_1(t_1) & z_1(t_2) & \cdots & z_1(t_n) \\ \vdots & \vdots & & \vdots \\ z_m(t_1) & z_m(t_2) & \cdots & z_m(t_n) \end{bmatrix}$$

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  no longer independent and now more Gauß distributed.

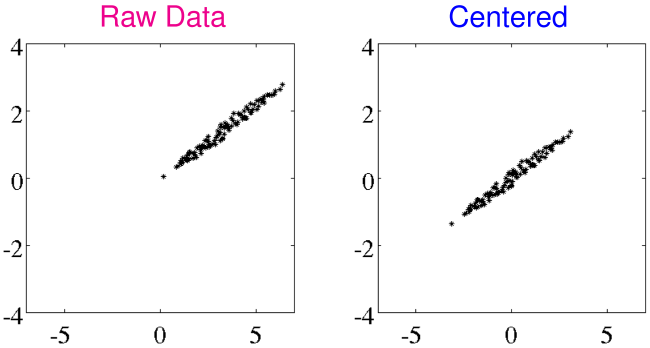
- Goal is to undo the trend toward Gaußianity to recover the sources

$$X = WY$$

  with $W = U\Lambda^{-\frac{1}{2}}V^{\mathrm{T}} \approx A^{-1}$ but unavoidable ambiguities.

Steps of PCA/ICA

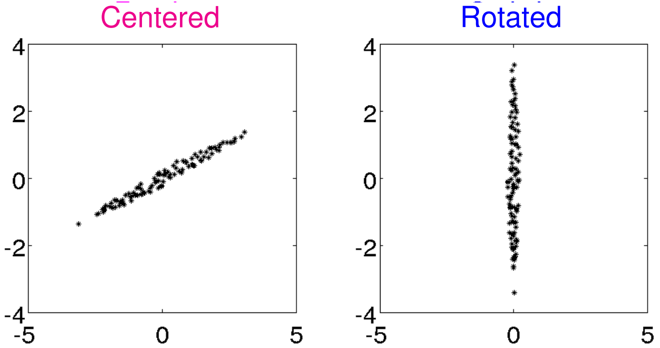
- Centering:



$$Y_{\mathrm{c}} = Y - \overline{Y}, \quad \overline{Y} = \begin{bmatrix} \overline{\boldsymbol{y}}_1 \\ \overline{\boldsymbol{y}}_2 \end{bmatrix}, \quad \overline{\boldsymbol{y}}_i = \frac{1}{n}\sum_{j=1}^{n}(\boldsymbol{y}_i)_j$$

Steps of PCA/ICA

- First rotation:

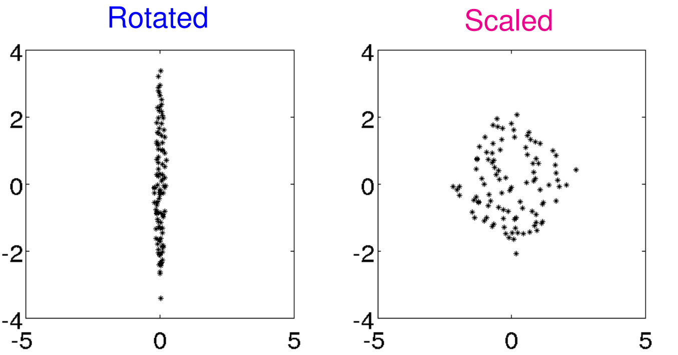


$$K = \frac{1}{n} Y_c Y_c^{\mathrm{T}} = \frac{1}{n} \begin{bmatrix} \boldsymbol{y}_1^{\mathrm{T}} - \overline{\boldsymbol{y}}_1 \\ \boldsymbol{y}_2^{\mathrm{T}} - \overline{\boldsymbol{y}}_2 \end{bmatrix} \begin{bmatrix} \boldsymbol{y}_1^{\mathrm{T}} - \overline{\boldsymbol{y}}_1 \\ \boldsymbol{y}_2^{\mathrm{T}} - \overline{\boldsymbol{y}}_2 \end{bmatrix}^{\mathrm{T}} = \begin{bmatrix} \sigma^2(\boldsymbol{y}_1) & \kappa(\boldsymbol{y}_1, \boldsymbol{y}_2) \\ \kappa(\boldsymbol{y}_2, \boldsymbol{y}_1) & \sigma^2(\boldsymbol{y}_2) \end{bmatrix}$$

$$V^{\mathrm{T}} K V = \Lambda, \quad V^{\mathrm{T}} V = I, \quad \Lambda = \mathrm{diag}\{\lambda_1, \lambda_2\}, \quad Y_r = V^{\mathrm{T}} Y_c$$

Steps of PCA/ICA

- Scaling:

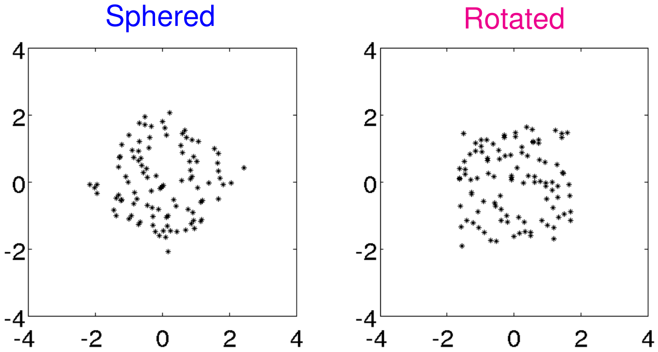


$$K = \frac{1}{n} Y_{\mathrm{c}} {Y_{\mathrm{c}}}^{\mathrm{T}}, \quad V^{\mathrm{T}} K V = \Lambda, \quad Y_{\mathrm{r}} = V^{\mathrm{T}} Y_{\mathrm{c}}, \quad Y_{\mathrm{s}} = \Lambda^{-\frac{1}{2}} Y_{\mathrm{r}}$$

The data Y_{s} are *sphered*: $\frac{1}{n} Y_{\mathrm{s}} {Y_{\mathrm{s}}}^{\mathrm{T}} = I$.

Steps of PCA/ICA

- Second rotation:



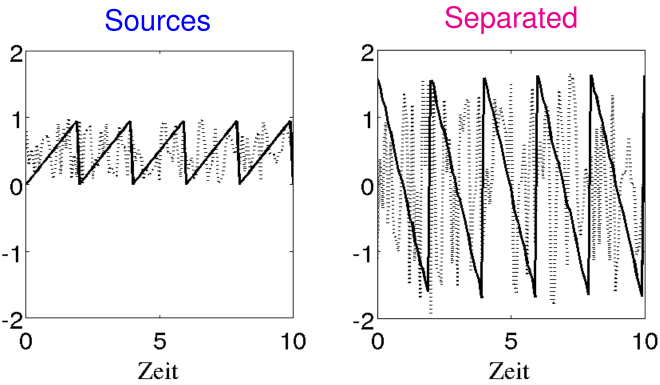
where

$$X_c = UY_s, \quad U = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix}, \quad U^T U = I$$

and θ minimizes the *Gaußianity*...

Steps of PCA/ICA

- The result:



With unavoidable ambiguities,

$$X_c = U\Lambda^{-\frac{1}{2}} V^{\mathrm{T}} Y_c \approx Z, \quad \overline{X}_c = \langle 0, 0 \rangle^{\mathrm{T}}, \quad \frac{1}{n} X_c {X_c}^{\mathrm{T}} = I$$

Minimization of Gaußianity

- A Gauß distributed sampling $\boldsymbol{n} = \{n_i\}_{i=1}^{n}$ with mean μ and variance σ^2 has the *Moments*

$$M_k(\boldsymbol{n}) = \frac{1}{n}\sum_{i=1}^{n} |n_i - \mu|^k \overset{n\to\infty}{\longrightarrow} \begin{cases} \sigma^2, & k = 2 \\ 3 \cdot \sigma^4, & k = 4 \\ 5 \cdot 3 \cdot \sigma^6, & k = 6 \quad \text{usw.} \end{cases}$$

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$$\mathcal{K}(\boldsymbol{n}) = M_4(\boldsymbol{n}) - 3[M_2(\boldsymbol{n})]^2 = 0$$

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- A sampling $\boldsymbol{x}(\theta)$ is given depending upon a parameter θ.

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- A sampling $\boldsymbol{x}(\theta)$ is given depending upon a parameter θ.
- The Gaußianity of $\boldsymbol{x}(\theta)$ can be minimized with respect to θ according to:

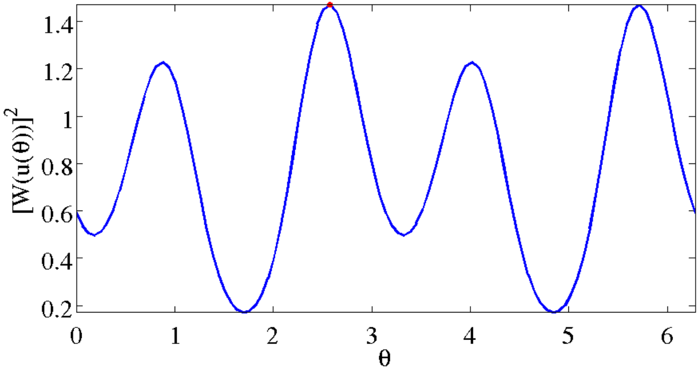
$$\theta^\star = \underset{\theta\in[0,2\pi]}{\operatorname{argmax}}[\mathcal{K}(\boldsymbol{x}(\theta))]^2$$

Minimization of Gaußianity

The landscape for the objective function with rotation $\boldsymbol{u}(\theta)$

$$[\mathcal{K}(\boldsymbol{u}(\theta)^{\mathrm{T}} Y_{\mathrm{s}})]^2, \quad \boldsymbol{u}(\theta) = \langle \cos(\theta), \sin(\theta) \rangle^{\mathrm{T}}$$

appears as follows, where the maximizing $\theta^\star$ is marked with $\bullet$.



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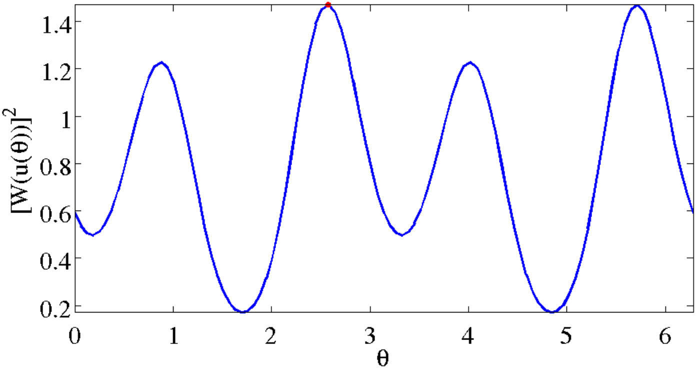

If there are *m* sources, there are polar coordinates $\{\theta_1, \ldots, \theta_{m-1}\}$.

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Summary of Steps:

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- Rotation:
$$X_{\mathrm{c}} = U Y_{\mathrm{s}}, \quad U^{\mathrm{T}} = \{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m\}$$
where each $\boldsymbol{u}_k$ minimizes Gaußianity.

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  For example, kurtosis
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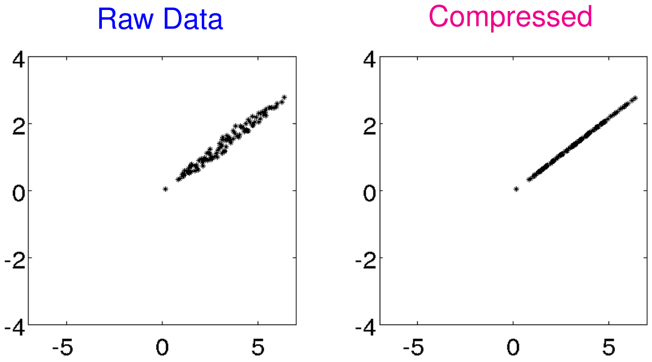
So $J(\boldsymbol{u}) = [\mathcal{K}(Y_{\mathrm{s}}^{\mathrm{T}}\boldsymbol{u})]^2$ may be maximized with $\boldsymbol{u}_k^{\mathrm{T}}\boldsymbol{u}_l = \delta_{kl}$.

Factor Analysis

The data can be compressed,



when the components with small λ_i are set to zero:

$$\Lambda = \mathrm{diag}\{\lambda_1, \lambda_2\}, \quad \lambda_1 \ll \lambda_2, \quad P = \mathrm{diag}\{0, 1\}$$

$$Y_P = \overline{Y} + V P V^{\mathrm{T}} (Y - \overline{Y})$$

Formulation of PCA/ICA

(PCA) Let the data be so decomposed,

$$Y_{\mathrm{c}} = Y - \overline{Y}, \quad K = \frac{1}{n} Y_{\mathrm{c}} Y_{\mathrm{c}}^{\mathrm{T}}, \quad KV = V\Lambda, \quad Y_{\mathrm{s}} = \Lambda^{-\frac{1}{2}} V^{\mathrm{T}} Y_{\mathrm{c}}$$

Let $\Lambda = \mathrm{diag}\{\lambda_1, \ldots, \lambda_m\}$ with $\lambda_1 \geq \cdots \geq \lambda_m$. With $P \in \mathbb{R}^{r \times m}$, $r < m$, $P_{i,j} = \delta_{i,j}$, the data Y are so projected to its r strongest principal components,

$$Y \approx Y_P = \overline{Y} + V\Lambda^{\frac{1}{2}} P^{\mathrm{T}} P Y_{\mathrm{s}} = \overline{Y} + \frac{1}{n}(PY_{\mathrm{s}})^{\mathrm{T}}(PY_{\mathrm{s}})$$

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(ICA) Let the data be further so decomposed,

$$X_{\mathrm{c}} = UY_{\mathrm{s}}$$

With $Q \in \mathbb{R}^{r \times m}$, $r < m$, $Q_{i,j} = \delta_{q_i,j}$, the data Y are so projected to the r independent components $\{q_1, \ldots, q_r\}$,

$$Y \approx Y_Q = \overline{Y} + V\Lambda^{\frac{1}{2}} U^{\mathrm{T}} Q^{\mathrm{T}} Q X_{\mathrm{c}} = \overline{Y} + \frac{1}{n}(QX_{\mathrm{c}})^{\mathrm{T}}(QX_{\mathrm{c}})$$

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&= \arg\min_{\mu} \left[(\mu - 0)^2 + (m-1)(\mu - 1)^2 \right] = (m-1)/m
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\mu_1(\boldsymbol{x}) &= \arg\min_{\mu} \sum_{i=1}^{m} |\mu - x_i| \\
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&= \arg \min_{a \le \mu \le b} [(\mu - 0) + (m-1)(1-\mu)] = 1 \quad \text{(robust!)}
\end{aligned}
$$

Best generalization for higher dimensional data,
$Y = \{\boldsymbol{c}_1, \ldots, \boldsymbol{c}_n\} \in \mathbb{R}^{m \times n}$,

$$
\boldsymbol{\mu}_1(Y) = \arg \min_{\boldsymbol{\mu} \in \mathbb{R}^m} \sum_{j=1}^{n} \|\boldsymbol{\mu} - \boldsymbol{c}_j\|_{\ell_2}
$$

Benefits of ℓ_1 Formulations

Sphering. The ℓ_2 approach is obtained by minimizing

$$R_k(\boldsymbol{v}) = \frac{\frac{1}{n}\langle Y_k Y_k^{\mathrm{T}} \boldsymbol{v}, \boldsymbol{v}\rangle}{\langle \boldsymbol{v}, \boldsymbol{v}\rangle} = \left[\frac{\| Y_k^{\mathrm{T}} \boldsymbol{v}\|_{\ell_2}}{\sqrt{n}\|\boldsymbol{v}\|_{\ell_2}}\right]^2$$

where

$$Y_k = (I - V_{k-1} V_{k-1}^{\mathrm{T}}) Y_{\mathrm{c}}, \quad k = 2, \ldots, m-1, \quad Y_1 = Y_{\mathrm{c}}$$

and setting

$\boldsymbol{v}_k = \mathrm{argmin}_{\boldsymbol{v}} R_k(\boldsymbol{v})$, $\lambda_k = R_k(\boldsymbol{v}_k)$, $V_k = \{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\}$, $V = V_m$.

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Best generalization for ℓ_1 is obtained by minimizing

$$F_k(\boldsymbol{v}) = \frac{\| Y_k^{\mathrm{T}} \boldsymbol{v}\|_{\ell_1}}{\sqrt{n}\|\boldsymbol{v}\|_{\ell_2}}$$

where

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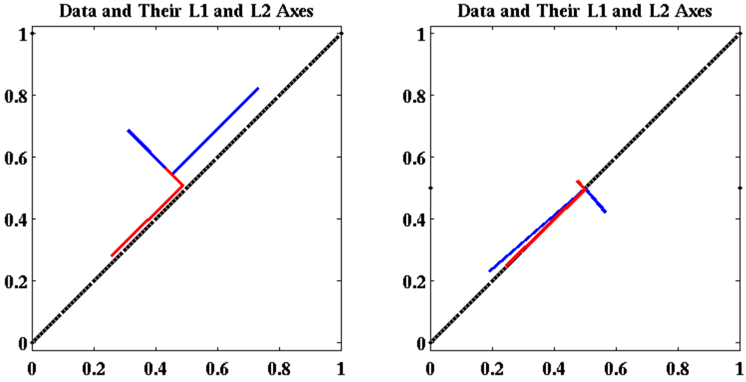
$$\boldsymbol{v}_k = \mathrm{argmin}_{\boldsymbol{v}} F_k(\boldsymbol{v}),\ \lambda_k = F_k(\boldsymbol{v}_k),\ V_k = \{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\},\ V = V_m.$$

Benefits of ℓ_1 Formulations

Outliers accumulated at $(0,1)$, then at $(0,\frac{1}{2})$ and $(1,\frac{1}{2})$,



Blue is for ℓ_2, Red is for $\ell_1(\ell_2)$.

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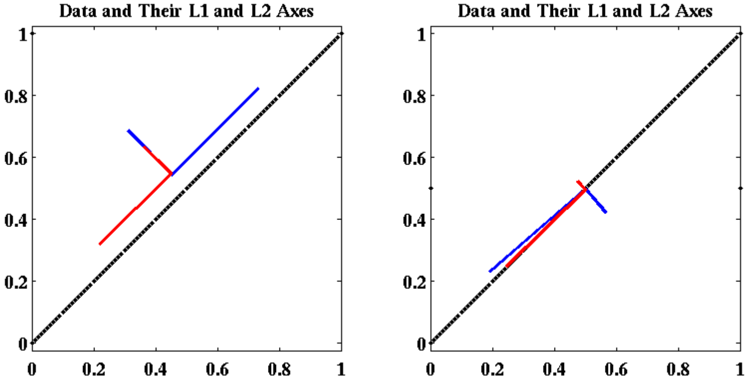

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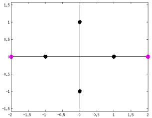
Benefits of ℓ_1 Formulations

Test data $Y = \{\boldsymbol{y}_1, \boldsymbol{y}_2\}^{\mathrm{T}} \in \mathbb{R}^{2\times n}$, each pair in $\{(\pm 1, 0), (0, \pm 1)\}$ except for outliers

$$\begin{aligned} (\boldsymbol{y}_1)_1 &= \alpha, \quad (\boldsymbol{y}_2)_1 = 0 \\ (\boldsymbol{y}_1)_2 &= -\alpha, \quad (\boldsymbol{y}_2)_2 = 0 \end{aligned}$$



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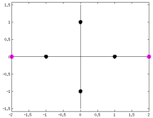
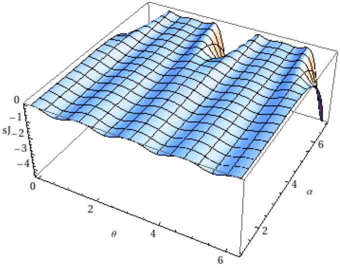


Then $\overline{Y} = (0, 0)$ and $V = I$.

The Kurtosis objective function $J(\boldsymbol{u}) = -\mathcal{K}^2(Y_{\mathrm{s}}^{\mathrm{T}}\boldsymbol{u})$ has the following landscape for the test data:



$\boldsymbol{u} = \{\cos(\theta), \sin(\theta)\}$ with $\theta = \frac{\pi}{4}$ is the robust solution.

This solution is obtained for $\alpha \approx 0$, but not for α moderately larger.

Benefits of ℓ_1 Formulations

An alternative objection function is based on the ℓ_1 moment,

$$\mathcal{F}(\boldsymbol{x}) = M_1(\boldsymbol{x}) - \sqrt{M_2(\boldsymbol{x})}\sqrt{\frac{2}{\pi}}$$

where $\mathcal{F}(\boldsymbol{n}) = \sigma\sqrt{2/\pi} - \sigma\sqrt{2/\pi} = 0$ for $\boldsymbol{n} \sim N(\mu, \sigma^2)$.

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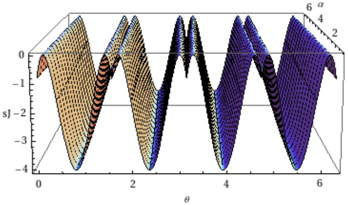
The new objective function

$$J(\boldsymbol{u}) = -\mathcal{F}^2(Y_{\mathrm{s}}^{\mathrm{T}}\boldsymbol{u})$$

has the following landscape for the test data:



$\boldsymbol{u} = \{\cos(\theta), \sin(\theta)\}$ with $\theta = \frac{\pi}{4}$ is the robust solution.

This solution is obtained for a large range of $\alpha > 0$.

Minimizing the Robust Objective Function for ICA

The robust objective function

$$J(\boldsymbol{u}) = -\mathcal{F}^2(Y_{\mathrm{s}}^{\mathrm{T}}\boldsymbol{u}) = -[M_1(Y_{\mathrm{s}}\boldsymbol{u}) - \sqrt{2/\pi}]^2$$

$(M_2(Y_{\mathrm{s}}^{\mathrm{T}}\boldsymbol{u}) = 1)$ is minimized under the condition $\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u} = 1$.

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The solution is obtained from a stationary point of

$$L(\boldsymbol{u}, \lambda) = -[M_1(Y_{\mathrm{s}}^{\mathrm{T}}\boldsymbol{u}) - \sqrt{2/\pi}]^2 + \lambda(\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u} - 1)/2$$

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$$\phi(\boldsymbol{u}) = 2[M_1(Y_{\mathrm{s}}^{\mathrm{T}}\boldsymbol{u}) - \sqrt{2/\pi}] \quad \text{and} \quad G(\boldsymbol{u}) = \frac{1}{n}\sum_{i=1}^{n}\frac{Y_{\mathrm{s}}\boldsymbol{e}_i\boldsymbol{e}_i^{\mathrm{T}}Y_{\mathrm{s}}^{\mathrm{T}}}{|\boldsymbol{e}_i^{\mathrm{T}}Y_{\mathrm{s}}^{\mathrm{T}}\boldsymbol{u}|}$$

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A stationary point $(\boldsymbol{u}^\star, \lambda^\star)$ satisfies $-D_{\boldsymbol{u}}J(\boldsymbol{u}^\star) = \lambda^\star\boldsymbol{u}^\star$ or with $\lambda^\star = \mu^\star(\boldsymbol{u}^\star)\phi(\boldsymbol{u}^\star)$ the nonlinear eigenspace problem,

$$G(\boldsymbol{u}^\star)\boldsymbol{u}^\star = \mu^\star(\boldsymbol{u}^\star)\boldsymbol{u}^\star, \quad \boldsymbol{u}^{\star\mathrm{T}}\boldsymbol{u}^\star = 1$$

Minimizing the Robust Objective Function for ICA

The nonlinear eigenspace problem is solved by a vector iteration.

Let $\boldsymbol{u}_l \approx \boldsymbol{u}^\star$ with $\|\boldsymbol{u}_l\| = 1$ and an update $\boldsymbol{u}_{l+1}$ is determined by,

$$\boldsymbol{u} = G(\boldsymbol{u}_l)\boldsymbol{u}_l, \quad \boldsymbol{u}_{l+1} = \boldsymbol{u}/\|\boldsymbol{u}\|, \quad l = 1, 2, \ldots$$

After convergence

$$\boldsymbol{u}^\star = \lim_{l\to\infty} \boldsymbol{u}_l$$

is the first column of U^{T}.

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$$\boldsymbol{u}^\star = \lim_{l\to\infty} \boldsymbol{u}_l$$

is the first column of U^{T}.

The next column of U^{T} is determined by a modified vector iteration.

For this, the projected data

$$Y_{\mathrm{p}} = (I - \boldsymbol{u}^\star \boldsymbol{u}^{\star\mathrm{T}}) Y_{\mathrm{s}}$$

have columns which are linearly independent from $\boldsymbol{u}^\star$.

Minimizing the Robust Objective Function for ICA

With the modified matrix,

$$\tilde{G}(\boldsymbol{u}) = \frac{1}{n}\sum_{i=1}^{n} \frac{Y_{\mathrm{p}}\boldsymbol{e}_i\boldsymbol{e}_i^{\mathrm{T}} Y_{\mathrm{p}}^{\mathrm{T}}}{|\boldsymbol{e}_i^{\mathrm{T}} Y_{\mathrm{p}}^{\mathrm{T}}\boldsymbol{u}|}$$

the modified vector iteration is,

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The remaining columns of U^T are determined similarly, where $\boldsymbol{u}^\star$ above is replaced with the matrix $[\boldsymbol{u}_1^\star, \ldots, \boldsymbol{u}_k^\star]$, when k columns $\{\boldsymbol{u}_1^\star, \ldots, \boldsymbol{u}_k^\star\}$ of U^T have already been calculated.

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Claim: Convergence to a constrained minimum can be proved with appropriate step size control.

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Observation: Robust convergence is seen in practice.

Application to DCE-MRI sequences

For each time $t = 1, \ldots, T$, the matrix of pixel values,

$$B(t) = \{B_{i,j}(t)\}_{1 \leq i,j \leq N}$$

is an image in the [Video].

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With $n = T = 134$ and $m = N^2 = 400^2$ the images are represented as long vectors:

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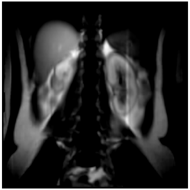
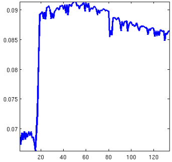
To the left is the first column of V (displayed as image),





To the right is the first row of Y_{s}.

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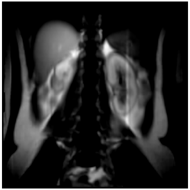

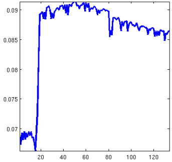

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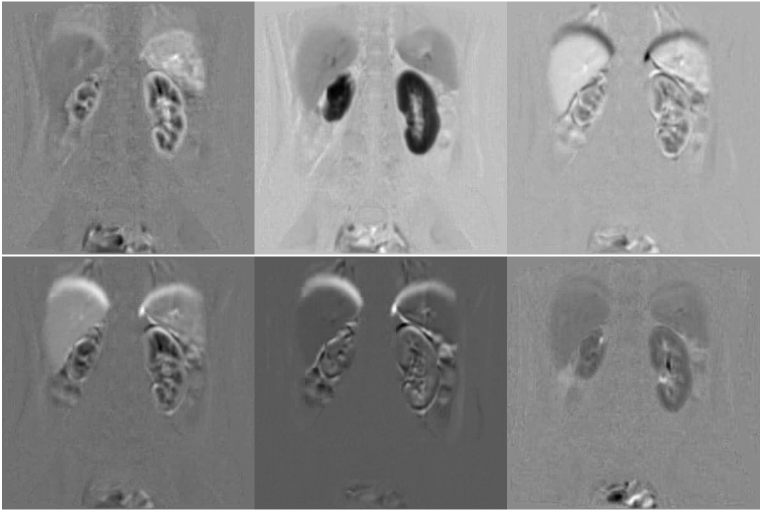
Compressed to 10 principal components: [Video]

Anwendung für DCE-MRI Folgen

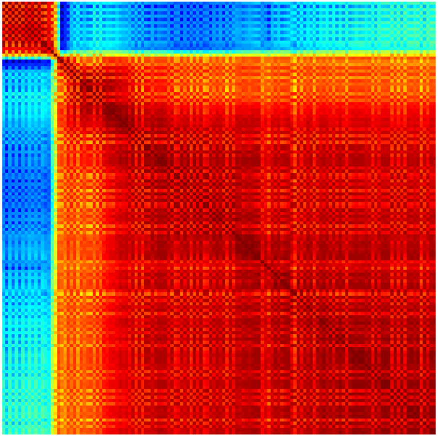
The 6 most significant independent components:



Separate intensity changes due to motion or contrast agent and eliminate motion: [Video]

Application to DCE-MRI sequences

Virtual Gating, through segmentation of correlations:



Three groups [Video], stabilized further by PCA/ICA [Video].

Formulation in Function Space

Based upon the imaging examples:

- Sampling occurs continuously in time . . . ?
- Same number of sources as pixels,
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Consequence: The function space setting resembles the finite dimensional setting but with infinite matrices operating between bases in separable spaces.

Thank You!