

l_1 Approaches to PCA and ICA

S. Keeling and K. Kunisch

Institute for Mathematics and Scientific Computing
Karl Franzens University of Graz
Graz, Austria

ACMAC, FORTH, University of Crete, Heraklion
February 21, 2013



Steierische Modellierungswoche 2012

Projekt: Signalverarbeitung

Tutorium: Trennung von Datenquellen in unkorrelierte und unabhängige Komponenten

a.o.Univ.Prof. Mag.Dr. Stephen Keeling

<http://math.uni-graz.at/keeling/>

Literatur:

[http://cis.legacy.ics.tkk.fi/aapo/papers/
IJCNN99_tutorialweb/](http://cis.legacy.ics.tkk.fi/aapo/papers/IJCNN99_tutorialweb/)

Dokumentation:

[http://math.uni-graz.at/keeling/skripten/
Tutorium.pdf](http://math.uni-graz.at/keeling/skripten/Tutorium.pdf)

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

Inhaltsverzeichnis

Matrixalgebra

- Lineare Gleichungen
- Lösung von Systemen Linearer Gleichungen
- Effekt der Matrix-Multiplikation
- Eigenräume
- Eigenwerte und Eigenvektoren
- Eigenraum-Zerlegung

Statistik

- Mittelwert und Varianz einer Abtastung
- Zentraler Grenzwertsatz
- Kovarianz zweier Abtastungen
- Zentrierte und Gesphärte Daten
- Korrelation
- Unabhängigkeit
- Mischungen von Abtastungen
- Gaußianität
- Hauptkomponentenanalyse (PCA) und Unabhängigkeitsanalyse (ICA)

Optimierung

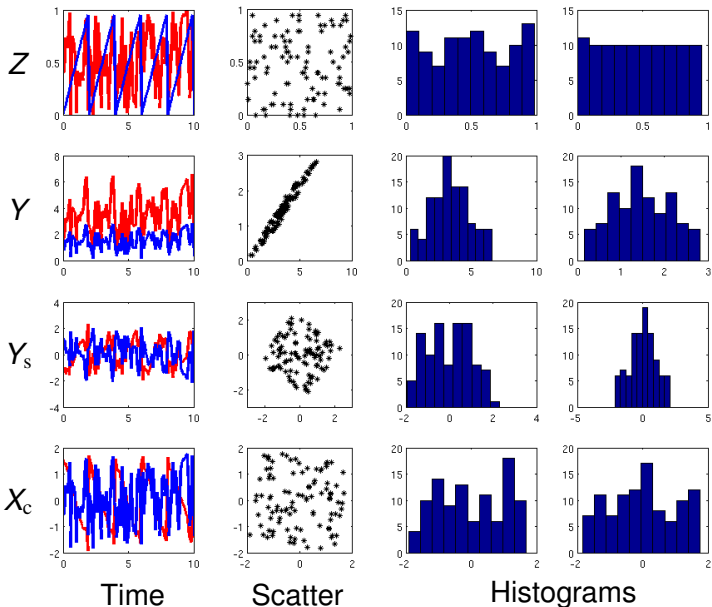
- Nelder-Mead Verfahren
- `fminsearch`
- Optimierung der Wölbung mit Nelder-Mead
- Abstiegsverfahren
- Abstiegsverfahren für Systeme
- Optimierung der Wölbung mit Roher Gewalt
- Optimierung der Wölbung mit Abstiegsverfahren
- Newton Verfahren
- Newton Verfahren für Systeme
- Optimierung der Wölbung mit Newton Verfahren

Fortgeschrittene Themen

- Robuste Zielfunktion
- Optimierung der Robusten Zielfunktion
- Formulierung im Funktionenraum

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**.

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

Formulation of PCA/ICA

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

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

- ▶ Rows of Y are measured samples of unknown **mixtures** of the sources

$$Y = AZ$$

no longer independent and now **more Gauß distributed**.

Formulation of PCA/ICA

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

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

- ▶ Rows of Y are measured samples of unknown **mixtures** of the sources

$$Y = AZ$$

no longer independent and now **more Gauß distributed**.

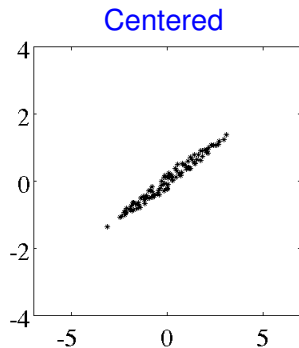
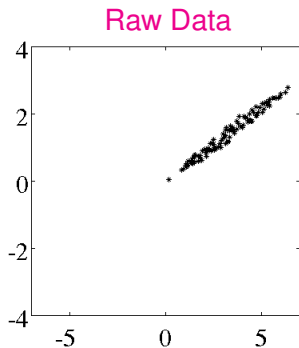
- ▶ Goal is to **undo** the trend toward **Gaußianity** to recover the sources

$$X = WY$$

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

Steps of PCA/ICA

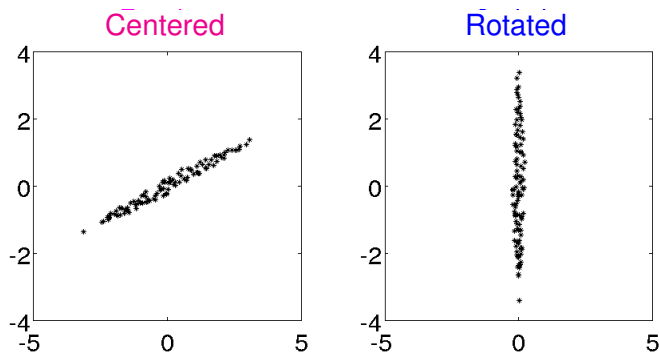
- ▶ Centering:



$$Y_c = Y - \bar{Y}, \quad \bar{Y} = \begin{bmatrix} \bar{y}_1 \\ \bar{y}_2 \end{bmatrix}, \quad \bar{y}_i = \frac{1}{n} \sum_{j=1}^n (y_i)_j$$

Steps of PCA/ICA

- First rotation:

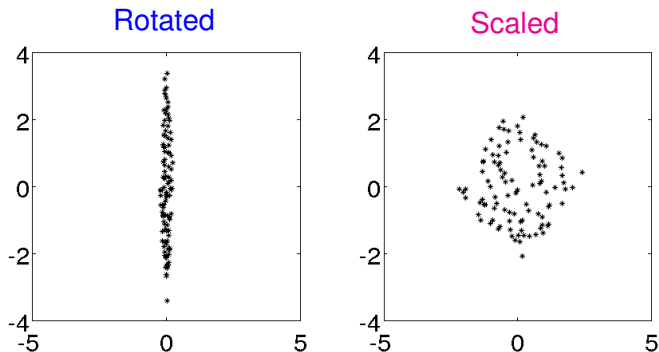


$$K = \frac{1}{n} \mathbf{Y}_c \mathbf{Y}_c^T = \frac{1}{n} \begin{bmatrix} \mathbf{y}_1^T - \bar{\mathbf{y}}_1 \\ \mathbf{y}_2^T - \bar{\mathbf{y}}_2 \end{bmatrix} \begin{bmatrix} \mathbf{y}_1^T - \bar{\mathbf{y}}_1 \\ \mathbf{y}_2^T - \bar{\mathbf{y}}_2 \end{bmatrix}^T = \begin{bmatrix} \sigma^2(\mathbf{y}_1) & \kappa(\mathbf{y}_1, \mathbf{y}_2) \\ \kappa(\mathbf{y}_2, \mathbf{y}_1) & \sigma^2(\mathbf{y}_2) \end{bmatrix}$$

$$\mathbf{V}^T \mathbf{K} \mathbf{V} = \Lambda, \quad \mathbf{V}^T \mathbf{V} = \mathbf{I}, \quad \Lambda = \text{diag}\{\lambda_1, \lambda_2\}, \quad \mathbf{Y}_r = \mathbf{V}^T \mathbf{Y}_c$$

Steps of PCA/ICA

- Scaling:

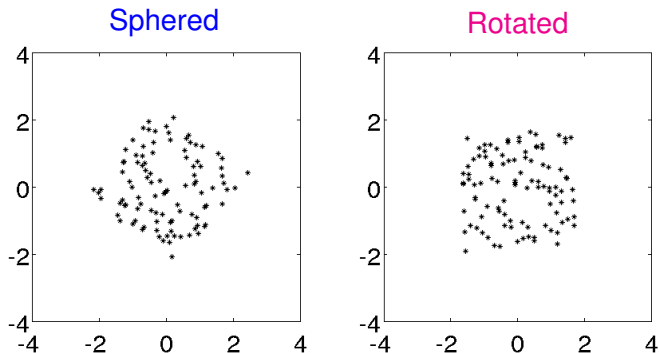


$$K = \frac{1}{n} Y_c Y_c^T, \quad V^T K V = \Lambda, \quad Y_r = V^T Y_c, \quad Y_s = \Lambda^{-\frac{1}{2}} Y_r$$

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

Steps of PCA/ICA

- ▶ Second rotation:



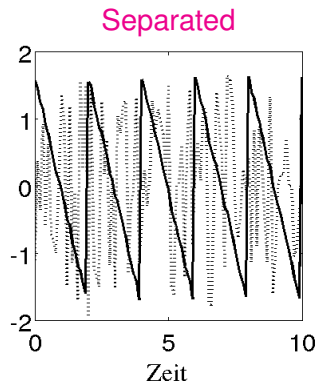
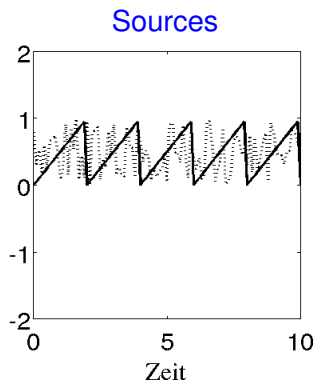
where

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

and θ minimizes the *Gaussianity*...

Steps of PCA/ICA

- ▶ The result:



With unavoidable ambiguities,

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

Minimization of Gaußianity

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

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

Minimization of Gaußianity

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

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

- ▶ So \mathbf{n} has the *kurtosis*,

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

Minimization of Gaußianity

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

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

- ▶ So \mathbf{n} has the *kurtosis*,

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

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

Minimization of Gaußianity

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

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

- ▶ So \mathbf{n} has the *kurtosis*,

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

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

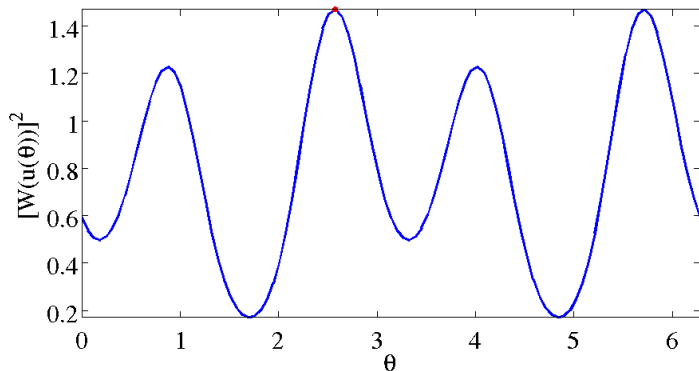
$$\theta^* = \operatorname{argmax}_{\theta \in [0, 2\pi]} [\mathcal{K}(\mathbf{x}(\theta))]^2$$

Minimization of Gaußianity

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

$$[\mathcal{K}(\mathbf{u}(\theta)^T \mathbf{Y}_s)]^2, \quad \mathbf{u}(\theta) = \langle \cos(\theta), \sin(\theta) \rangle^T$$

appears as follows, where the maximizing θ^* is marked with \bullet .

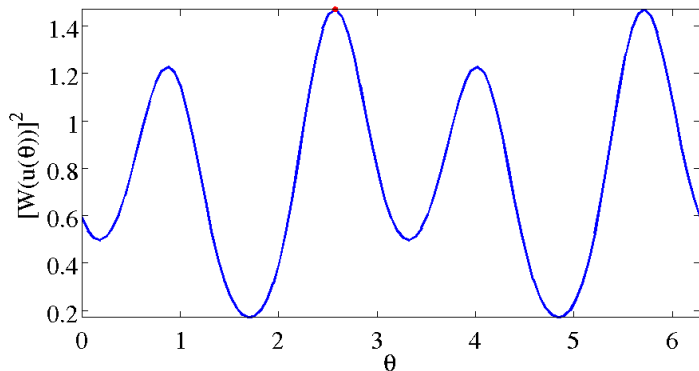


Minimization of Gaußianity

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

$$[\mathcal{K}(\mathbf{u}(\theta)^T \mathbf{Y}_s)]^2, \quad \mathbf{u}(\theta) = \langle \cos(\theta), \sin(\theta) \rangle^T$$

appears as follows, where the maximizing θ^* is marked with \bullet .



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

Formulation of PCA/ICA

Summary of Steps:

- ▶ Centering:

$$Y_c = Y - \bar{Y}$$

Formulation of PCA/ICA

Summary of Steps:

- ▶ Centering:

$$Y_c = Y - \bar{Y}$$

- ▶ Rotation:

$$K = \frac{1}{n} Y_c Y_c^T, \quad KV = V\Lambda, \quad Y_r = V^T Y_c$$

Formulation of PCA/ICA

Summary of Steps:

- ▶ Centering:

$$Y_c = Y - \bar{Y}$$

- ▶ Rotation:

$$K = \frac{1}{n} Y_c Y_c^T, \quad KV = V\Lambda, \quad Y_r = V^T Y_c$$

- ▶ Scaling:

$$Y_s = \Lambda^{-\frac{1}{2}} Y_r$$

Formulation of PCA/ICA

Summary of Steps:

- ▶ Centering:

$$Y_c = Y - \bar{Y}$$

- ▶ Rotation:

$$K = \frac{1}{n} Y_c Y_c^T, \quad KV = V\Lambda, \quad Y_r = V^T Y_c$$

- ▶ Scaling:

$$Y_s = \Lambda^{-\frac{1}{2}} Y_r$$

- ▶ Rotation:

$$X_c = UY_s, \quad U^T = \{\mathbf{u}_1, \dots, \mathbf{u}_m\}$$

where each \mathbf{u}_k minimizes Gaussianity.

Formulation of PCA/ICA

Summary of Steps:

- ▶ Centering:

$$Y_c = Y - \bar{Y}$$

- ▶ Rotation:

$$K = \frac{1}{n} Y_c Y_c^T, \quad KV = V\Lambda, \quad Y_r = V^T Y_c$$

- ▶ Scaling:

$$Y_s = \Lambda^{-\frac{1}{2}} Y_r$$

- ▶ Rotation:

$$X_c = UY_s, \quad U^T = \{\mathbf{u}_1, \dots, \mathbf{u}_m\}$$

where each \mathbf{u}_k minimizes Gaussianity.

For example, **kurtosis**

$$\mathcal{K}(\mathbf{x}) = M_4(\mathbf{x}) - 3M_2^2(\mathbf{x})$$

satisfies $\mathcal{K}(\mathbf{n}) = 3\sigma^4 - 3\sigma^4 = 0$ for $\mathbf{n} \sim N(\mu, \sigma^2)$.

Formulation of PCA/ICA

Summary of Steps:

- ▶ Centering:

$$Y_c = Y - \bar{Y}$$

- ▶ Rotation:

$$K = \frac{1}{n} Y_c Y_c^T, \quad KV = V\Lambda, \quad Y_r = V^T Y_c$$

- ▶ Scaling:

$$Y_s = \Lambda^{-\frac{1}{2}} Y_r$$

- ▶ Rotation:

$$X_c = UY_s, \quad U^T = \{\mathbf{u}_1, \dots, \mathbf{u}_m\}$$

where each \mathbf{u}_k minimizes Gaussianity.

For example, **kurtosis**

$$\mathcal{K}(\mathbf{x}) = M_4(\mathbf{x}) - 3M_2^2(\mathbf{x})$$

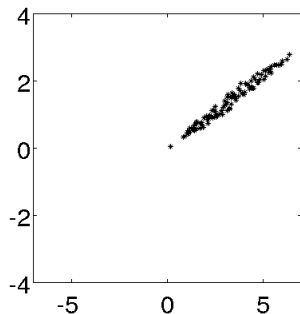
satisfies $\mathcal{K}(\mathbf{n}) = 3\sigma^4 - 3\sigma^4 = 0$ for $\mathbf{n} \sim N(\mu, \sigma^2)$.

So $J(\mathbf{u}) = [\mathcal{K}(Y_s^T \mathbf{u})]^2$ may be maximized with $\mathbf{u}_k^T \mathbf{u}_l = \delta_{kl}$.

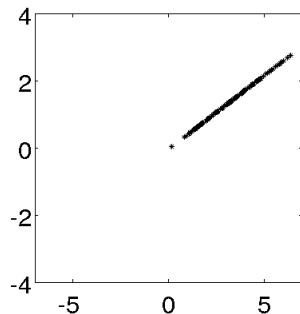
Factor Analysis

The data can be compressed,

Raw Data



Compressed



when the components with small λ_i are set to zero:

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

$$Y_P = \bar{Y} + VPV^T(Y - \bar{Y})$$

Formulation of PCA/ICA

(PCA) Let the data be so decomposed,

$$Y_c = Y - \bar{Y}, \quad K = \frac{1}{n} Y_c Y_c^T, \quad KV = V\Lambda, \quad Y_s = \Lambda^{-\frac{1}{2}} V^T Y_c$$

Let $\Lambda = \text{diag}\{\lambda_1, \dots, \lambda_m\}$ with $\lambda_1 \geq \dots \geq \lambda_m$. 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,

$$Y \approx Y_P = \bar{Y} + V\Lambda^{\frac{1}{2}} P^T P Y_s = \bar{Y} + \frac{1}{n} (P Y_s)^T (P Y_s)$$

Formulation of PCA/ICA

(PCA) Let the data be so decomposed,

$$Y_c = Y - \bar{Y}, \quad K = \frac{1}{n} Y_c Y_c^T, \quad KV = V\Lambda, \quad Y_s = \Lambda^{-\frac{1}{2}} V^T Y_c$$

Let $\Lambda = \text{diag}\{\lambda_1, \dots, \lambda_m\}$ with $\lambda_1 \geq \dots \geq \lambda_m$. 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**,

$$Y \approx Y_P = \bar{Y} + V\Lambda^{\frac{1}{2}} P^T P Y_s = \bar{Y} + \frac{1}{n} (P Y_s)^T (P Y_s)$$

(ICA) Let the data be further so decomposed,

$$X_c = U Y_s$$

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** $\{q_1, \dots, q_r\}$,

$$Y \approx Y_Q = \bar{Y} + V\Lambda^{\frac{1}{2}} U^T Q^T Q X_c = \bar{Y} + \frac{1}{n} (Q X_c)^T (Q X_c)$$

Benefits of ℓ_1 Formulations

Centering. Given data $\mathbf{x} = \langle 0, 1, \dots, 1 \rangle \in \mathbb{R}^m$,

Benefits of ℓ_1 Formulations

Centering. Given data $\mathbf{x} = \langle 0, 1, \dots, 1 \rangle \in \mathbb{R}^m$,

$$\begin{aligned}\mu_2(\mathbf{x}) &= \arg \min_{\mu} \sum_{i=1}^m (\mu - x_i)^2 \\ &= \arg \min_{\mu} \left[(\mu - 0)^2 + (m - 1)(\mu - 1)^2 \right] = (m - 1)/m\end{aligned}$$

Benefits of ℓ_1 Formulations

Centering. Given data $\mathbf{x} = \langle 0, 1, \dots, 1 \rangle \in \mathbb{R}^m$,

$$\begin{aligned}\mu_2(\mathbf{x}) &= \arg \min_{\mu} \sum_{i=1}^m (\mu - x_i)^2 \\ &= \arg \min_{\mu} \left[(\mu - 0)^2 + (m - 1)(\mu - 1)^2 \right] = (m - 1)/m\end{aligned}$$

$$\begin{aligned}\mu_1(\mathbf{x}) &= \arg \min_{\mu} \sum_{i=1}^m |\mu - x_i| \\ &= \arg \min_{a \leq \mu \leq b} [(\mu - 0) + (m - 1)(1 - \mu)] = 1 \quad (\text{robust!})\end{aligned}$$

Benefits of ℓ_1 Formulations

Centering. Given data $\mathbf{x} = \langle 0, 1, \dots, 1 \rangle \in \mathbb{R}^m$,

$$\begin{aligned}\mu_2(\mathbf{x}) &= \arg \min_{\mu} \sum_{i=1}^m (\mu - x_i)^2 \\ &= \arg \min_{\mu} \left[(\mu - 0)^2 + (m-1)(\mu - 1)^2 \right] = (m-1)/m\end{aligned}$$

$$\begin{aligned}\mu_1(\mathbf{x}) &= \arg \min_{\mu} \sum_{i=1}^m |\mu - x_i| \\ &= \arg \min_{a \leq \mu \leq b} [(\mu - 0) + (m-1)(1 - \mu)] = 1 \quad (\text{robust!})\end{aligned}$$

Best generalization for higher dimensional data,

$Y = \{\mathbf{c}_1, \dots, \mathbf{c}_n\} \in \mathbb{R}^{m \times n}$,

$$\mu_1(Y) = \arg \min_{\mu \in \mathbb{R}^m} \sum_{j=1}^n \|\mu - \mathbf{c}_j\|_{\ell_2}$$

Benefits of ℓ_1 Formulations

Sphering. The ℓ_2 approach is obtained by minimizing

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

where

$$Y_k = (I - V_{k-1} V_{k-1}^T) Y_c, \quad k = 2, \dots, m-1, \quad Y_1 = Y_c$$

and setting

$$\mathbf{v}_k = \operatorname{argmin}_{\mathbf{v}} R_k(\mathbf{v}), \quad \lambda_k = R_k(\mathbf{v}_k), \quad V_k = \{\mathbf{v}_1, \dots, \mathbf{v}_k\}, \quad V = V_m.$$

Benefits of ℓ_1 Formulations

Sphering. The ℓ_2 approach is obtained by minimizing

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

where

$$Y_k = (I - V_{k-1} V_{k-1}^T) Y_c, \quad k = 2, \dots, m-1, \quad Y_1 = Y_c$$

and setting

$$\mathbf{v}_k = \operatorname{argmin}_{\mathbf{v}} R_k(\mathbf{v}), \quad \lambda_k = R_k(\mathbf{v}_k), \quad V_k = \{\mathbf{v}_1, \dots, \mathbf{v}_k\}, \quad V = V_m.$$

Best generalization for ℓ_1 is obtained by minimizing

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

where

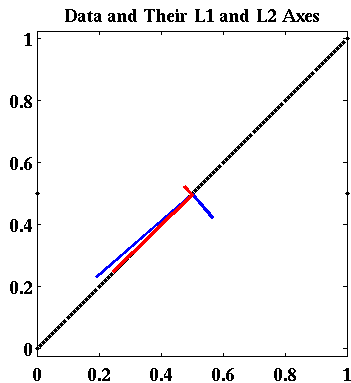
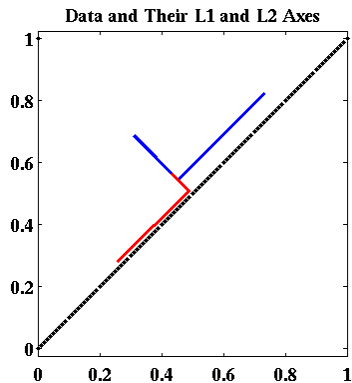
$$Y_k = (I - V_{k-1} V_{k-1}^T) Y_c, \quad k = 2, \dots, m-1, \quad Y_1 = Y_c$$

and setting

$$\mathbf{v}_k = \operatorname{argmin}_{\mathbf{v}} F_k(\mathbf{v}), \quad \lambda_k = F_k(\mathbf{v}_k), \quad V_k = \{\mathbf{v}_1, \dots, \mathbf{v}_k\}, \quad V = V_m.$$

Benefits of ℓ_1 Formulations

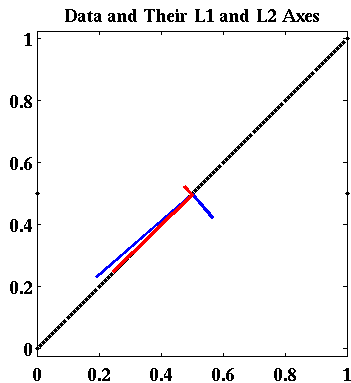
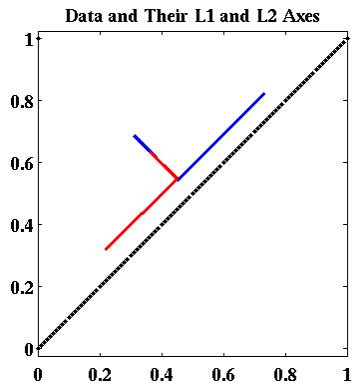
Outliers accumulated at $(0, 1)$, then at $(0, \frac{1}{2})$ and $(1, \frac{1}{2})$,



Blue is for ℓ_2 , Red is for ℓ_1 (ℓ_2).

Benefits of ℓ_1 Formulations

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

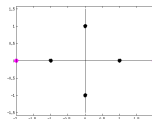


Blue is for ℓ_2 , Red is for ℓ_1 (ℓ_1).

Benefits of ℓ_1 Formulations

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

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

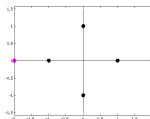


Then $\bar{Y} = (0, 0)$ and $V = I$.

Benefits of ℓ_1 Formulations

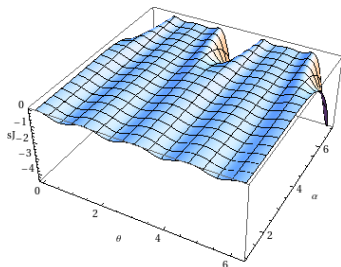
Test data $Y = \{\mathbf{y}_1, \mathbf{y}_2\}^T \in \mathbb{R}^{2 \times n}$, each pair in $\{(\pm 1, 0), (0, \pm 1)\}$ except for outliers

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



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

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



$\mathbf{u} = \{\cos(\theta), \sin(\theta)\}$ 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,

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

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

Benefits of ℓ_1 Formulations

An alternative objection function is based on the ℓ_1 moment,

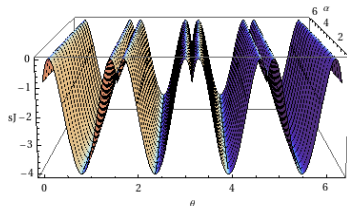
$$\mathcal{F}(\mathbf{x}) = M_1(\mathbf{x}) - \sqrt{M_2(\mathbf{x})} \sqrt{\frac{2}{\pi}}$$

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

The new objective function

$$J(\mathbf{u}) = -\mathcal{F}^2(Y_s^T \mathbf{u})$$

has the following landscape for the test data:



$\mathbf{u} = \{\cos(\theta), \sin(\theta)\}$ 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

$$J(\mathbf{u}) = -\mathcal{F}^2(Y_s^T \mathbf{u}) = -[M_1(Y_s \mathbf{u}) - \sqrt{2/\pi}]^2$$

$(M_2(Y_s^T \mathbf{u}) = 1)$ is minimized under the condition $\mathbf{u}^T \mathbf{u} = 1$.

Minimizing the Robust Objective Function for ICA

The robust objective function

$$J(\mathbf{u}) = -\mathcal{F}^2(Y_s^T \mathbf{u}) = -[M_1(Y_s \mathbf{u}) - \sqrt{2/\pi}]^2$$

$(M_2(Y_s^T \mathbf{u}) = 1)$ is minimized under the condition $\mathbf{u}^T \mathbf{u} = 1$.

The solution is obtained from a stationary point of

$$L(\mathbf{u}, \lambda) = -[M_1(Y_s^T \mathbf{u}) - \sqrt{2/\pi}]^2 + \lambda(\mathbf{u}^T \mathbf{u} - 1)/2$$

Minimizing the Robust Objective Function for ICA

The robust objective function

$$J(\mathbf{u}) = -\mathcal{F}^2(Y_s^T \mathbf{u}) = -[M_1(Y_s \mathbf{u}) - \sqrt{2/\pi}]^2$$

$(M_2(Y_s^T \mathbf{u}) = 1)$ is minimized under the condition $\mathbf{u}^T \mathbf{u} = 1$.

The solution is obtained from a stationary point of

$$L(\mathbf{u}, \lambda) = -[M_1(Y_s^T \mathbf{u}) - \sqrt{2/\pi}]^2 + \lambda(\mathbf{u}^T \mathbf{u} - 1)/2$$

We have $D_{\mathbf{u}}J(\mathbf{u}) = -\phi(\mathbf{u})G(\mathbf{u})\mathbf{u}$ with

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

Minimizing the Robust Objective Function for ICA

The robust objective function

$$J(\mathbf{u}) = -\mathcal{F}^2(Y_s^T \mathbf{u}) = -[M_1(Y_s \mathbf{u}) - \sqrt{2/\pi}]^2$$

$(M_2(Y_s^T \mathbf{u}) = 1)$ is minimized under the condition $\mathbf{u}^T \mathbf{u} = 1$.

The solution is obtained from a stationary point of

$$L(\mathbf{u}, \lambda) = -[M_1(Y_s^T \mathbf{u}) - \sqrt{2/\pi}]^2 + \lambda(\mathbf{u}^T \mathbf{u} - 1)/2$$

We have $D_{\mathbf{u}}J(\mathbf{u}) = -\phi(\mathbf{u})G(\mathbf{u})\mathbf{u}$ with

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

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

$$G(\mathbf{u}^*)\mathbf{u}^* = \mu^*(\mathbf{u}^*)\mathbf{u}^*, \quad \mathbf{u}^{*T} \mathbf{u}^* = 1$$

Minimizing the Robust Objective Function for ICA

The nonlinear eigenspace problem is solved by a **vector iteration**.

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

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

After convergence

$$\mathbf{u}^* = \lim_{l \rightarrow \infty} \mathbf{u}_l$$

is the first column of U^T .

Minimizing the Robust Objective Function for ICA

The nonlinear eigenspace problem is solved by a **vector iteration**.

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

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

After convergence

$$\mathbf{u}^* = \lim_{l \rightarrow \infty} \mathbf{u}_l$$

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**

$$Y_p = (I - \mathbf{u}^* \mathbf{u}^{*T}) Y_s$$

have columns which are linearly independent from \mathbf{u}^* .

Minimizing the Robust Objective Function for ICA

With the **modified matrix**,

$$\tilde{G}(\mathbf{u}) = \frac{1}{n} \sum_{i=1}^n \frac{Y_p \mathbf{e}_i \mathbf{e}_i^T Y_p^T}{|\mathbf{e}_i^T Y_p^T \mathbf{u}|}$$

the modified vector iteration is,

$$\mathbf{u} = (I - \mathbf{u}^* \mathbf{u}^{*\top}) \tilde{G}(\mathbf{u}_l) \mathbf{u}_l, \quad \mathbf{u}_{l+1} = \mathbf{u} / \|\mathbf{u}\|, \quad l = 1, 2, \dots$$

Minimizing the Robust Objective Function for ICA

With the **modified matrix**,

$$\tilde{G}(\mathbf{u}) = \frac{1}{n} \sum_{i=1}^n \frac{Y_p \mathbf{e}_i \mathbf{e}_i^T Y_p^T}{|\mathbf{e}_i^T Y_p^T \mathbf{u}|}$$

the modified vector iteration is,

$$\mathbf{u} = (I - \mathbf{u}^* \mathbf{u}^{*\top}) \tilde{G}(\mathbf{u}_l) \mathbf{u}_l, \quad \mathbf{u}_{l+1} = \mathbf{u} / \|\mathbf{u}\|, \quad l = 1, 2, \dots$$

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

Minimizing the Robust Objective Function for ICA

With the **modified matrix**,

$$\tilde{G}(\mathbf{u}) = \frac{1}{n} \sum_{i=1}^n \frac{Y_p \mathbf{e}_i \mathbf{e}_i^T Y_p^T}{|\mathbf{e}_i^T Y_p^T \mathbf{u}|}$$

the modified vector iteration is,

$$\mathbf{u} = (I - \mathbf{u}^* \mathbf{u}^{*\top}) \tilde{G}(\mathbf{u}_l) \mathbf{u}_l, \quad \mathbf{u}_{l+1} = \mathbf{u} / \|\mathbf{u}\|, \quad l = 1, 2, \dots$$

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

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

Minimizing the Robust Objective Function for ICA

With the **modified matrix**,

$$\tilde{G}(\mathbf{u}) = \frac{1}{n} \sum_{i=1}^n \frac{Y_p \mathbf{e}_i \mathbf{e}_i^T Y_p^T}{|\mathbf{e}_i^T Y_p^T \mathbf{u}|}$$

the modified vector iteration is,

$$\mathbf{u} = (I - \mathbf{u}^* \mathbf{u}^{*T}) \tilde{G}(\mathbf{u}_l) \mathbf{u}_l, \quad \mathbf{u}_{l+1} = \mathbf{u} / \|\mathbf{u}\|, \quad l = 1, 2, \dots$$

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

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

Observation: **Robust convergence** is seen in practice.

Application to DCE-MRI sequences

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

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

is an image in the [\[Video\]](#).

Application to DCE-MRI sequences

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

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

is an image in the [Video]. Eliminate motion? Noise? Artifacts?

Application to DCE-MRI sequences

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

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

is an image in the [Video]. Eliminate motion? Noise? Artifacts?

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

$$\mathbf{c}_t = \{ B_{1,1}(t), \dots, B_{N,1}(t), B_{1,2}(t), \dots, B_{N,2}(t), \dots, B_{1,N}(t), \dots, B_{N,N}(t) \}^T$$

and PCA/ICA is carried out with $Y = \{\mathbf{c}_1, \dots, \mathbf{c}_n\}$.

Application to DCE-MRI sequences

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

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

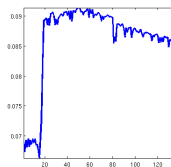
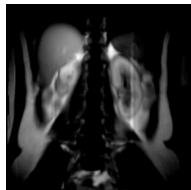
is an image in the [Video]. Eliminate motion? Noise? Artifacts?

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

$$\mathbf{c}_t = \{ B_{1,1}(t), \dots, B_{N,1}(t), B_{1,2}(t), \dots, B_{N,2}(t), \dots, B_{1,N}(t), \dots, B_{N,N}(t) \}^T$$

and PCA/ICA is carried out with $Y = \{\mathbf{c}_1, \dots, \mathbf{c}_n\}$.

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



To the right is the first row of Y_s .

Application to DCE-MRI sequences

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

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

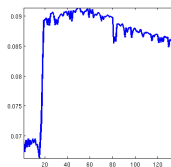
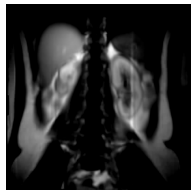
is an image in the [\[Video\]](#). Eliminate motion? Noise? Artifacts?

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

$$\mathbf{c}_t = \{ B_{1,1}(t), \dots, B_{N,1}(t), B_{1,2}(t), \dots, B_{N,2}(t), \dots, B_{1,N}(t), \dots, B_{N,N}(t) \}^T$$

and PCA/ICA is carried out with $Y = \{\mathbf{c}_1, \dots, \mathbf{c}_n\}$.

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

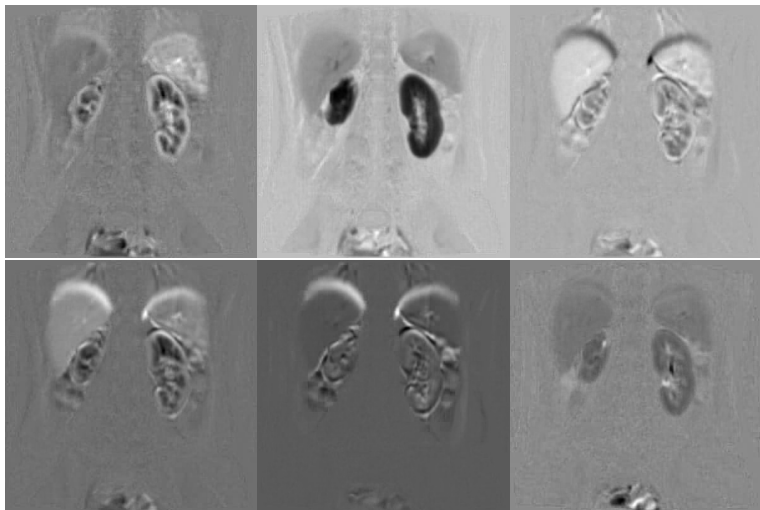


To the [right](#) is the first row of Y_s .

Compressed to 10 principal components: [\[Video\]](#)

Anwendung für DCE-MRI Folgen

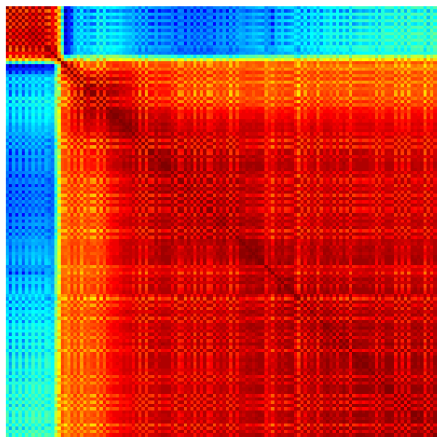
The 6 most significant independent components:



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,
which refine to a continuum ... ?

Formulation in Function Space

Based upon the imaging examples:

- ▶ Sampling occurs continuously in time ... ?
- ▶ Same number of sources as pixels,
which refine to a continuum ... ?

Claim: That the sources be statistically independent requires that that they be **countable**.

Formulation in Function Space

Based upon the imaging examples:

- ▶ Sampling occurs continuously in time ... ?
- ▶ Same number of sources as pixels,
which refine to a continuum ... ?

Claim: That the sources be statistically independent requires that that they be **countable**.

Consequence: The function space setting resembles the finite dimensional setting but with **infinite matrices** operating between bases in **separable spaces**.

Thank You!