

# PCA and ICA

Julie Nutini

*Machine Learning Reading Group*

February 6, 2017

# What is PCA?

- Principal Component Analysis (PCA) is a **statistical procedure** that allows **better analysis and interpretation of unstructured data**.

# What is PCA?

- Principal Component Analysis (PCA) is a **statistical procedure** that allows **better analysis and interpretation of unstructured data**.
- Uses an **orthogonal linear transformation** to convert a set of observations to a **new coordinate system** that **maximizes the variance**.

# What is PCA?

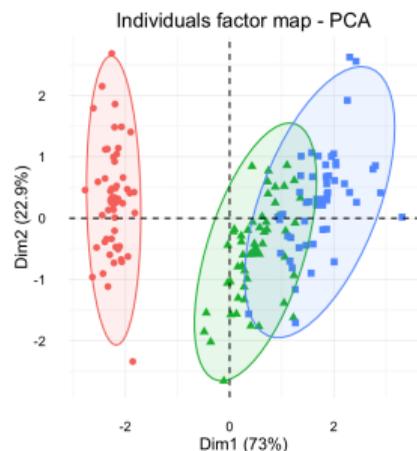
- Principal Component Analysis (PCA) is a **statistical procedure** that allows **better analysis and interpretation of unstructured data**.
- Uses an **orthogonal linear transformation** to convert a set of observations to a **new coordinate system** that **maximizes the variance**.
- The new coordinates are called **principal components**.

# What is PCA?

- Principal Component Analysis (PCA) is a **statistical procedure** that allows **better analysis and interpretation of unstructured data**.
- Uses an **orthogonal linear transformation** to convert a set of observations to a **new coordinate system** that **maximizes the variance**.
- The new coordinates are called **principal components**.

Example:

- Fit  $n$ -dimensional **ellipsoid** to data.
- By omitting axis with smallest variance (smallest principal component), we lose **smallest amount of info**.

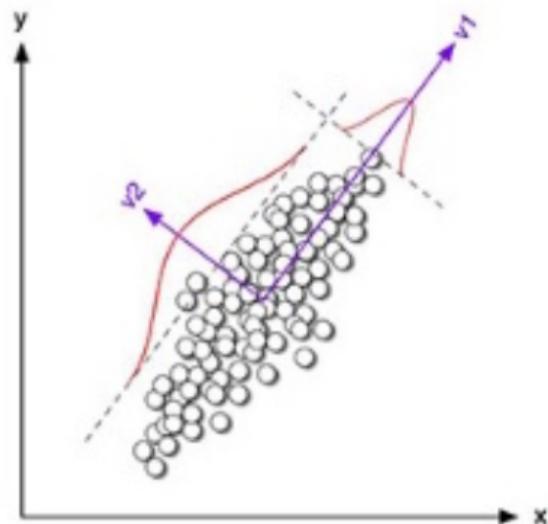


# Principal Component Analysis (PCA) aka...

- Signal processing: discrete Kosambi-Karhunen-Loève transform (KLT)
- Multivariate quality control: the Hotelling transform
- Mechanical engineering: proper orthogonal decomposition (POD)
- Linear algebra: singular value decomposition (SVD) of  $X$  (Golub and Van Loan, 1983)
- Linear algebra: eigenvalue decomposition (EVD) of  $X^T X$
- Psychometrics: factor analysis, Eckart-Young theorem (Harman, 1960), or Schmidt-Mirsky theorem
- Meteorological science: empirical orthogonal functions (EOF)
- Noise and vibration: empirical eigenfunction decomposition (Sirovich, 1987), empirical component analysis (Lorenz, 1956), quasiharmonic modes (Brooks et al., 1988), spectral decomposition
- Structural dynamics: empirical modal analysis
- ...

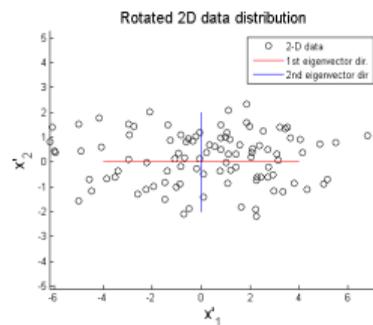
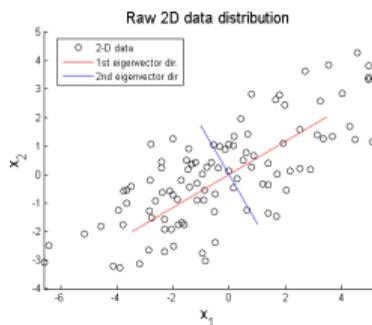
# Applications of PCA

- Dimension construction
- Feature extraction
- Data visualization
- Image compression
- Medical imaging
- Lossy data compression
- ...



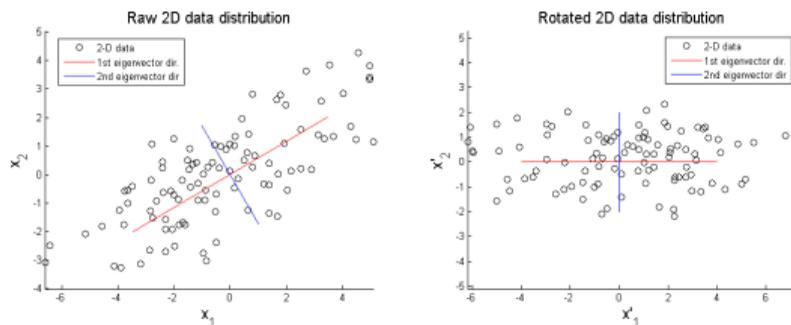
# Application: 2D Data Analysis

- Data matrix  $X$  can be **rotated** to align principal axes with  $x$  and  $y$  axis.

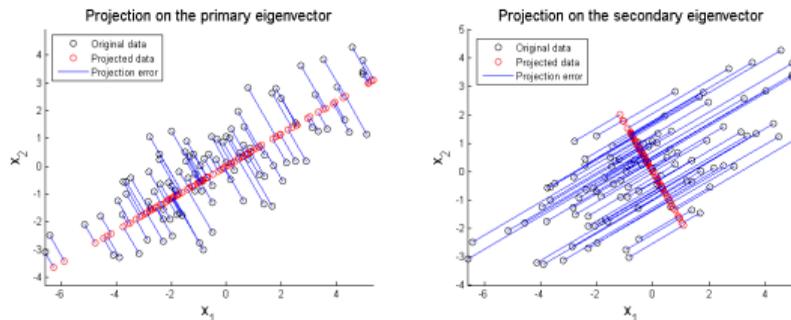


# Application: 2D Data Analysis

- Data matrix  $X$  can be **rotated** to align principal axes with x and y axis.

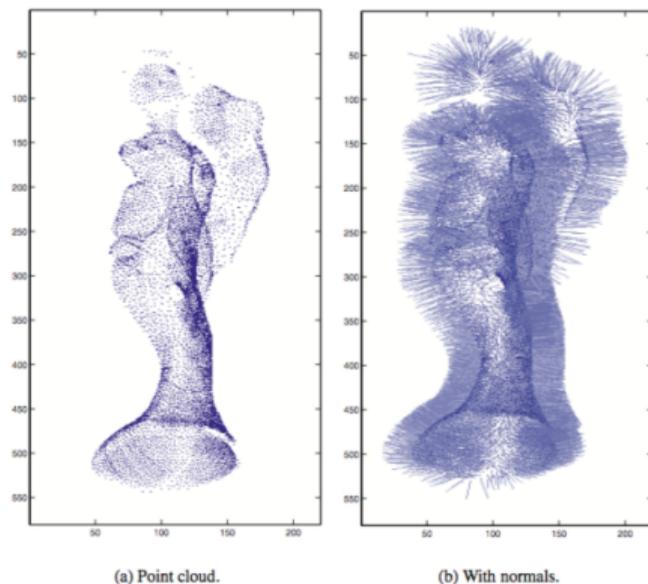


- **Project**  $X$  on the primary and secondary principal direction.



# Application: Data Visualization

- Scattered set of points, presumably forms coherent surface.
- Display point cloud data in a pleasing way.



**Figure 4.9.** Example 4.18: a point cloud representing (a) a surface in three-dimensional space, and (b) together with its unsigned normals.

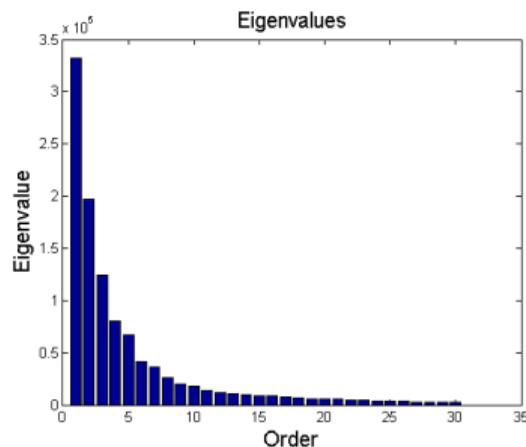
# Application: Image Compression

- Effectively represent image with limited number of principal components.



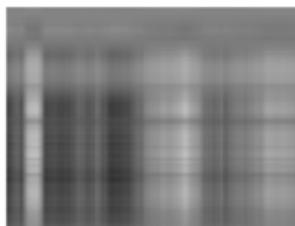
# Application: Image Compression

- Effectively represent image with limited number of principal components.

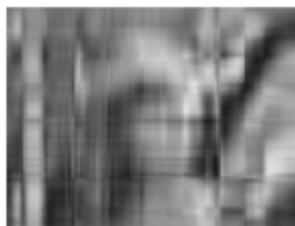


- Do not know # of principal components needed for **successful reconstruction**.

# Application: Image Compression



(a) 1 principal component



(b) 5 principal component



(c) 9 principal component



(d) 13 principal component



(e) 17 principal component



(f) 21 principal component



(g) 25 principal component



(h) 29 principal component

# The Problem

Let  $X$  be a  $D$ -dimensional random vector with **covariance matrix**  $S$ .

# The Problem

Let  $X$  be a  $D$ -dimensional random vector with **covariance matrix**  $S$ .

- **Problem:** Consecutively find the unit vectors  $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_D$  such that

$$Y_i = X^T \mathbf{u}_i$$

satisfies:

- 1  $\text{var}(Y_1)$  is the maximum.
- 2  $\text{var}(Y_2)$  is the maximum subject to  $\text{cov}(Y_2, Y_1) = 0$ .
- 3  $\text{var}(Y_k)$  is the maximum subject to  $\text{cov}(Y_k, Y_i) = 0$ , where  $k = 3, 4, \dots, D$  and  $k > i$ .

# The Solutions

- Let  $(\lambda_i, \mathbf{u}_i)$  be the pairs of **eigenvalues** and **eigenvectors** of the **covariance matrix**  $S$  such that

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_D (\geq 0)$$

and

$$\|\mathbf{u}_i\|_2 = 1, \quad \text{for all } 1 \leq i \leq D.$$

# The Solutions

- Let  $(\lambda_i, \mathbf{u}_i)$  be the pairs of **eigenvalues** and **eigenvectors** of the **covariance matrix**  $S$  such that

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_D (\geq 0)$$

and

$$\|\mathbf{u}_i\|_2 = 1, \quad \text{for all } 1 \leq i \leq D.$$

- Then  $\text{var}(Y_i) = \lambda_i$  for  $1 \leq i \leq D$ .
- The principal components of  $X$  are the eigenvectors of  $S$ .
- The variance will be a maximum when we **set  $\mathbf{u}_1$  to the eigenvector having the largest eigenvalue.**

# The Solutions

- Let  $(\lambda_i, \mathbf{u}_i)$  be the pairs of **eigenvalues** and **eigenvectors** of the **covariance matrix**  $S$  such that

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_D (\geq 0)$$

and

$$\|\mathbf{u}_i\|_2 = 1, \quad \text{for all } 1 \leq i \leq D.$$

- Then  $\text{var}(Y_i) = \lambda_i$  for  $1 \leq i \leq D$ .
- The principal components of  $X$  are the eigenvectors of  $S$ .
  - The variance will be a maximum when we **set  $\mathbf{u}_1$  to the eigenvector having the largest eigenvalue.**
- The **proportion of variance** each eigenvector represents is given by the **ratio of the given eigenvalue to the sum of all the eigenvalues.**

- Linear, nonparametric analysis that **cannot incorporate prior knowledge**.

# Restrictions of PCA

- Linear, nonparametric analysis that **cannot incorporate prior knowledge**.
- Important that **variance** can be used to **differentiate/imply similarity**.

# Restrictions of PCA

- Linear, nonparametric analysis that cannot incorporate prior knowledge.
- Important that variance can be used to differentiate/imply similarity.
- If the given data set is nonlinear or multimodal distribution, PCA fails to provide meaningful data reduction.

# Restrictions of PCA

- Linear, nonparametric analysis that **cannot incorporate prior knowledge**.
- Important that **variance** can be used to **differentiate/ imply similarity**.
- If the given data set is **nonlinear** or **multimodal distribution**, **PCA fails to provide meaningful data reduction**.
- To incorporate the **prior knowledge of data to PCA**, researchers have proposed **dimension reduction techniques** as extensions of PCA:
  - e.g., kernel PCA, multilinear PCA, and independent component analysis (ICA).

# General: How to do PCA?

**Goal:** Find the axes of the ellipse (i.e., the principal components).

# General: How to do PCA?

**Goal:** Find the axes of the ellipse (i.e., the principal components).

Consider a data matrix  $X$ .

- 1 Subtract the sample mean from each column of  $X$  (data has mean 0).

# General: How to do PCA?

**Goal:** Find the axes of the ellipse (i.e., the principal components).

Consider a data matrix  $X$ .

- 1 Subtract the sample mean from each column of  $X$  (data has mean 0).
- 2 Compute covariance matrix of the data.

# General: How to do PCA?

**Goal:** Find the axes of the ellipse (i.e., the principal components).

Consider a data matrix  $X$ .

- 1 Subtract the sample mean from each column of  $X$  (data has mean 0).
- 2 Compute covariance matrix of the data.
- 3 Calculate the eigenvalues/corresponding eigenvectors of covariance matrix,

$$Xv = \lambda v$$

\*  $Xv$  does not change direction of  $v$ .

# General: How to do PCA?

**Goal:** Find the axes of the ellipse (i.e., the principal components).

Consider a data matrix  $X$ .

- 1 Subtract the sample mean from each column of  $X$  (data has mean 0).
- 2 Compute covariance matrix of the data.
- 3 Calculate the eigenvalues/corresponding eigenvectors of covariance matrix,

$$Xv = \lambda v$$

\*  $Xv$  does not change direction of  $v$ .

- 4 Orthogonalize the set of eigenvectors, normalize each to unit vectors.

# Formulations of PCA

There are two main formulations of PCA:

# Formulations of PCA

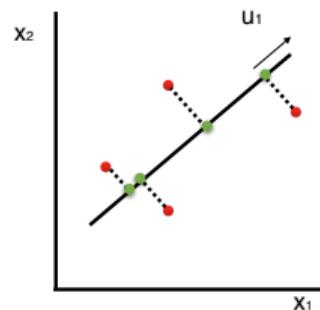
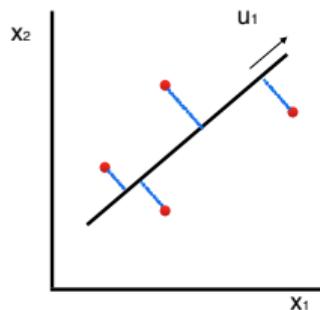
There are two main formulations of PCA:

- **Maximum variance formulation:** The orthogonal projection of the data onto a lower dimensional linear space (principal subspace) such that the **variance of the projected data is maximized**.

# Formulations of PCA

There are two main formulations of PCA:

- **Maximum variance formulation:** The orthogonal projection of the data onto a lower dimensional linear space (principal subspace) such that the **variance of the projected data is maximized**.
- **Minimum-error formulation:** The linear projection that **minimizes the average projection cost**, defined as the mean squared distance between the data points and their projections.



# Maximum Variance Formulation

**Goal:** Project data onto space having dimensionality  $M < D$  while **maximizing variance of projected data**.

# Maximum Variance Formulation

**Goal:** Project data onto space having dimensionality  $M < D$  while **maximizing variance of projected data**.

- Consider a data set of observations  $\{x_n\}$  where  $n = 1, \dots, N$ .
- Each  $x_n$  is a Euclidean variable with dimensionality  $D$ .

# Maximum Variance Formulation

**Goal:** Project data onto space having dimensionality  $M < D$  while **maximizing variance of projected data**.

- Consider a data set of observations  $\{x_n\}$  where  $n = 1, \dots, N$ .
- Each  $x_n$  is a Euclidean variable with dimensionality  $D$ .
- Assume projecting onto a one-dimensional space ( $M = 1$ ).

# Maximum Variance Formulation

**Goal:** Project data onto space having dimensionality  $M < D$  while **maximizing variance of projected data**.

- Consider a data set of observations  $\{x_n\}$  where  $n = 1, \dots, N$ .
- Each  $x_n$  is a Euclidean variable with dimensionality  $D$ .
- Assume projecting onto a one-dimensional space ( $M = 1$ ).
- Define the direction of this space using  $\mathbf{u}_1$ .
- Assume  $\mathbf{u}_1$  is a unit vector ( $\mathbf{u}_1^T \mathbf{u}_1 = 1$ ).

# Maximum Variance Formulation

- The **mean** of the projected data is  $\mathbf{u}_1^T \bar{x}$  where  $\bar{x}$  is the sample set mean

$$\bar{x} = \frac{1}{N} \sum_{n=1}^N x_n$$

# Maximum Variance Formulation

- The **mean** of the projected data is  $\mathbf{u}_1^T \bar{x}$  where  $\bar{x}$  is the sample set mean

$$\bar{x} = \frac{1}{N} \sum_{n=1}^N x_n$$

- The **variance** of the projected data is given by

$$\frac{1}{N} \sum_{n=1}^N (\mathbf{u}_1^T x_n - \mathbf{u}_1^T \bar{x})^2 = \mathbf{u}_1^T S \mathbf{u}_1$$

where  $S$  is the **covariance matrix** of the data,

$$S = \frac{1}{N} \sum_{n=1}^N (x_n - \bar{x})(x_n - \bar{x})^T.$$

# Maximum Variance Formulation

- To maximize the variance, we solve the following constrained problem

$$\underset{\mathbf{u}_1}{\text{maximize}} \quad \mathbf{u}_1^T S \mathbf{u}_1 \quad \text{s.t.} \quad \mathbf{u}_1^T \mathbf{u}_1 = 1$$

# Maximum Variance Formulation

- To maximize the variance, we solve the following constrained problem

$$\underset{\mathbf{u}_1}{\text{maximize}} \quad \mathbf{u}_1^T S \mathbf{u}_1 \quad \text{s.t.} \quad \mathbf{u}_1^T \mathbf{u}_1 = 1$$

- The Lagrangian of this problem is given by

$$\mathcal{L}(\mathbf{u}_1, \lambda_1) = \mathbf{u}_1^T S \mathbf{u}_1 + \lambda_1(1 - \mathbf{u}_1^T \mathbf{u}_1).$$

# Maximum Variance Formulation

- To maximize the variance, we solve the following constrained problem

$$\underset{\mathbf{u}_1}{\text{maximize}} \quad \mathbf{u}_1^T S \mathbf{u}_1 \quad \text{s.t.} \quad \mathbf{u}_1^T \mathbf{u}_1 = 1$$

- The Lagrangian of this problem is given by

$$\mathcal{L}(\mathbf{u}_1, \lambda_1) = \mathbf{u}_1^T S \mathbf{u}_1 + \lambda_1(1 - \mathbf{u}_1^T \mathbf{u}_1).$$

- Differentiating with respect to  $\mathbf{u}_1$ , we have a stationary point when

$$S \mathbf{u}_1 = \lambda_1 \mathbf{u}_1.$$

# Maximum Variance Formulation

- By left-multiplying by  $\mathbf{u}_1$  and using  $\mathbf{u}_1^T \mathbf{u}_1 = 1$ , we have

$$\mathbf{u}_1^T S \mathbf{u}_1 = \lambda_1.$$

# Maximum Variance Formulation

- By left-multiplying by  $\mathbf{u}_1$  and using  $\mathbf{u}_1^T \mathbf{u}_1 = 1$ , we have

$$\mathbf{u}_1^T S \mathbf{u}_1 = \lambda_1.$$

- Thus, the **maximum variance** will occur when we set  $\mathbf{u}_1$  to the **eigenvector** having the largest eigenvalue  $\lambda_1$ .

# Maximum Variance Formulation

- By left-multiplying by  $\mathbf{u}_1$  and using  $\mathbf{u}_1^T \mathbf{u}_1 = 1$ , we have

$$\mathbf{u}_1^T S \mathbf{u}_1 = \lambda_1.$$

- Thus, the **maximum variance** will occur when we set  $\mathbf{u}_1$  to the **eigenvector having the largest eigenvalue  $\lambda_1$** .
- Additional principal components can be defined in an incremental fashion.
- A similar problem can be formed for the **minimum error formulation**.
  - Solution is in terms of the  $D - M$  smallest eigenvalues of the eigenvectors that are **orthogonal to the principal subspace**.

- The **singular value decomposition** of a matrix  $A \in \mathbb{R}^{m \times n}$  is given by

$$A = U\Sigma V^T$$

where

- $U \in \mathbb{R}^{m \times m}$  and  $V \in \mathbb{R}^{n \times n}$  are orthogonal matrices (i.e.,  $U^T U = U U^T = I$ )
- $D \in \mathbb{R}^{m \times n}$  diagonal matrix with the singular values of  $A$  along the diagonal.

- The **singular value decomposition** of a matrix  $A \in \mathbb{R}^{m \times n}$  is given by

$$A = U\Sigma V^T$$

where

- $U \in \mathbb{R}^{m \times m}$  and  $V \in \mathbb{R}^{n \times n}$  are orthogonal matrices (i.e.,  $U^T U = U U^T = I$ )
- $D \in \mathbb{R}^{m \times n}$  diagonal matrix with the singular values of  $A$  along the diagonal.
- The **largest variance is in the direction of the first column of  $U$**  (the first **principal component**)
- The largest variance on the subspace **orthogonal to the first principal component** is the direction of the second column of  $U$
- ...

- Therefore,

$$B = U^T A = \Sigma V^T$$

represents a better alignment than the given  $A$  in terms of **variance differentiation**.

- Therefore,

$$B = U^T A = \Sigma V^T$$

represents a better alignment than the given  $A$  in terms of **variance differentiation**.

- Covariance matrix of  $A$  is a positive semi-definite matrix,

$$C = AA^T = U\Sigma\Sigma^T U^T$$

and the **eigenvectors are the columns of  $U$**  (namely, the **singular vectors** which are the principal components).

- Therefore,

$$B = U^T A = \Sigma V^T$$

represents a better alignment than the given  $A$  in terms of **variance differentiation**.

- Covariance matrix of  $A$  is a positive semi-definite matrix,

$$C = AA^T = U\Sigma\Sigma^T U^T$$

and the **eigenvectors are the columns of  $U$**  (namely, the **singular vectors** which are the principal components).

- Application of PCA with respect to SVD:
  - Solving **almost singular linear systems**
    - If the problem is too ill-conditioned, then regularize it.

# Computing the Principal Components

Eigenvalues:

- QR algorithm: costs  $O(D^3)$ .
- Power Method: Finds first  $M$  principal components, costs  $O(MD^2)$ .

# Computing the Principal Components

Eigenvalues:

- QR algorithm: costs  $O(D^3)$ .
- Power Method: Finds first  $M$  principal components, costs  $O(MD^2)$ .

Singular values:

- SVD costs  $O(m^2n + mn^2 + n^3)$  for general matrix  $A$  of dimension  $m \times n$ .

# Computing the Principal Components

Eigenvalues:

- QR algorithm: costs  $O(D^3)$ .
- Power Method: Finds first  $M$  principal components, costs  $O(MD^2)$ .

Singular values:

- SVD costs  $O(m^2n + mn^2 + n^3)$  for general matrix  $A$  of dimension  $m \times n$ .

→ When  $D$  is **large**, a direct application of PCA will be **computationally infeasible**.

# PCA for High-Dimensional Data

Let  $X$  be an  $(N \times D)$ -dimensional centered matrix.

- The  $n$ th row is  $(x_n - \bar{x})^T$ .
- The covariance matrix can be written as  $S = \frac{1}{N} X^T X$ .

- The corresponding eigenvector equation becomes

$$\frac{1}{N} X^T X \mathbf{u}_i = \lambda_i \mathbf{u}_i.$$

# PCA for High-Dimensional Data

- The corresponding eigenvector equation becomes

$$\frac{1}{N}X^T X \mathbf{u}_i = \lambda_i \mathbf{u}_i.$$

- Multiply both sides by  $X$ ,

$$\frac{1}{N}X X^T (X \mathbf{u}_i) = \lambda_i (X \mathbf{u}_i).$$

# PCA for High-Dimensional Data

- The corresponding eigenvector equation becomes

$$\frac{1}{N}X^T X \mathbf{u}_i = \lambda_i \mathbf{u}_i.$$

- Multiply both sides by  $X$ ,

$$\frac{1}{N}X X^T (X \mathbf{u}_i) = \lambda_i (X \mathbf{u}_i).$$

- Let  $\mathbf{v}_i = X \mathbf{u}_i$  to get

$$\frac{1}{N}X X^T \mathbf{v}_i = \lambda_i \mathbf{v}_i,$$

which is the eigenvector equation for the  $N \times N$  matrix  $\frac{1}{N}X X^T$ .

# PCA for High-Dimensional Data

- The corresponding eigenvector equation becomes

$$\frac{1}{N}X^T X \mathbf{u}_i = \lambda_i \mathbf{u}_i.$$

- Multiply both sides by  $X$ ,

$$\frac{1}{N}X X^T (X \mathbf{u}_i) = \lambda_i (X \mathbf{u}_i).$$

- Let  $\mathbf{v}_i = X \mathbf{u}_i$  to get

$$\frac{1}{N}X X^T \mathbf{v}_i = \lambda_i \mathbf{v}_i,$$

which is the eigenvector equation for the  $N \times N$  matrix  $\frac{1}{N}X X^T$ .

- This has the **same  $N - 1$  eigenvalues as the original covariance matrix.**
- We can solve the eigenvalue problem for cost of  $O(N^3)$ .

- PCA is a statistical procedure that uses an **orthogonal linear transformation** to reduce the dimension of a dataset while **maximizing the variance**.

- PCA is a statistical procedure that uses an **orthogonal linear transformation** to reduce the dimension of a dataset while **maximizing the variance**.
- PCs of a dataset  $X$  are the eigenvectors of its covariance matrix.

- PCA is a statistical procedure that uses an **orthogonal linear transformation** to reduce the dimension of a dataset while **maximizing the variance**.
- PCs of a dataset  $X$  are the eigenvectors of its covariance matrix.
- Formulated as a maximum variance problem or a minimum error problem.

- PCA is a statistical procedure that uses an **orthogonal linear transformation** to reduce the dimension of a dataset while **maximizing the variance**.
- PCs of a dataset  $X$  are the eigenvectors of its covariance matrix.
- Formulated as a maximum variance problem or a minimum error problem.
- Transformation for high-dimensional data.
  - Allows you to find principal components in smaller subspace.

- PCA is a statistical procedure that uses an **orthogonal linear transformation** to reduce the dimension of a dataset while **maximizing the variance**.
- PCs of a dataset  $X$  are the eigenvectors of its covariance matrix.
- Formulated as a maximum variance problem or a minimum error problem.
- Transformation for high-dimensional data.
  - Allows you to find principal components in smaller subspace.
- Extensions:
  - Probabilistic PCA
    - Maximum likelihood PCA, EM algorithm for PCA, Bayesian PCA, Factor analysis
  - Kernel PCA

# Independent Component Analysis

- PCA focuses on models with latent variables based on linear-Gaussian distributions.
  - The PCs represent a **rotation** of the coordinate system in data space.
  - Data distribution in the new coordinates is **uncorrelated**.

# Independent Component Analysis

- PCA focuses on models with latent variables based on linear-Gaussian distributions.
  - The PCs represent a **rotation** of the coordinate system in data space.
  - Data distribution in the new coordinates is **uncorrelated**.
  - This is a **necessary condition for independence, but not a sufficient condition**.

# Independent Component Analysis

- Independent Component Analysis (ICA):
  - Similar to PCA, finds a **new basis** to represent data.

# Independent Component Analysis

- Independent Component Analysis (ICA):
  - Similar to PCA, finds a **new basis** to represent data.
  - Computational method for separating multivariate signal into **additive subcomponents** that are **maximally independent**.

# Independent Component Analysis

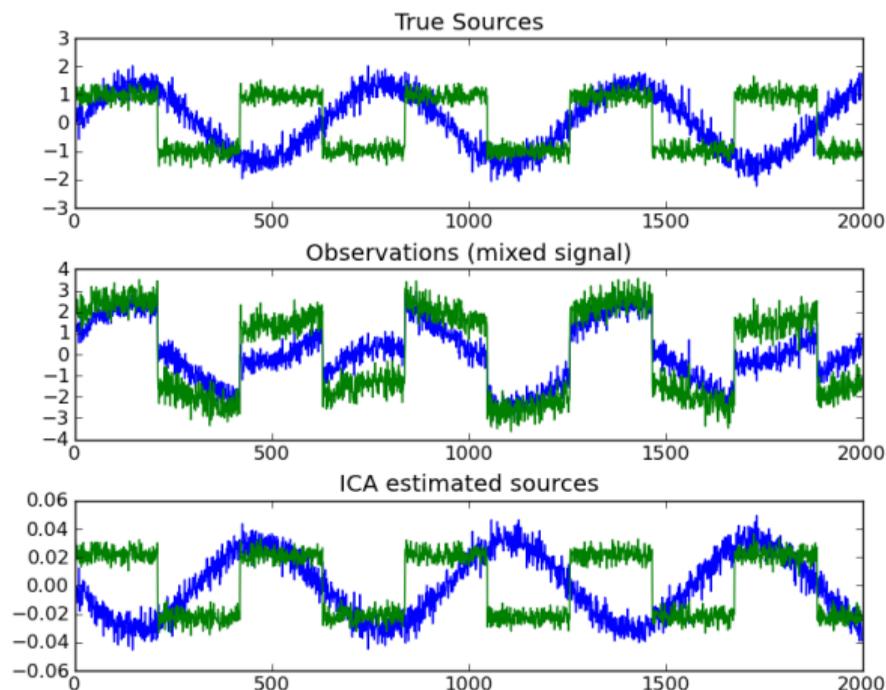
- Independent Component Analysis (ICA):
  - Similar to PCA, finds a **new basis** to represent data.
  - Computational method for separating multivariate signal into **additive subcomponents** that are **maximally independent**.
  - Observed variables are **linear combination of the latent variables**.

# Independent Component Analysis

- Independent Component Analysis (ICA):
  - Similar to PCA, finds a **new basis** to represent data.
  - Computational method for separating multivariate signal into **additive subcomponents** that are **maximally independent**.
  - Observed variables are **linear combination of the latent variables**.
  - Assumes **subcomponents are non-Gaussian signals** and are **statistically independent**.

# Example: blind source separation

## Example: blind source separation



- ICA is used to recover the sources.

## Example: blind source separation

- Consider some data  $s \in \mathbb{R}^n$  that is generated via  $n$  independent sources

$$x = As,$$

where  $A$  is an unknown matrix (mixing matrix),  $x$  received signal.

## Example: blind source separation

- Consider some data  $s \in \mathbb{R}^n$  that is generated via  $n$  independent sources

$$x = As,$$

where  $A$  is an unknown matrix (mixing matrix),  $x$  received signal.

- Repeated observations gives a data set  $\{x^{(i)}, i = 1, \dots, m\}$ .

# Example: blind source separation

- Consider some data  $s \in \mathbb{R}^n$  that is generated via  $n$  independent sources

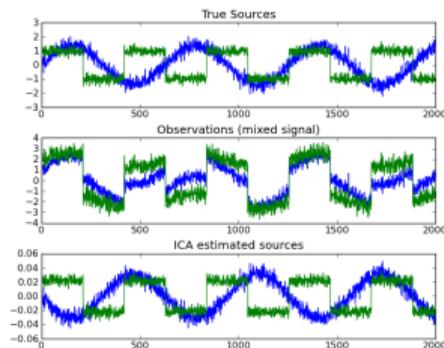
$$x = As,$$

where  $A$  is an unknown matrix (mixing matrix),  $x$  received signal.

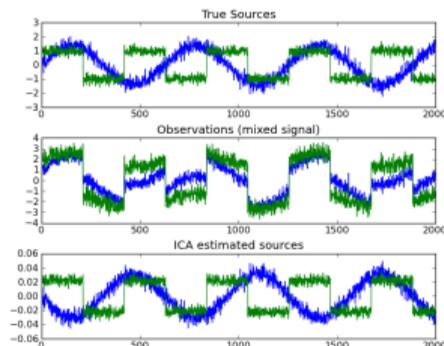
- Repeated observations gives a data set  $\{x^{(i)}, i = 1, \dots, m\}$ .
- **Goal:** Recover  $s^{(i)}$ .

- Given no prior knowledge about the sources or the mixing matrix, some inherent ambiguities in  $A$  are impossible to recover.
- Permutation of the sources is ambiguous.

- Given no prior knowledge about the sources or the mixing matrix, some inherent ambiguities in  $A$  are impossible to recover.
- Permutation of the sources is ambiguous.
- Scalings of  $W = A^{-1}$  cannot be recovered.
  - Might not matter depending on the application.
- We cannot determine the order of the independent components.



- Given no prior knowledge about the sources or the mixing matrix, some inherent ambiguities in  $A$  are impossible to recover.
- Permutation of the sources is ambiguous.
- Scalings of  $W = A^{-1}$  cannot be recovered.
  - Might not matter depending on the application.
- We cannot determine the order of the independent components.
- These are the ONLY ambiguities assuming the sources  $s_i$  are non-Gaussian.
- As long as the data is non-Gaussian, we can recover the  $n$  independent sources.



# ICA Algorithm (Bell and Sejnowski)

- Suppose the distribution of each source  $s_i$  is given by a density  $p_s$ .
- The **joint distribution of the sources  $s$**  is given by

$$p(s) = \prod_{i=1}^n p_s(s_i).$$

# ICA Algorithm (Bell and Sejnowski)

- Suppose the distribution of each source  $s_i$  is given by a density  $p_s$ .
- The **joint distribution of the sources**  $s$  is given by

$$p(s) = \prod_{i=1}^n p_s(s_i).$$

- By modelling the joint distribution as a product of the marginal, we capture the assumption that the sources are **independent**.

# ICA Algorithm (Bell and Sejnowski)

- Suppose the distribution of each source  $s_i$  is given by a density  $p_s$ .
- The **joint distribution of the sources**  $s$  is given by

$$p(s) = \prod_{i=1}^n p_s(s_i).$$

→ By modelling the joint distribution as a product of the marginal, we capture the assumption that the sources are **independent**.

- This implies the following density on  $x = As = W^{-1}s$  :

$$p(x) = \prod_{i=1}^n p_s(w_i^T x) \cdot |W|.$$

- Need to specify a density for the individual sources  $p_s$ .

# ICA Algorithm

- We need to specify a **cdf** for it that slowly increases from 0 to 1.
- Reasonable default: the **sigmoid function**

$$g(s) = \frac{1}{(1 + e^{-s})}.$$

- This yields  $p_s(s) = g'(s)$ .

- We need to specify a **cdf** for it that slowly increases from 0 to 1.
- Reasonable default: the **sigmoid function**

$$g(s) = \frac{1}{(1 + e^{-s})}.$$

- This yields  $p_s(s) = g'(s)$ .
- Given a training set  $\{x^{(i)}, i = 1, \dots, m\}$ , the **log likelihood** for our parameter **matrix  $W$**  is

$$\ell(W) = \sum_{i=1}^m \left( \sum_{j=1}^n \log g'(w_j^T x^{(i)}) + \log |W| \right).$$

- Maximizing this in terms of  $W$ , we derive a stochastic gradient ascent learning rule for training example  $x^{(i)}$ :

$$W := W + \alpha \left( \begin{bmatrix} 1 - 2g(w_1^T x^{(i)}) \\ 1 - 2g(w_2^T x^{(i)}) \\ \vdots \\ 1 - 2g(w_n^T x^{(i)}) \end{bmatrix} x^{(i)T} + (W^T)^{-1} \right)$$

where  $\alpha$  is the learning rate.

- Maximizing this in terms of  $W$ , we derive a stochastic gradient ascent learning rule for training example  $x^{(i)}$ :

$$W := W + \alpha \left( \begin{bmatrix} 1 - 2g(w_1^T x^{(i)}) \\ 1 - 2g(w_2^T x^{(i)}) \\ \vdots \\ 1 - 2g(w_n^T x^{(i)}) \end{bmatrix} x^{(i)T} + (W^T)^{-1} \right)$$

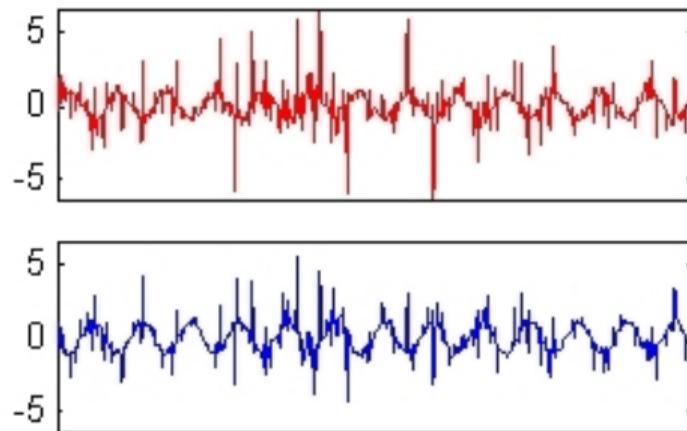
where  $\alpha$  is the learning rate.

- After the algorithm converges, we compute  $s^{(i)} = Wx^{(i)}$  to recover the original sources.

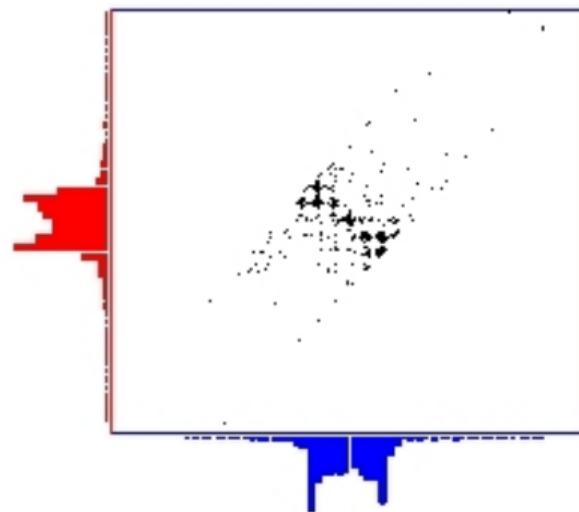
- FastICA [<http://research.ics.aalto.fi/ica/fastica/>]
- Implements the fast fixed-point algorithm for ICA and projection pursuit.
- Can download (for R, C++, Python and Matlab)

# FastICA Algorithm

SIGNALS



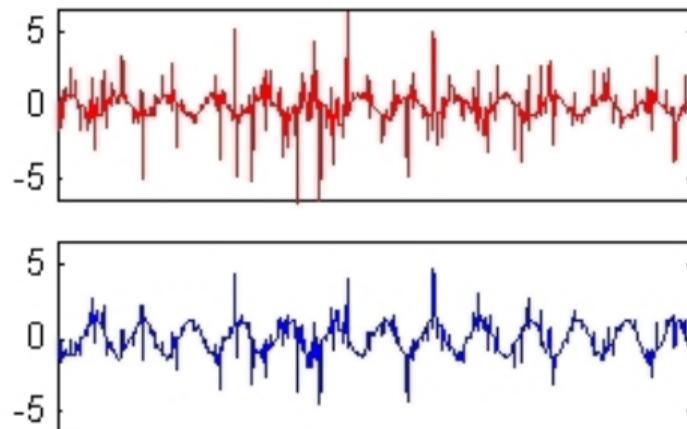
JOINT DENSITY



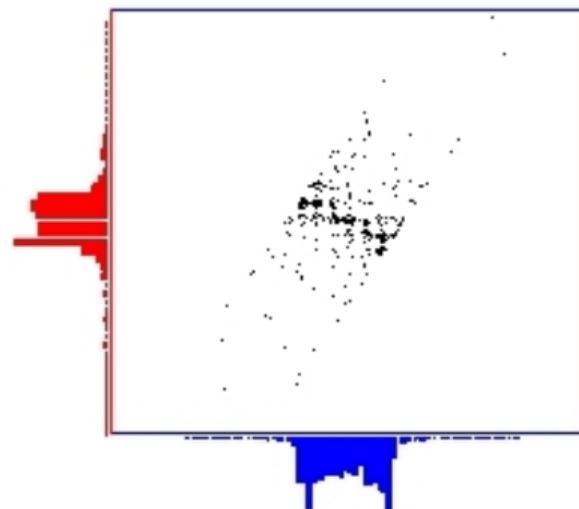
**Separated signals after 1 step of FastICA**

# FastICA Algorithm

SIGNALS



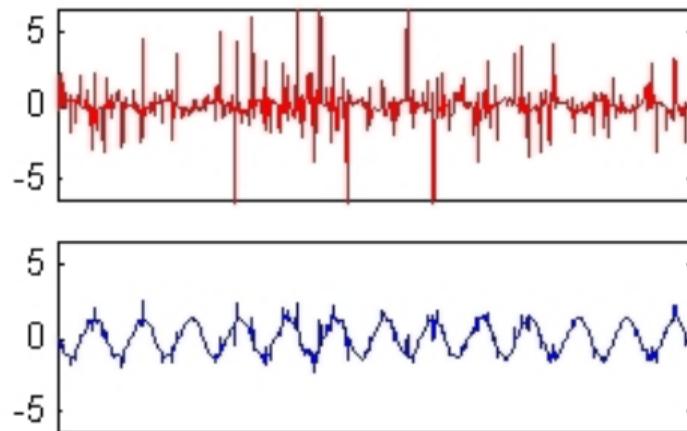
JOINT DENSITY



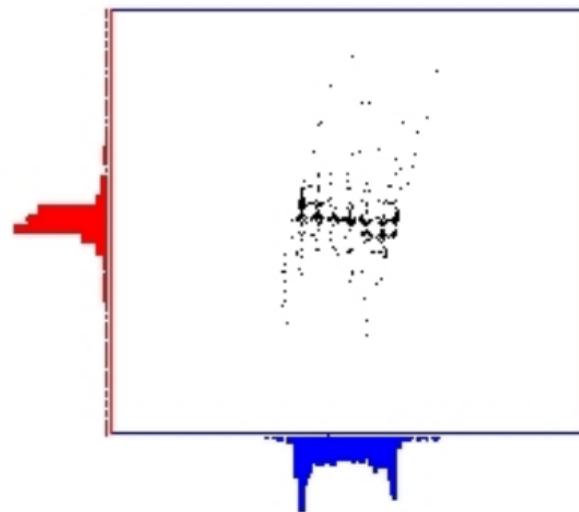
**Separated signals after 2 steps of FastICA**

# FastICA Algorithm

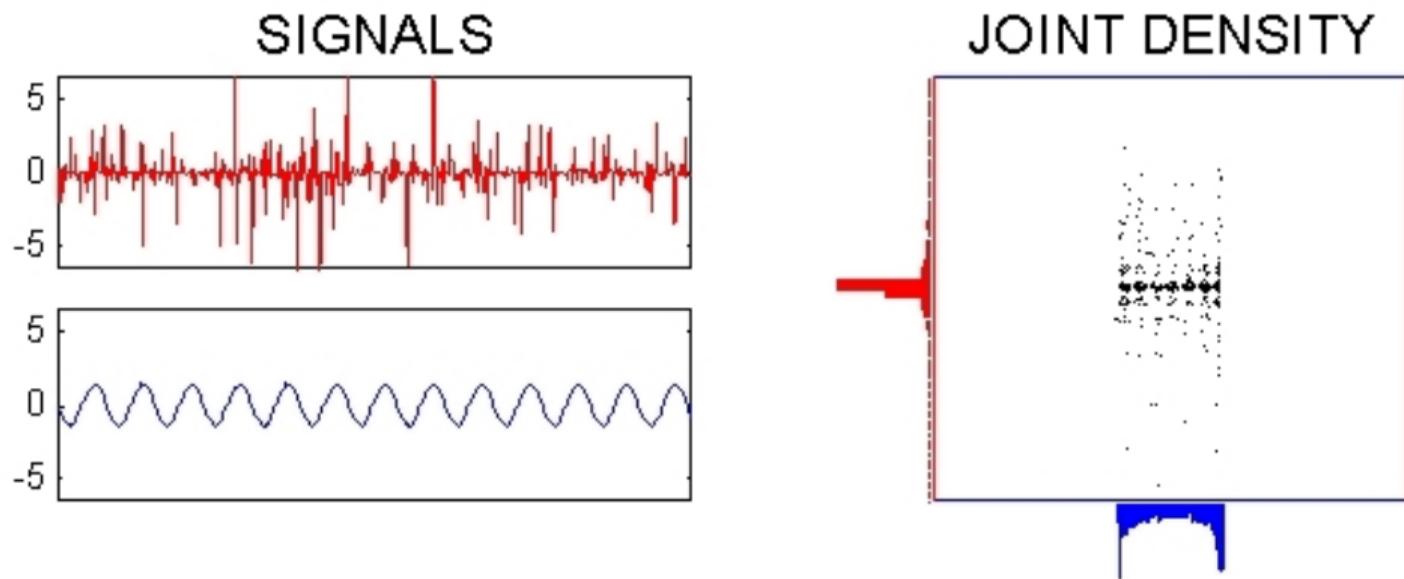
SIGNALS



JOINT DENSITY

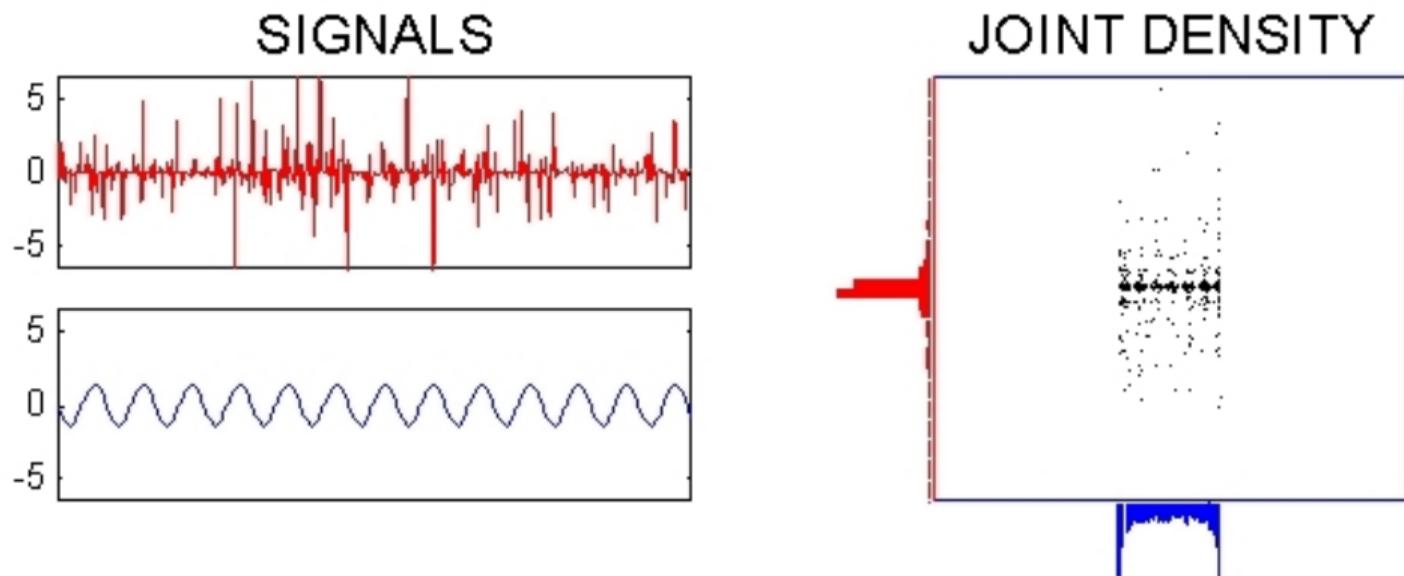


**Separated signals after 3 steps of FastICA**



**Separated signals after 4 steps of FastICA**

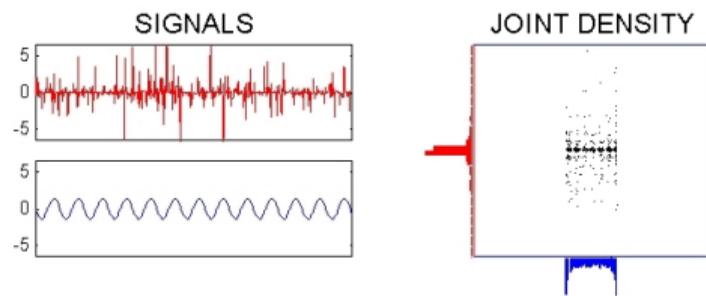
# FastICA Algorithm



**Separated signals after 5 steps of FastICA**

# FastICA Algorithm

- The source signals were **sinusoidal** and **impulsive noise**.
- The joint density is the product of the marginal densities.
  - Definition of **independence**.



Separated signals after 5 steps of FastICA

- ICA is a statistical and computational technique used to reveal hidden factors that underlie sets of random variables, measurements, or signals.

- ICA is a statistical and computational technique used to reveal hidden factors that underlie sets of random variables, measurements, or signals.
- Data assumed to be **linear combinations of some unknown latent variables**.
- Latent variables are assumed to be **non-Gaussian and independent**.

- ICA is a statistical and computational technique used to reveal hidden factors that underlie sets of random variables, measurements, or signals.
- Data assumed to be **linear combinations of some unknown latent variables**.
- Latent variables are assumed to be **non-Gaussian and independent**.
- ICA finds these **independent components**.

- ICA is a statistical and computational technique used to reveal hidden factors that underlie sets of random variables, measurements, or signals.
- Data assumed to be **linear combinations of some unknown latent variables**.
- Latent variables are assumed to be **non-Gaussian and independent**.
- ICA finds these **independent components**.
- Stochastic gradient ascent learning rule for training example  $x^{(i)}$ .
- FastICA
- ...

# Thank you!

- U. M. Ascher and C. Greif, *A First Course in Numerical Methods*, SIAM, 2011.
- C. M. Bishop. *Pattern Recognition and Machine Learning*, Springer, 2006.
- A. Hyvärinen. What is Independent Component Analysis?  
<https://www.cs.helsinki.fi/u/ahyvarin/whatisica.shtml>
- S. Jang. Basics and Examples of Principal Component Analysis (PCA), slecture, 2014  
[https://www.projectrhea.org/rhea/index.php/PCA\\_Theory\\_Examples](https://www.projectrhea.org/rhea/index.php/PCA_Theory_Examples).
- A. Ng. Independent Component Analysis, CS299 Lecture Notes.
- FastICA, <http://research.ics.aalto.fi/ica/fastica/>.