Principal Component Analysis (PCA)

and

PCA Neural Networks: An Application of Unsupervised Hebbian Learning

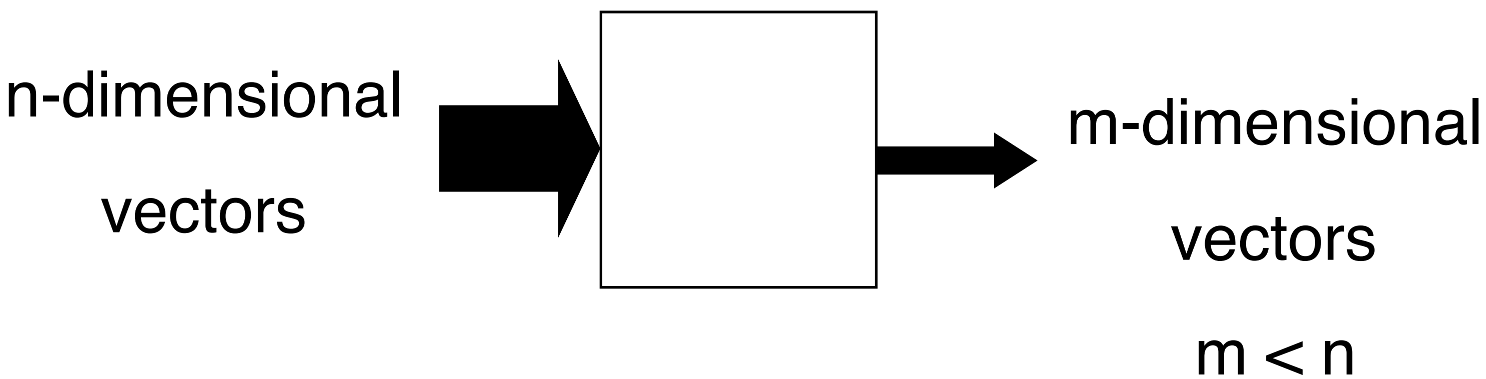
and intro to

Independent Components Analysis (ICA)

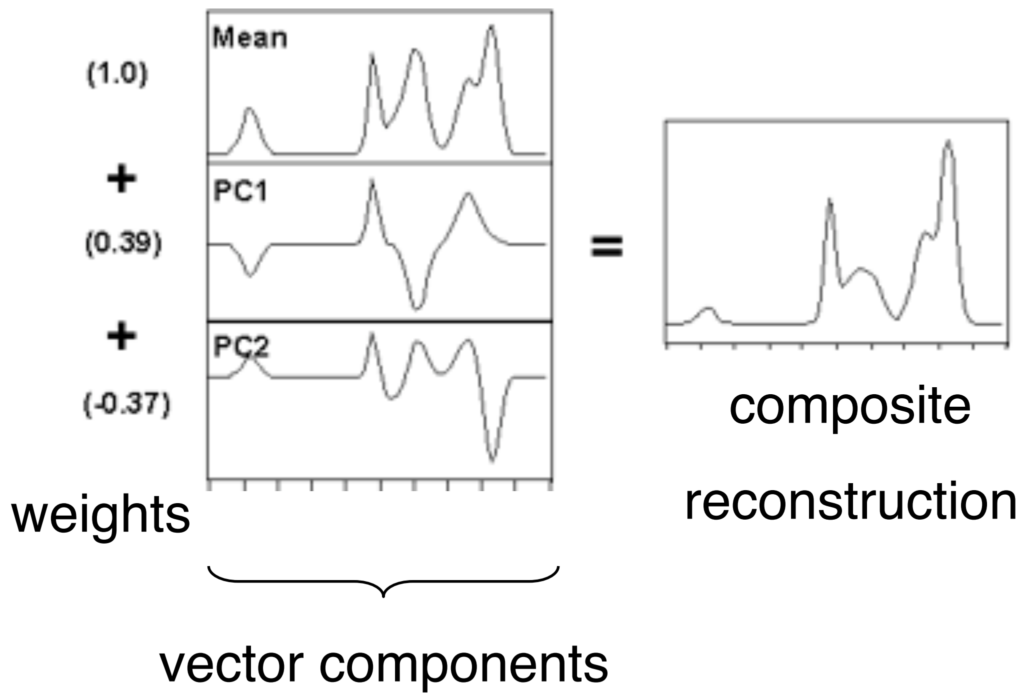
What is PCA?

- A standard statistical technique for reducing dimensionality of data (without using neural approach).
- Purpose: Better understanding or communication of data; used a lot in the sciences to select the most important features.
- In so reducing, we want to lose as little information as possible, given the before- and after- dimensions.
- Also known as **Karhuenen-Loeve (K-L) transformation** (Watanabe, 1969).
- Could be used to **preprocess** input to, say, MLP.

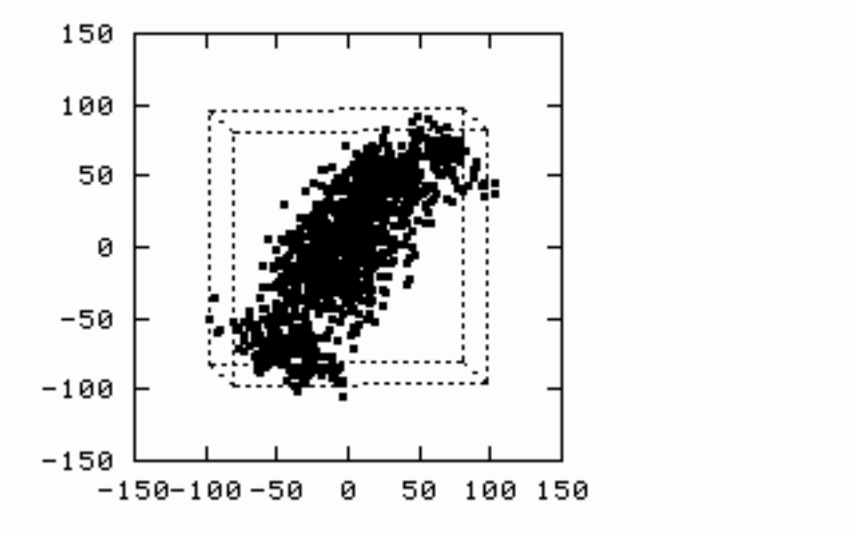
PCA



Reconstruction from Components

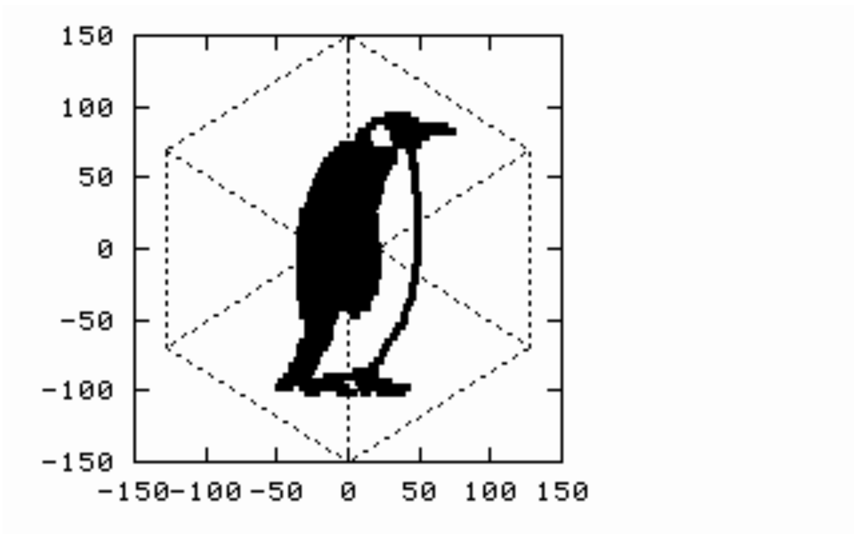


Scientific Uses



Transform coordinates to get a better understanding of the underlying phenomena.

Scientific Uses



Transform coordinates to get a better understanding of the underlying phenomena.

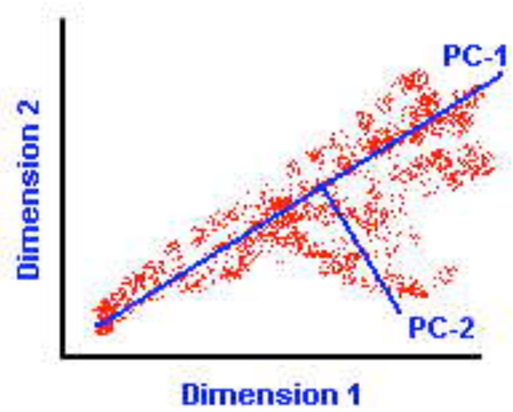
Comparison with Linear Regression

- Linear regression requires one to ***pre-identify*** dependent vs. independent variables.

- PCA does not.

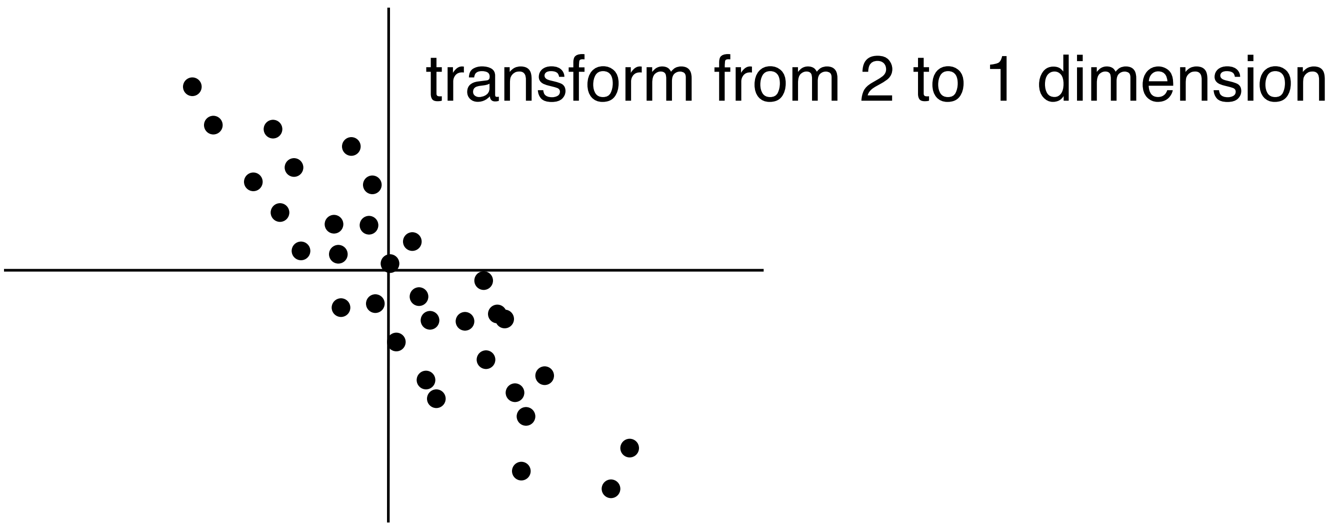
What is a "Principal Component"?

- If we were to plot the data, the **first principal component** would be the **predominant direction** in the data.
- The second principal component would be the second-most predominant direction, etc. up to the number of **dimensions** of the data points.



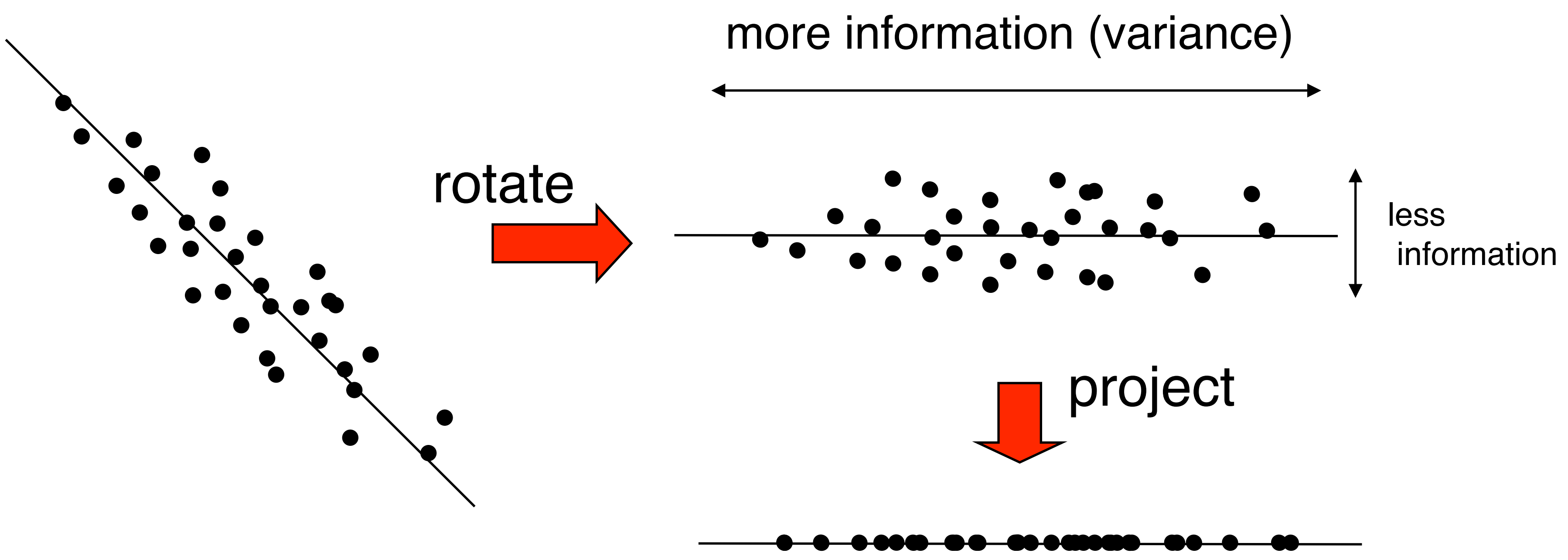
The main idea

- Transform the input data into fewer dimensions
- Preserve as much of the variance as possible



Transformation

- Preserve as much of the variance as possible



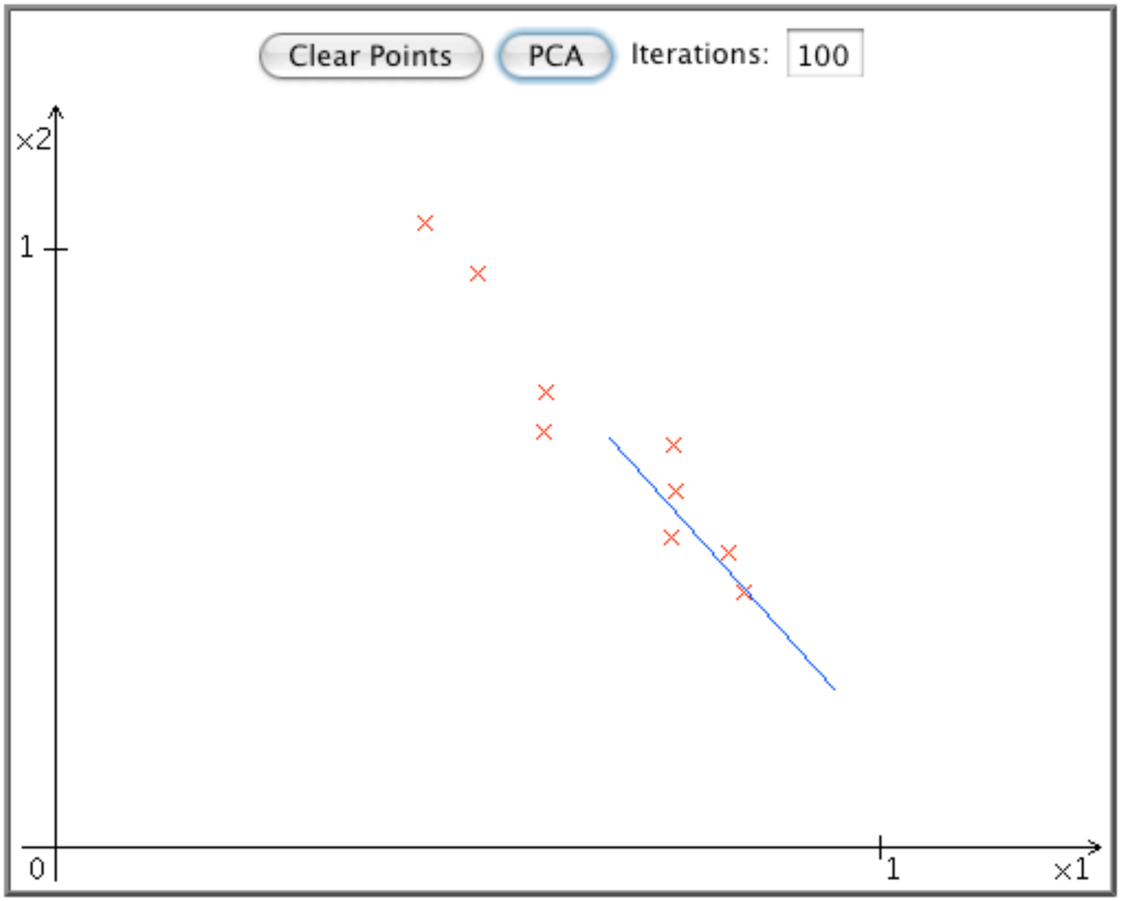
What is a Predominant Direction?

- This may seem subjective, but a mathematical definition can be provided.
- Let A be the matrix of data points:
  - Each point or observation is a column.
  - The rows correspond to the observed values of variables.

First P. C. Demo, you pick the points

http://www.igi.tugraz.at/lehre/CI/algorithms/pca_applet.html

This applet uses an iterative algorithm (APEX) to find the first PC.



Covariance vs. Correlation

- Most PCA presentations are based on **covariance**, which assumes input variables have **commensurate** units.
- Can also base PCA on **correlation**, which doesn't.
- To use covariance in general the general case, first normalize by dividing by each mean-adjusted variable by its variance.

Linear Transformation

- The types of transformations shown are linear:
  - B = WA
    where
    - A is the matrix of data (**each point as a column vector**), which is already mean-adjusted.
    - W is an m x n matrix, $m \leq n$
    - B is the transformed data matrix (called the "scores")
- We want the columns of W to be **orthonormal** (i.e. $WW^T = I$).
- The reconstruction A' of A from B will be obtained by:
  - $A' = W^TB$
    $= W^T(WA) = (W^TW)A.$

  (Note: W^TW won't generally be I, although WW^T is.)

Computing Principal Components

- PCA tries to minimize the *expectation* of reconstruction error:

  $E[\ || A - A' ||^2\ ] =$

  $E[\ tr(\ (A - A')(A-A')^T\ )] =$

  $tr(E[AA']) - tr(W\ E[AA']\ W^T) =$

  $tr(R) - tr(WRW^T)$, where

  $R = E[AA^T]$ is the *covariance matrix*
- E[ ] is the expectation, i.e. average over the data points
- tr is the trace (sum of diagonal elements).

What are the Principal Components, really?

- Want W such that **error** tr(R) - tr(WRW^T) is **minimized.**
- Equivalently, WRW^T (i.e. the **variance** of the transformed data) is **maximized**.
- The **eigenvectors** of the covariance matrix $R = AA^T$, ***ordered*** corresponding to largest to smallest eigenvalue, are the **principal components**.
- **PCA: Construct matrix W** as using the top so-many correspondingly-ordered eigenvectors as rows.

Example (worked in Matlab)
Turtle Shell Classification (D. Morrison)

data = (columns are data points)

1.3000	1.4000	1.5000	1.2000	1.1000	(Height)
3.2000	2.8000	3.1000	2.9000	3.0000	(Width)
3.7000	4.1000	4.6000	4.8000	4.8000	(Length)

Can fewer than 3 variables explain all?

means =

1.3000
3.0000
4.4000

```
[M,N] = size(data);

means = mean(data, 2);

mean_adjusted = data - repmat(means,1,N);
```

mean_adjusted =

0	0.1000	0.2000	-0.1000	-0.2000
0.2000	-0.2000	0.1000	-0.1000	0
-0.7000	-0.3000	0.2000	0.4000	0.4000

Example

covariance =

0.0250	0.0025	-0.0275
0.0025	0.0250	-0.0250
-0.0275	-0.0250	0.2350

variances =

0.2415
0.0225
0.0210

explained_variation =

0.8472
0.0791
0.0737

```
covariance = (mean_adjusted * mean_adjusted') / (N-1);

[eigenvectors, eigenvalues] = eig(covariance);

[junk, rindices] = sort(-1*eigenvalues);

variances = eigenvalues(rindices);

explained_variation = variances/sum(variances)
```

Example: Principal Components

PC = (column vectors)

-0.1265	0.5534	-0.8232
-0.1153	-0.8325	-0.5419
0.9852	-0.0263	-0.1691

```
PC = eigenvectors(:, rindices);

% transform the original data set by column

scores = PC * mean_adjusted;
```

scores = (transformed data, columns)

-0.4656	-0.3703	0.1947	0.2866	0.3546
-0.5459	-0.0076	0.0021	0.3116	0.2398
-0.1236	0.0531	0.2282	-0.0283	-0.1294

Example: Orthonormality Check

orthogonality_check =

1.0000	0.0000	0
0.0000	1.0000	0.0000
0	0.0000	1.0000

orthogonality_check = PC * PC'

Example: Reconstruction 1

subtracted_means =

1.3000	1.3000	1.3000	1.3000	1.3000
3.0000	3.0000	3.0000	3.0000	3.0000
4.4000	4.4000	4.4000	4.4000	4.4000

reconstruction_**using_all_components** =

1.3000	1.4000	1.5000	1.2000	1.1000
3.2000	2.8000	3.1000	2.9000	3.0000
3.7000	4.1000	4.6000	4.8000	4.8000

reconstruction_error =

0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

reconstruction_using_all_components = ...
(PC' * scores) + subtracted_means

reconstruction_error = reconstruction_using_all_components - data

Example: Reconstruction 2

reconstruction_**using_first_two_components** =

1.4218	1.3477	1.2751	1.2278	1.2275
3.1967	2.8014	3.1060	2.8993	2.9966
3.7209	4.0910	4.5614	4.8048	4.8219

reconstruction_error =

0.1218	-0.0523	-0.2249	0.0278	0.1275
-0.0033	0.0014	0.0060	-0.0007	-0.0034
0.0209	-0.0090	-0.0386	0.0048	0.0219

mse_reconstruction =

0.0058

```
reconstruction_using_first_two_components = ...
    (components(1:2, :)' *scores(1:2, :)) + subtracted_means

reconstruction_error = reconstruction_using_first_two_components - data

mse_reconstruction = mse(reconstruction_error)
```

Example: Reconstruction 3

reconstruction_**using_first_component_only** =

1.3589	1.3468	1.2754	1.2637	1.2551
2.7423	2.7951	3.1077	3.1586	3.1962
4.0167	4.0952	4.5603	4.6359	4.6919

reconstruction_error =

0.0589	-0.0532	-0.2246	0.0637	0.1551
-0.4577	-0.0049	0.0077	0.2586	0.1962
0.3167	-0.0048	-0.0397	-0.1641	-0.1081

mse_reconstruction =

0.0360

```
reconstruction_using_first_component_only = ...
    (components(1:1, :)' *scores(1:1, :)) + subtracted_means

reconstruction_error = reconstruction_using_first_component_only - data

mse_reconstruction = mse(reconstruction_error)
```

Matlab cov Function

```
A =            (mean adjusted, by row)

         0    0.2000   -0.7000
    0.1000   -0.2000   -0.3000
    0.2000    0.1000    0.2000
   -0.1000   -0.1000    0.4000
   -0.2000         0    0.4000

>> R = cov(A)

R =

    0.0250    0.0025   -0.0275
    0.0025    0.0250   -0.0250
   -0.0275   -0.0250    0.2350
```

Matlab pcacov function

```
>> [pc, variances, explained] = pcacov(R)

pc =

   -0.1265    0.5534    0.8232
   -0.1153   -0.8325    0.5419
    0.9852   -0.0263    0.1691

variances =

    0.2415
    0.0225
    0.0210

explained =

   84.7212
    7.9114
    7.3674
```

Eigenvalues

% Variance explained

Singular Value Decomposition: Another approach to computing PCs

- The singular-value decomposition (SVD) of A is:

  $A = USV^T$

- where:
  - The columns of U are the eigenvectors of $A A^T$.
  - The columns of V are the eigenvectors of $A^T A$, i.e. the PC's.
  - S is pseudo-diagonal (diagonal insofar as this is possible with a non-square matrix, the rest of the entries being 0).

- PC from SVD in Matlab:

  Y = mean_adjusted / sqrt(N-1)

  [U,S,PC] = svd(Y') [Note: Y' = U S PC']

Planets Example

(http://www.cs.mcgill.ca/~sqrt/dimr/dimreduction.html)

- Consider a 3-dimensional data set where the variables are the logarithms of
  - distance to the sun
  - equatorial diameter
  - density

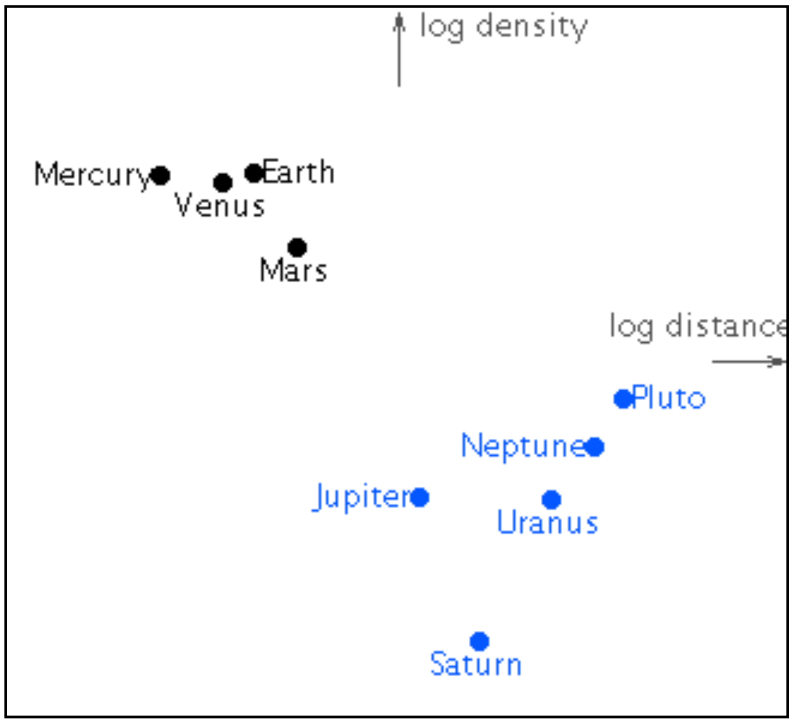
Data set (prior to taking logs)

planet	distance	diameter	density
Mercury	0.387	4878	5.42
Venus	0.723	12104	5.25
Earth	1.000	12756	5.52
Mars	1.524	6787	3.94
Jupiter	5.203	142800	1.314
Saturn	9.539	120660	0.69
Uranus	19.18	51118	1.29
Neptune	30.06	49528	1.64
Pluto	39.53	2300	2.03

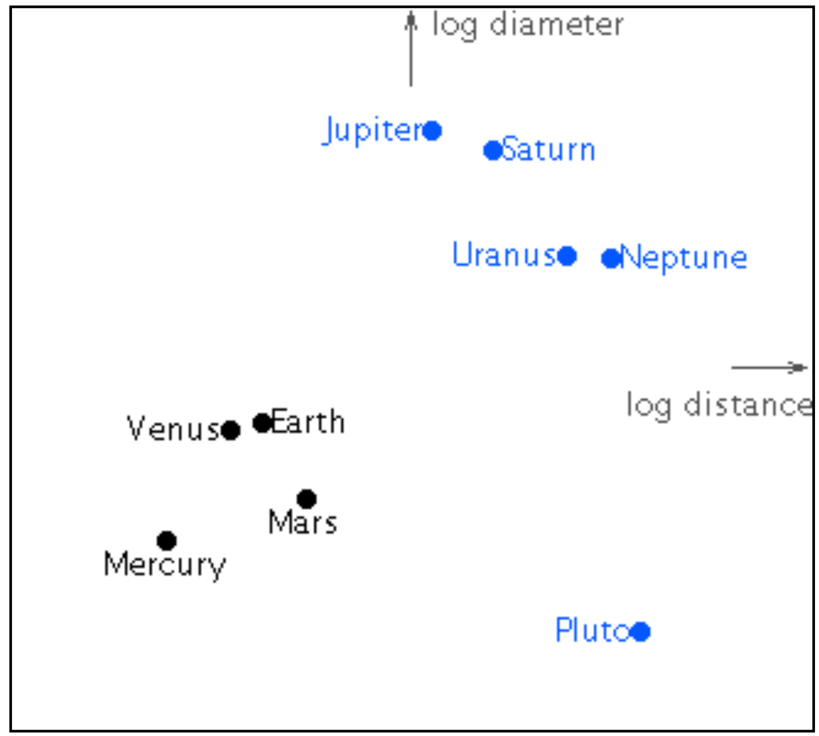
Log Data Projections

(projections being a special case of linear transformation)

In **two dimensions**, we can plot any one variable against another, e.g.



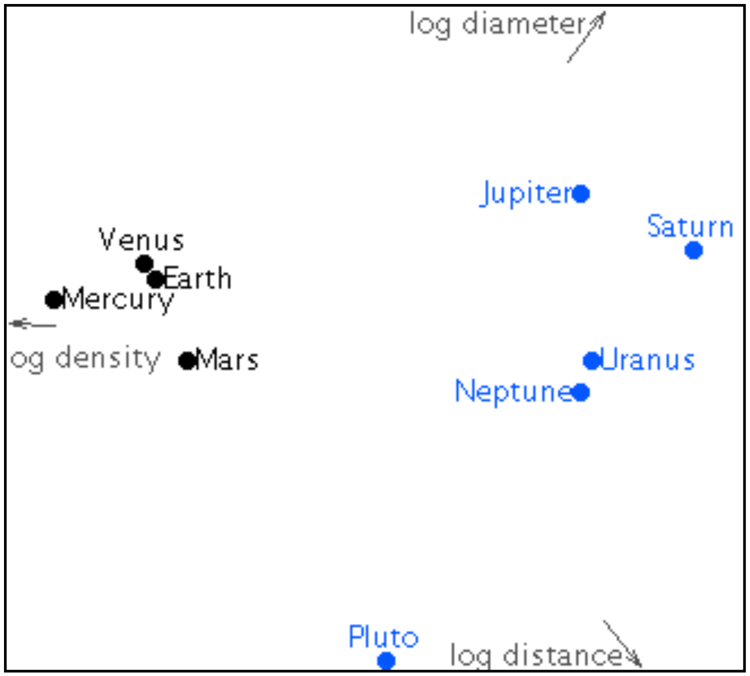
or



Of various possible plots, which show the widest variation among planets?

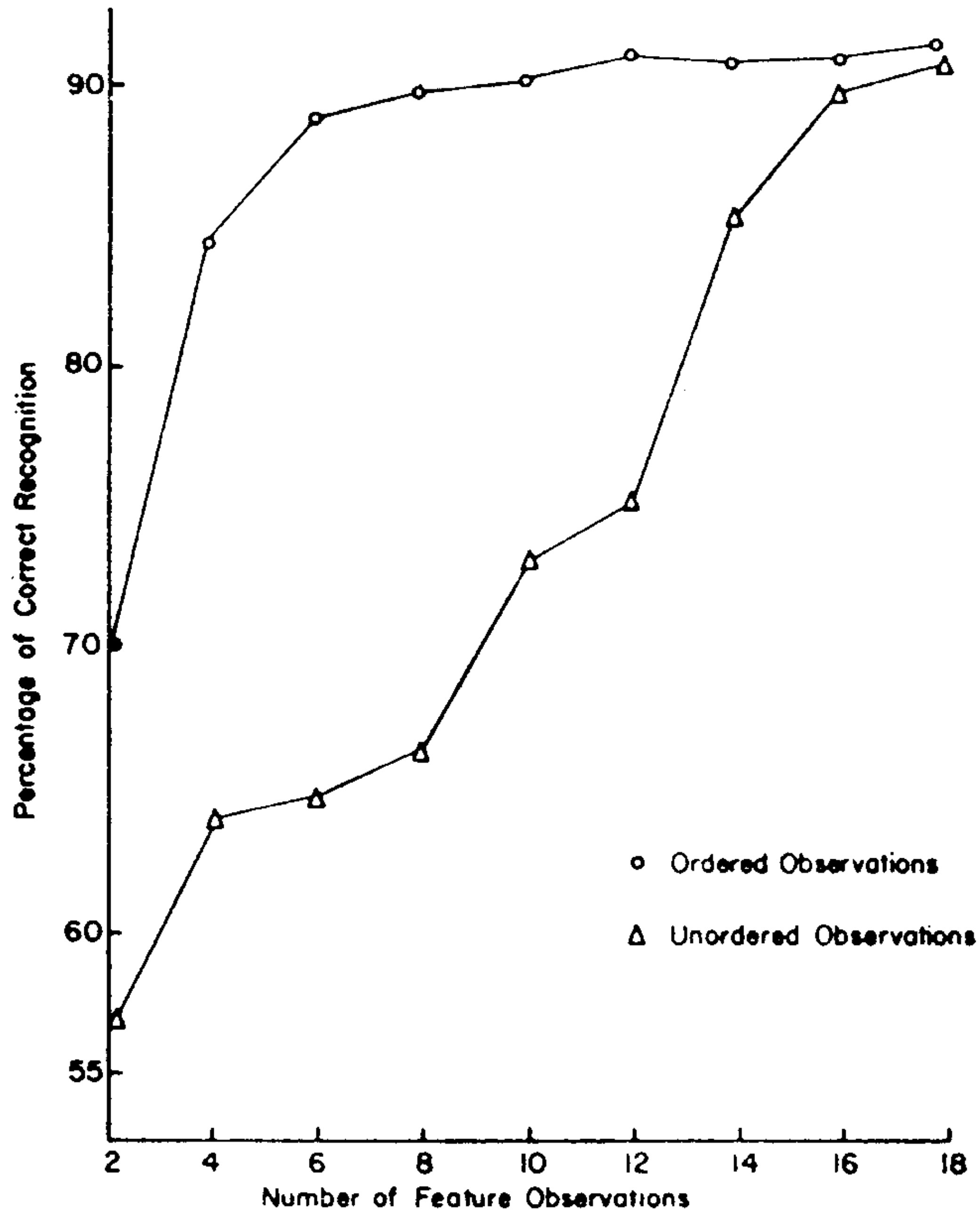
Maximizing Variance

- Transforming using first two principal components **preserves more of the variance** (summing variances in each dimension) in the projection than does projecting on any 2 variables:



Application: Handwritten Character recognition (K.S. Fu, 1968)

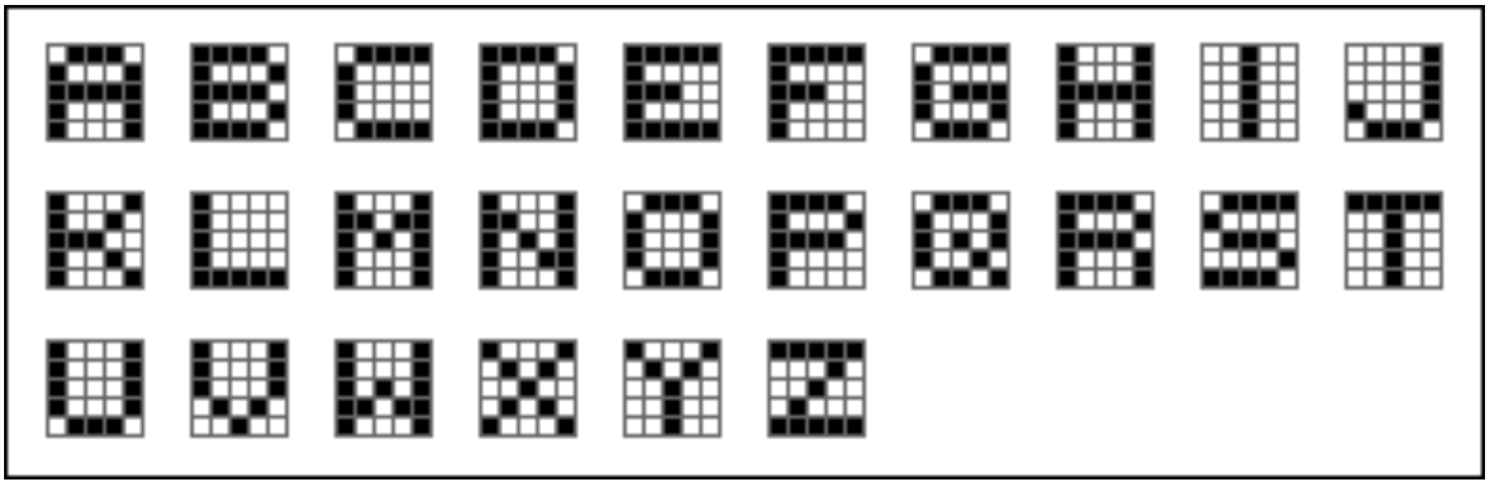
- Attempt recognition based upon **18 radial measurements**, spaced at 20 degree increments, of characters (240 samples).
- Recognition rate was computed vs. the number of measurements used (2, 4, 6, … out of 18) in no particular order.
- The same computation was done with the measurements **ordered by principal components**.
- The next slide compares the two approaches.


Percentage of Correct Recognition
90
80
70
60
55
2
4
6
8
10
12
14
16
18
Number of Feature Observations
Ordered Observations
Unordered Observations

A Related Example

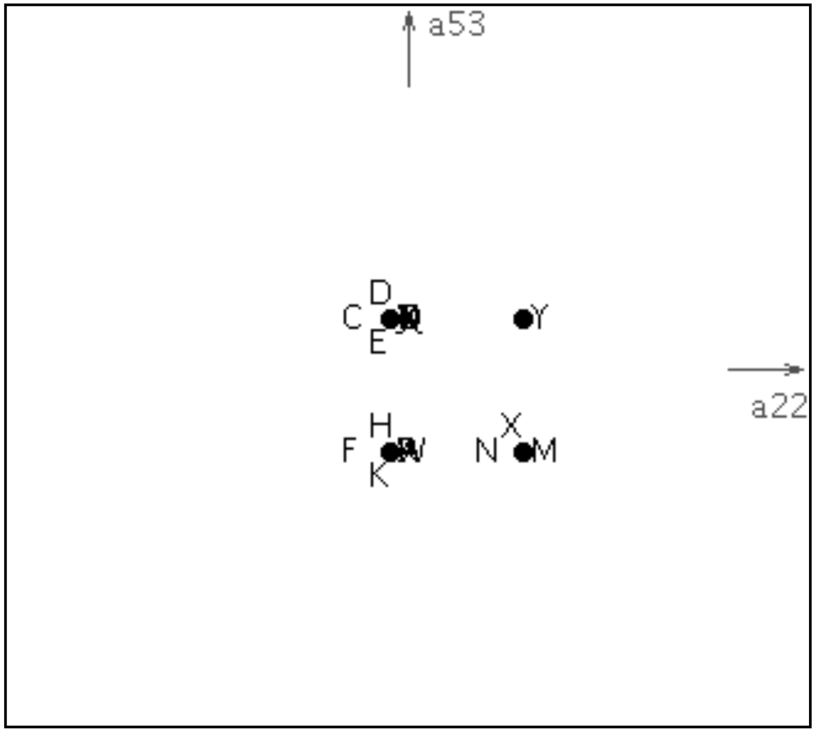
(http://www.cs.mcgill.ca/~sqrt/dimr/dimreduction.html)

- A 25-dimensional data set:



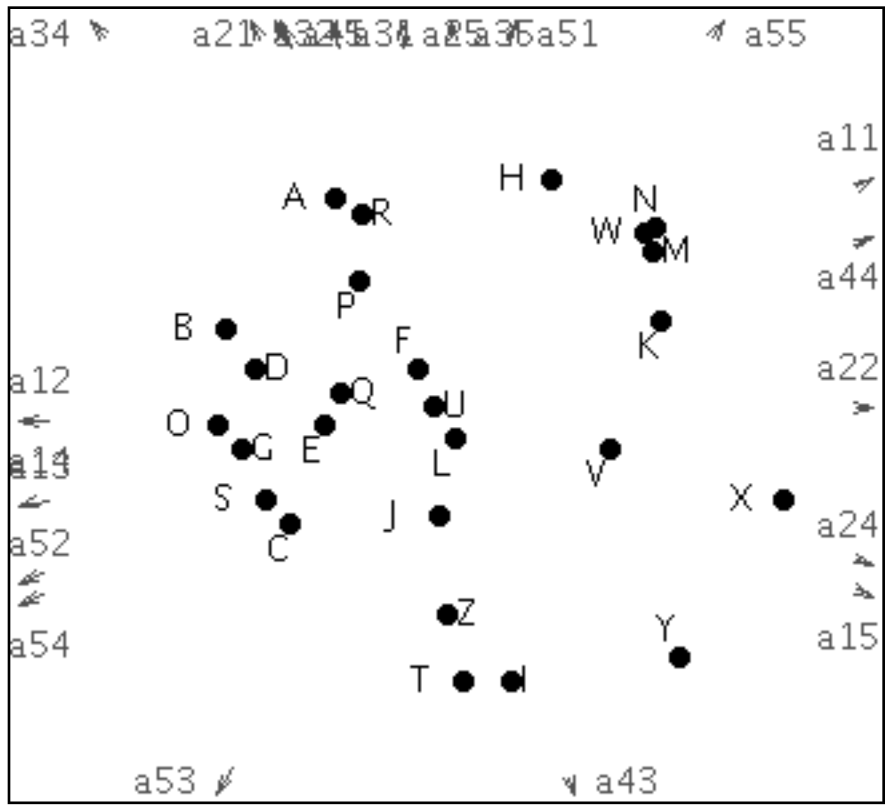
Projected Data

- Projecting on 2 variables does not help much in discriminating the points, e.g.



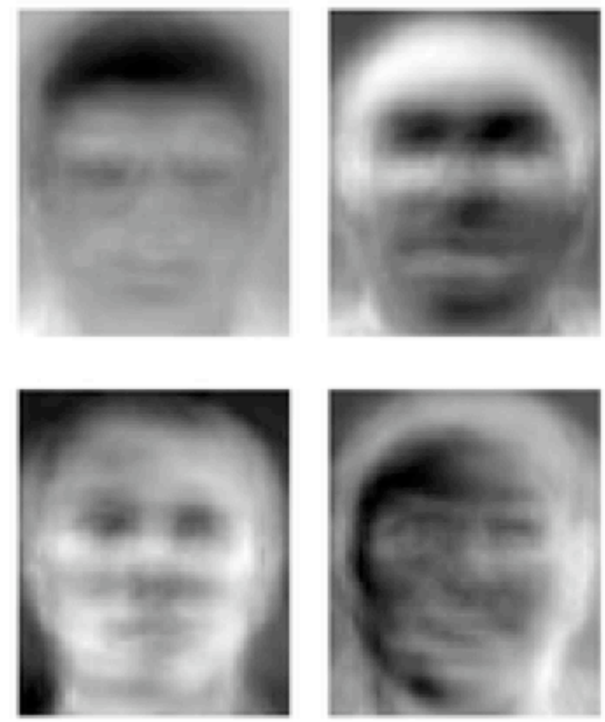
Projected Data

- Projecting on the first two principal components achieves the maximum variation in two dimensions:



Eigenfaces

Eigenfaces are a set of eigenvectors used in the computer vision problem of human face recognition. The approach of using eigenfaces for recognition was developed by Sirovich and Kirby (1987) and used by Matthew Turk and Alex Pentland in face classification. It is considered the first successful example of facial recognition technology. [*citation needed*] These eigenvectors are derived from the covariance matrix of the probability distribution of the high-dimensional vector space of *possible faces of human beings*.



Some eigenfaces from AT&T Laboratories Cambridge.

Eigenface Generation

To generate a set of eigenfaces, a large set of digitized images of human faces, taken under the same lighting conditions, are normalized to line up the eyes and mouths. They are then all resampled at the same pixel resolution. Eigenfaces can be extracted out of the image data by means of a mathematical tool called principal component analysis (PCA). Here are the steps involved in converting an image of a face into eigenfaces:

1. Prepare a training set. The faces constituting the training set T should be already prepared for processing.
2. Subtract the mean. The average matrix A has to be calculated and subtracted from the original in T. The results are stored in variable S.
3. Calculate the covariance matrix.
4. Calculate the eigenvectors and eigenvalues of this covariance matrix.
5. Choose the principal components.

Eigenface Selection

There will be a large number of eigenfaces created before step 5, and far fewer are really needed. Select from them those that have the highest eigenvalues. For instance, if we are working with a 100 x 100 image, then this system will create 10,000 eigenvectors. Since most individuals can be identified using a database with a size between 100 and 150, most of the 10,000 can be discarded, and only the most important should remain.

The eigenfaces that are created will appear as light and dark areas that are arranged in a specific pattern. This pattern is how different features of a face are singled out to be evaluated and scored. There will be a pattern to evaluate symmetry, if there is any style of facial hair, where the hairline is, or evaluate the size of the nose or mouth. Other eigenfaces have patterns that are less simple to identify, and the image of the eigenface may look very little like a face.

Eigenface Recognition Algorithm

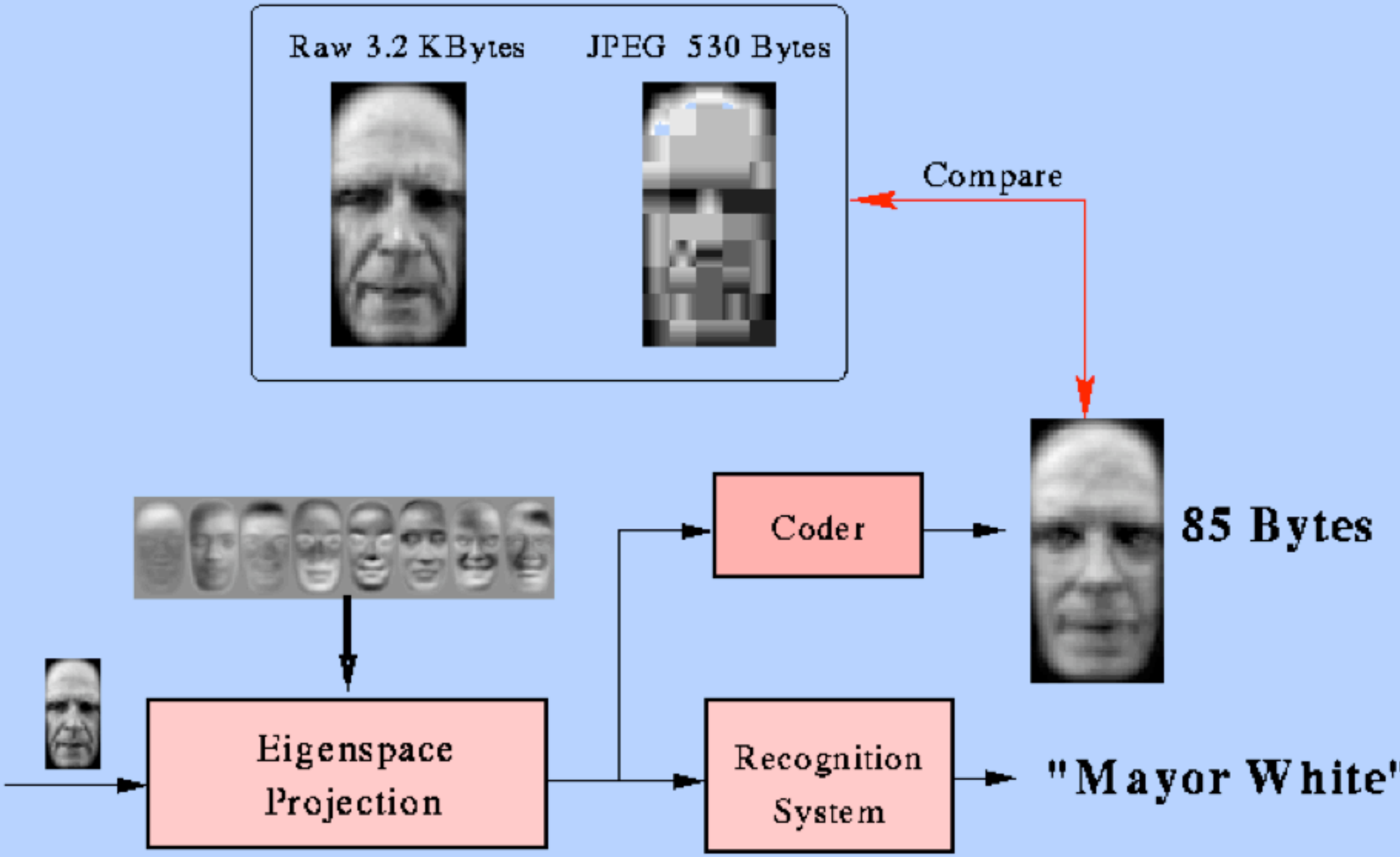
For an algorithm in more detail, see:

http://openbio.sourceforge.net/resources/eigenfaces/eigenfaces-html/facesOptions.html

Eigenfaces App: FERET Photobook

http://vismod.media.mit.edu/vismod/demos/facerec/basic.html

Recognition and Coding



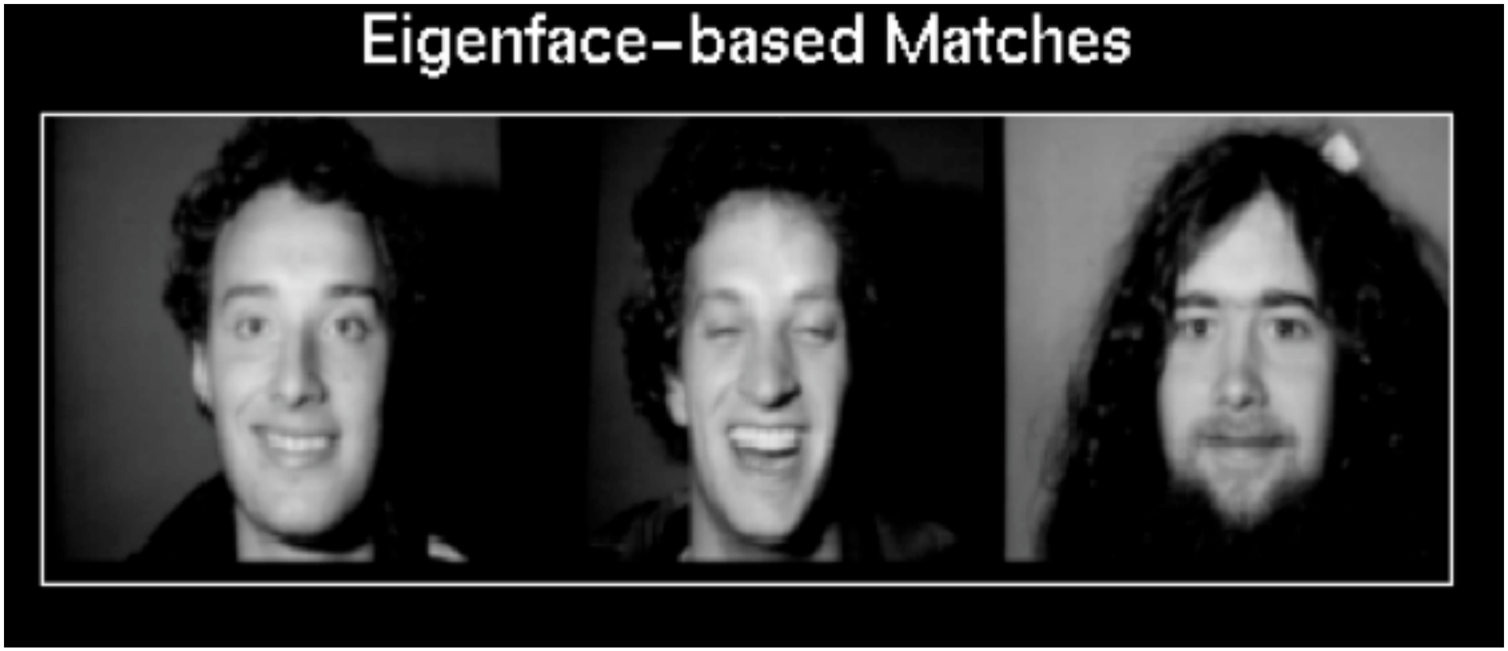
Recognition and Coding

Once the image is suitably normalized with respect to individual geometry and contrast, it is projected onto a set of normalized eigenfaces. The figure above shows the first few eigenfaces obtained from a KL expansion on an ensemble of 500 normalized faces. In our system, the projection coefficients are used to index through a database to perform identity verification and recognition using a nearest-neighbor search.

Here, the geometrically aligned and normalized image is projected onto a custom set of eigenfaces to obtain a feature vector which is used for recognition purposes as well as facial image coding.

See for Enhancements:

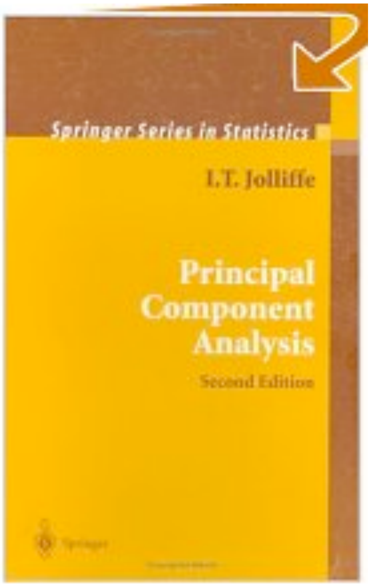
http://vismod.media.mit.edu/vismod/demos/facerec/basic.html



For the algorithm, see:

http://openbio.sourceforge.net/resources/eigenfaces/eigenfaces-html/facesOptions.html

PCA Source

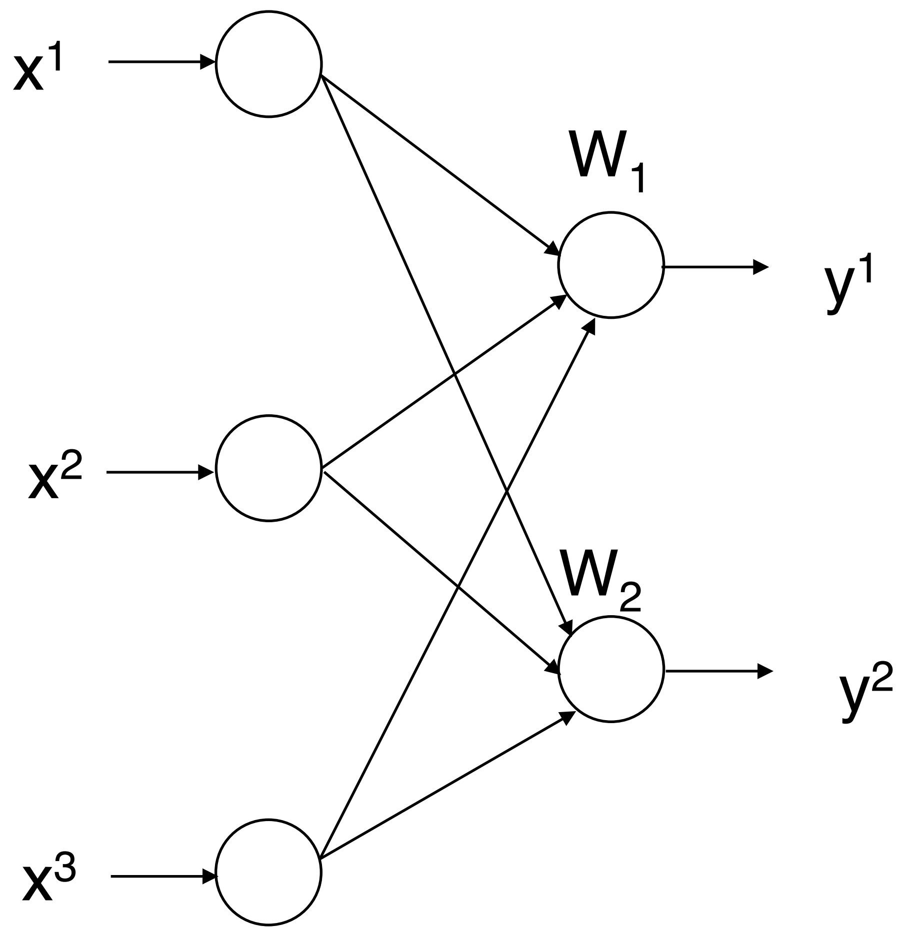


L.T. Jolliffe

What is a PCA Neural Network?

- The matrix W of PCA can be interpreted as **weights** of a 1-layer neural network, also known as an **autoencoder**.
- Training is by variants on Hebbian learning.
- The user pre-selects the number of output variables.
- The network effectively learns PCs by outputting the corresponding scores.
- The weights are the learned transformation matrix, however they will not necessarily be orthogonal.

3→2 PCA Network

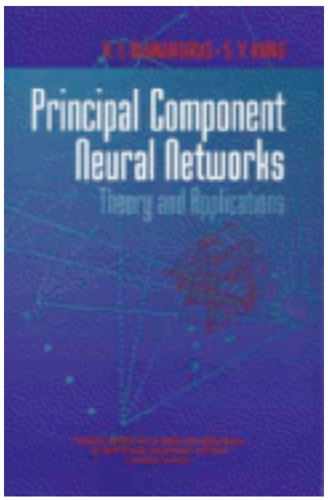


PCA Hebbian-Learning Rules

- $\Delta W = \eta\, y_i x_i^T - K_i W$, where
  - x_i is an input vector
  - y_i is the corresponding output vector ($= W x_i$)
  - $y_i x_i^T$ is the **Hebbian** component
  - K_i is **one of the following weight decay** components:
    - 0 — pure Hebbian (unbounded)
    - $y_i y_i^T$ — (Williams' rule, 1985)
    - $3D(y_i y_i^T) + 2L(y_i y_i^T)$ — (Oja and Karhunen rule, 1985)
    - $L(y_i y_i^T)$ — (Sanger's rule, 1989)

  where D(M) maps the **diagonal** entries of M to themselves, and other entries to 0, and
- L(M) maps entries **below** the main diagonal to themselves, and other entries to 0.

Other Variations Exist: Source for PCA NN



Diamantaras, K.I. / Kung, S.Y.

Principal Component Neural Networks
Theory and Applications

1996. 256 pages.
ISBN 0-471-05436-4 John Wiley & Sons

The coverage in this book is extensive. It gives several additional learning algorithms, including ones with **lateral** connections as well as feed-forward ones.

Other means of learning for dimensionality reduction

- Self-Organizing Map
  (# of dimensions in superstructure = reduced dimension)

- LVQ
  (# of neurons = reduced dimension)

- Projection pursuit, another statistical technique, effectively learns PC's sequentially

PCA Shortcomings

- The PCA user must select **how many** target dimensions to use.
- PCA only finds **linear** sub-spaces.
- PCA works best if the individual components are **Gaussian** -distributed.
- There are many variations, some of which partially resolve some of these issues.
- Related area: “Factor Analysis”

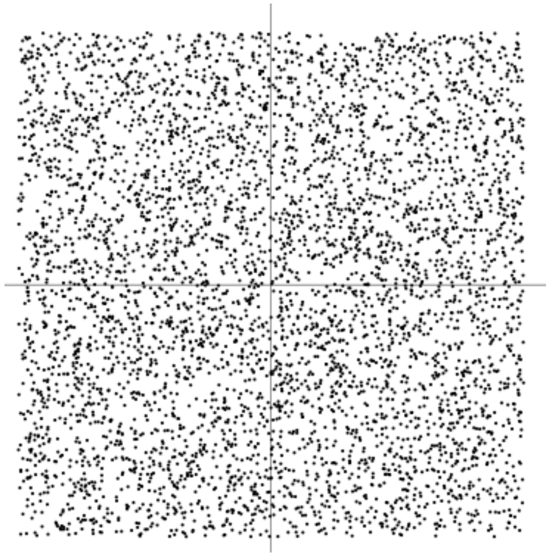
Independent Component Analysis (ICA)

- A technique for BSS (Blind Source Separation).
- Proposed for neuro-mimetic hardware in 1983 by Herault and Jutten.
- ICA seeks to extract components that are **statistically independent**.
- Two variables x, y are *statistically independent* iff
  $$P(x\ y) = P(x)P(y).$$
  Equivalently,
  $$E\{g(x)h(y)\} - E\{g(x)\}\,E\{h(y)\} = 0$$
  where g and h are **any** functions.

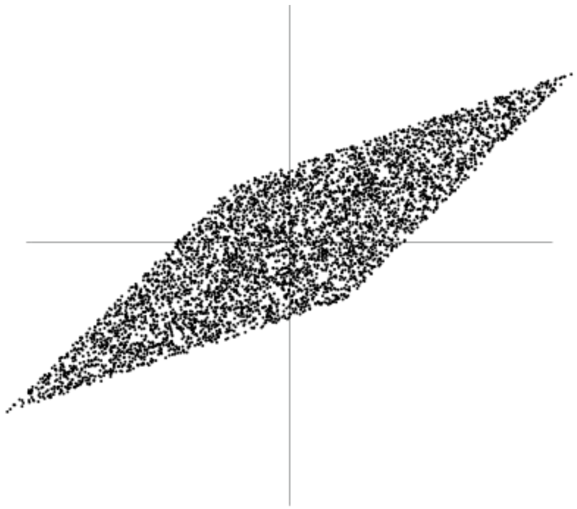
PCA vs. ICA

- PCA is finding **uncorrelated** components.
- ICA finds **independent** components.
- Independent implies uncorrelated, but not necessarily conversely.
- The input signals to ICA, being mixtures, will usually be correlated.
- The outputs, being independent, will not be.

Signals vs. Mixtures



Joint distribution of two independent signals



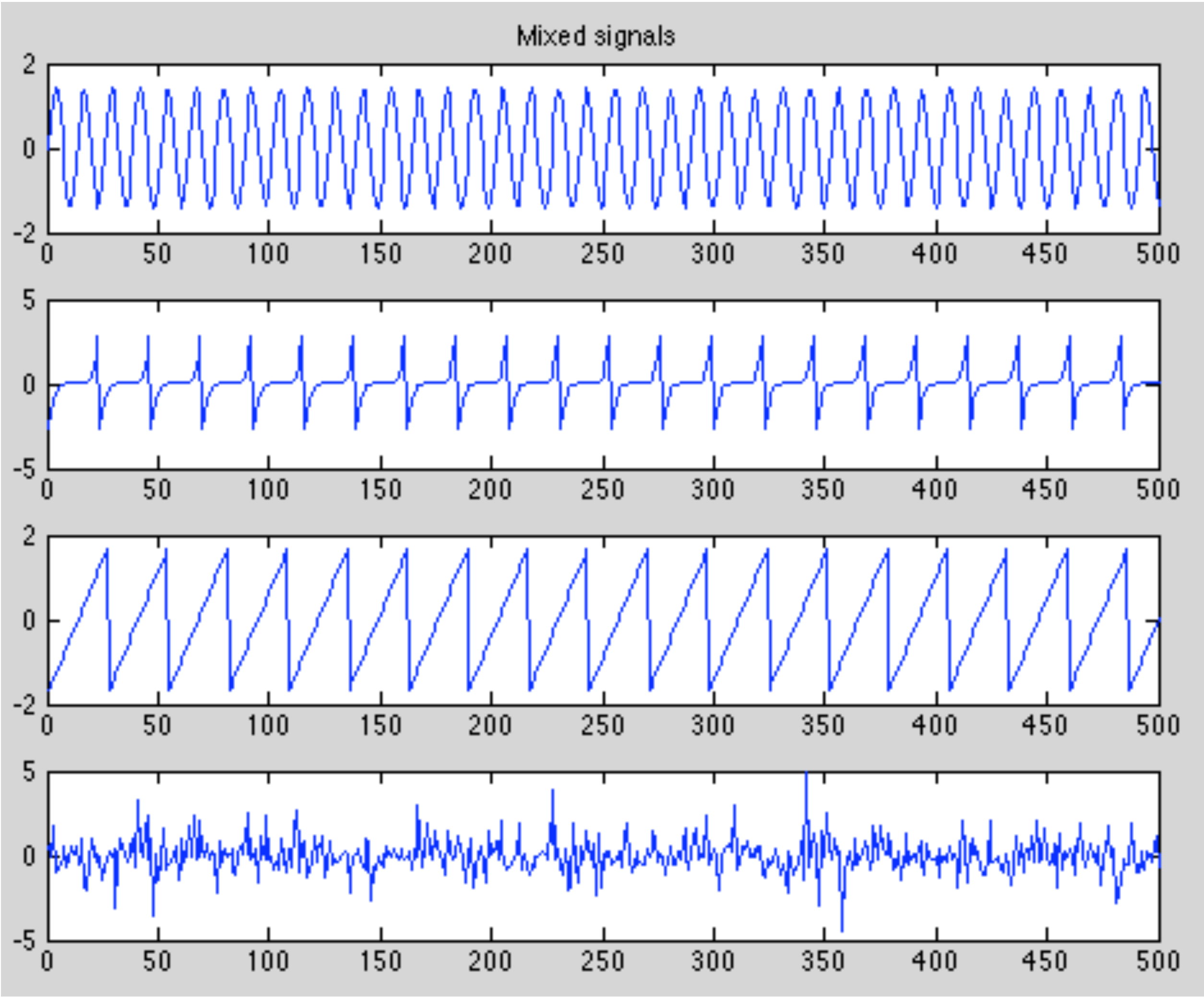
Joint distribution of a mixture of the same signals

ICA

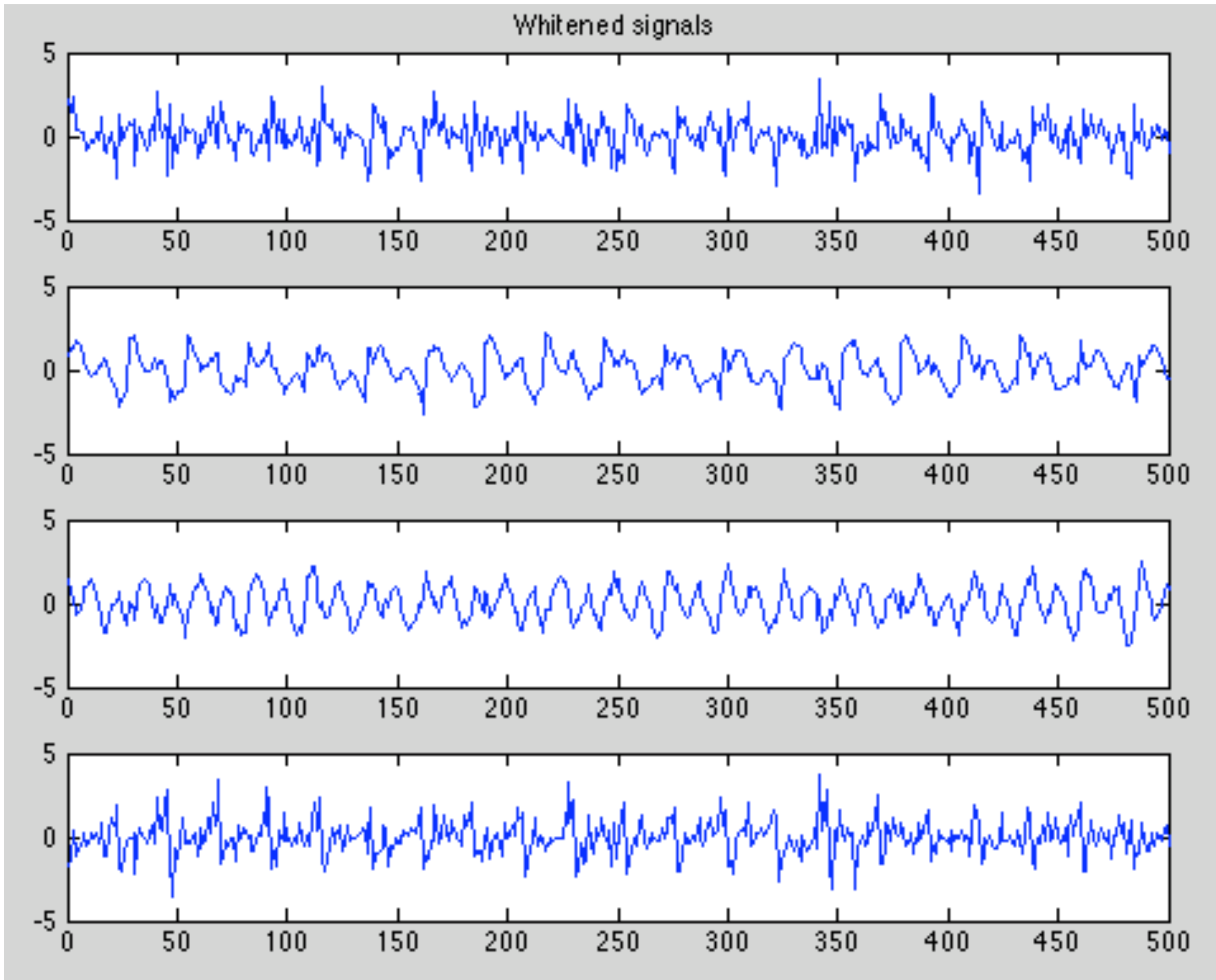
- Suppose we have n distinct mixtures of n statistically-independent signals.

- We wish to transform the mixtures to (signals as close as possible to) the original signals.

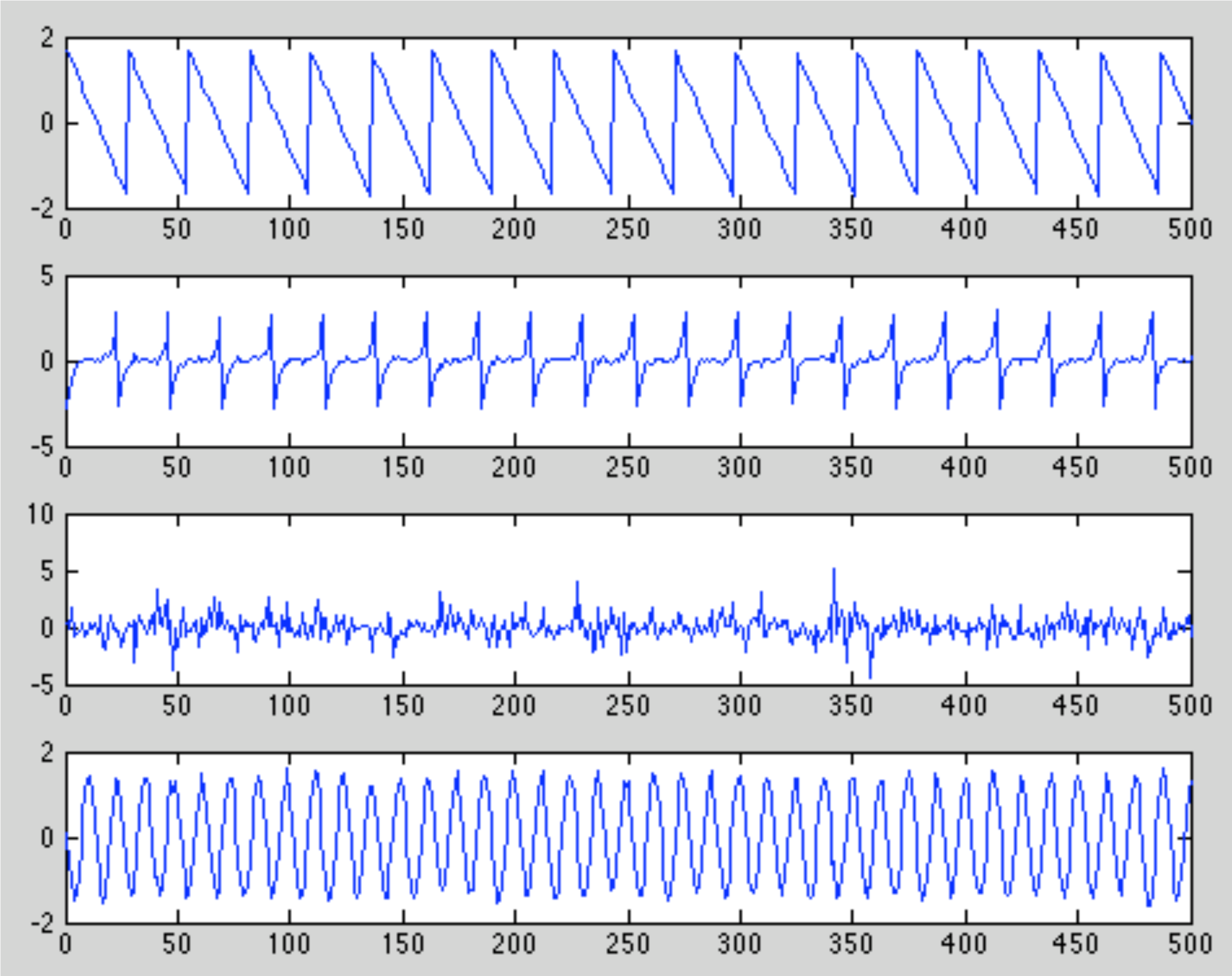
Fast-ICA Demo
Signals to be Mixed



Whitened Signals after Mixing

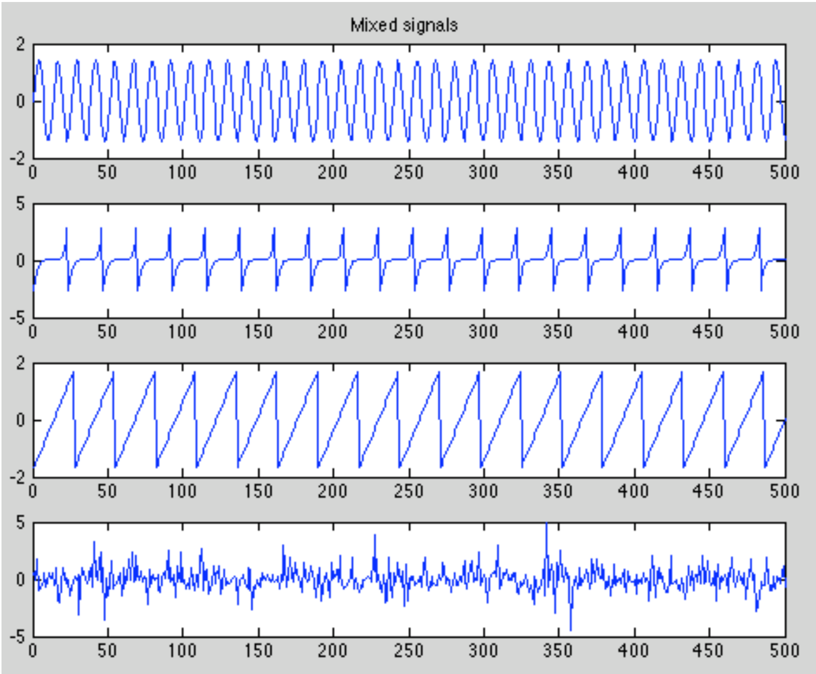


Extracted Independent Components

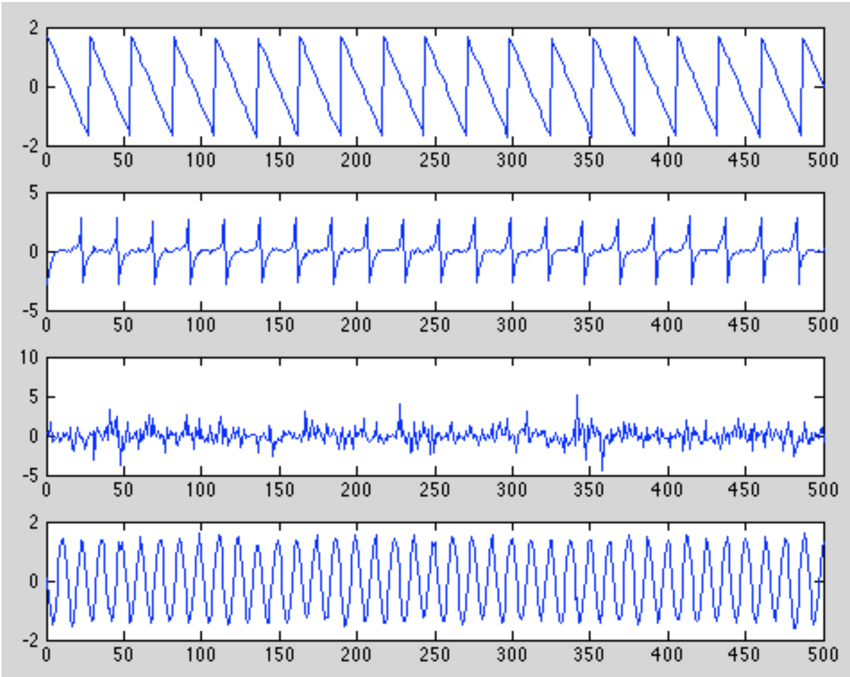


Comparison

Originals



Extractions from mixtures



ICA Demos

- http://www.cnl.salk.edu/~tewon/Blind/blind_audio.html
- http://www.cis.hut.fi/projects/ica/cocktail/cocktail_en.cgi

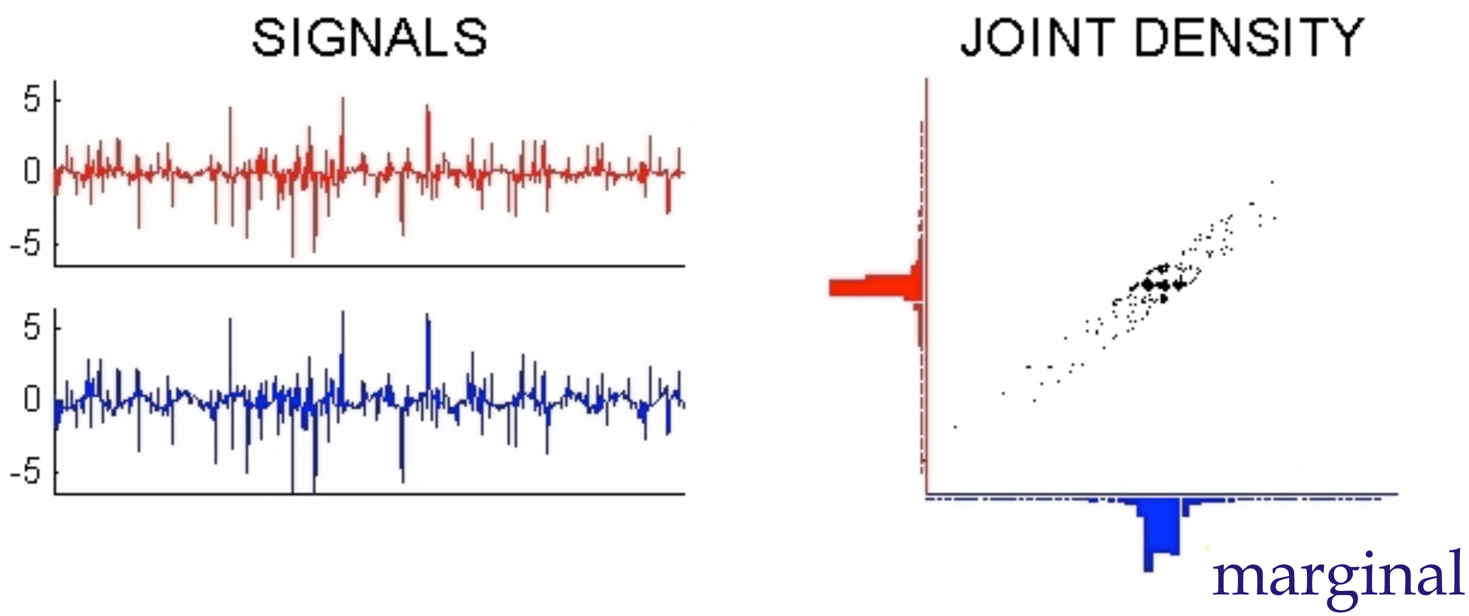
How can/does ICA work?

- One version: “Fast ICA”

- Throughout signals are assumed to be mean-adjusted.

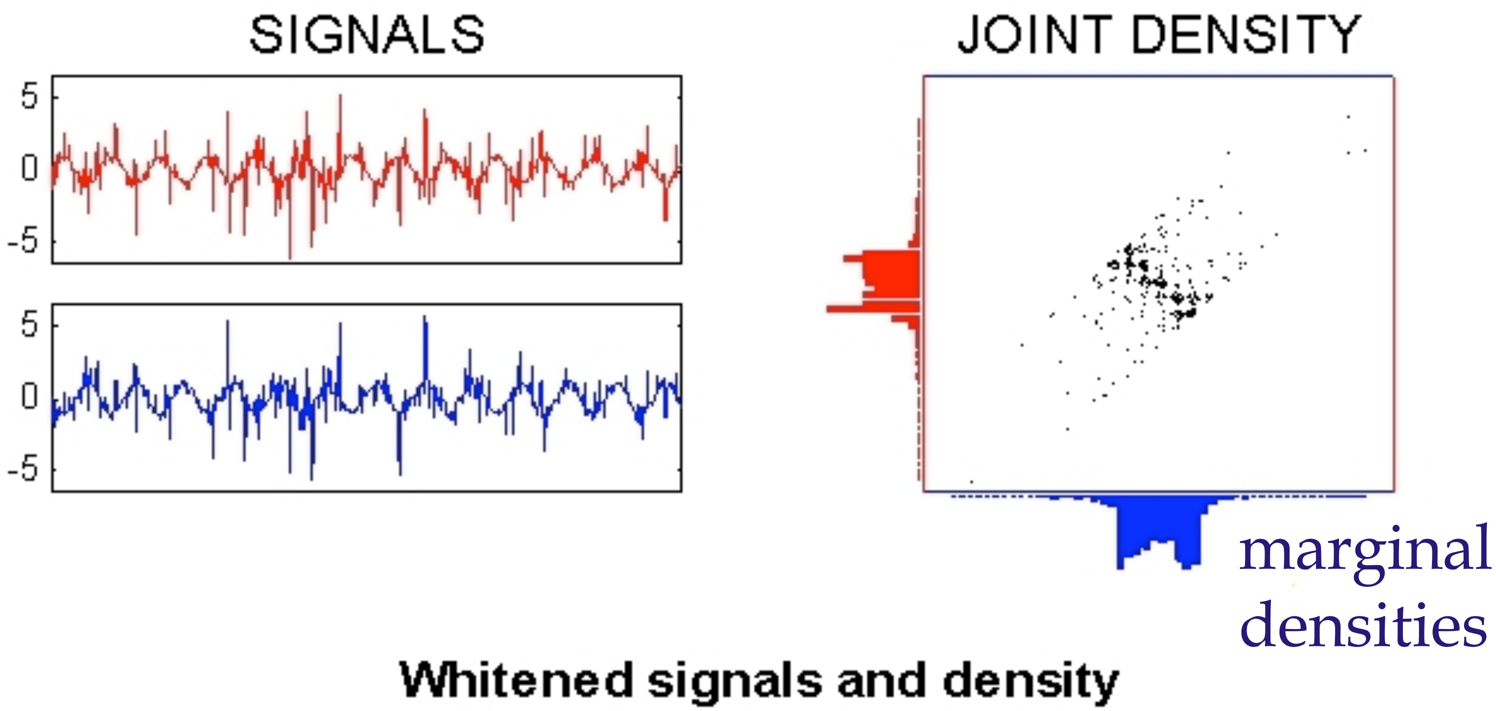
Correlation within Signal Mixture

(from http://www.cis.hut.fi/projects/ica/icademo/)



Input signals and density

Effect of whitening (aka "sphering"): removing correlations in mixed signals



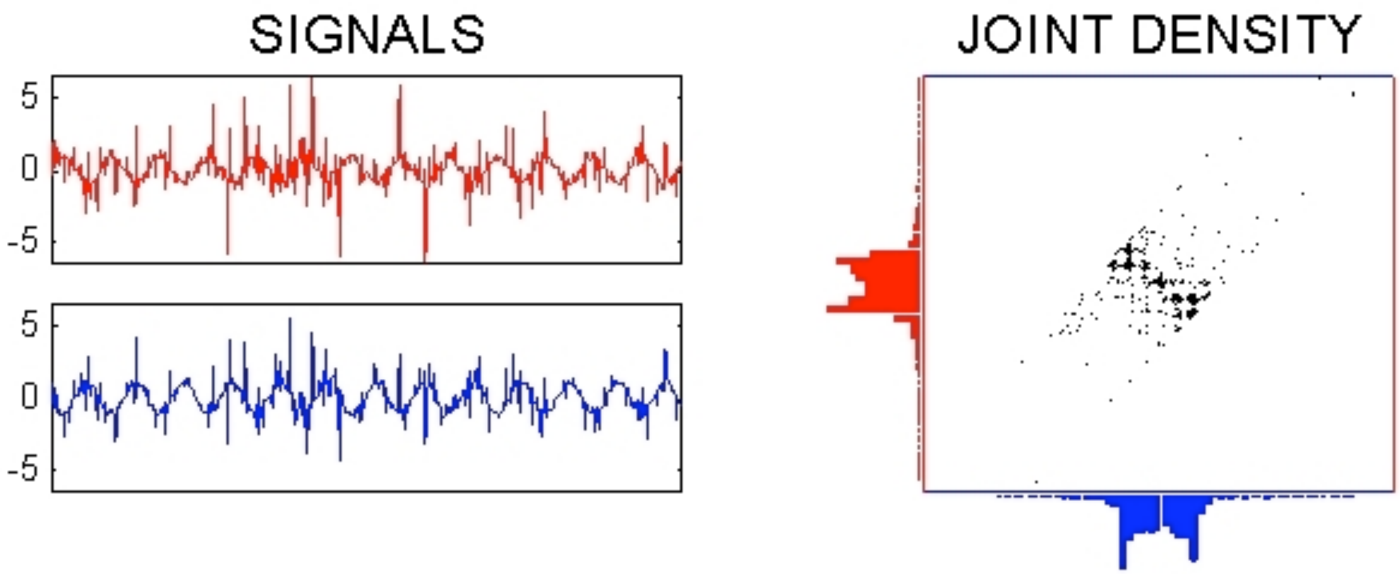
Whitening Transformation
(essentially a form of PCA)

- Seek a linear transformation V such that when y = Vx we get E{yy'} = I.
- Set $V = C^{-1/2}$, where C = E{xx'} is the correlation matrix of the data.
- Then $E\{yy'\} = E\{Vxx'V'\} = C^{-1/2}CC^{-1/2} = I$.
- For computational aspects, see: http://en.wikipedia.org /wiki/Square_root_of_a_matrix

Rotating the Whitened Signals

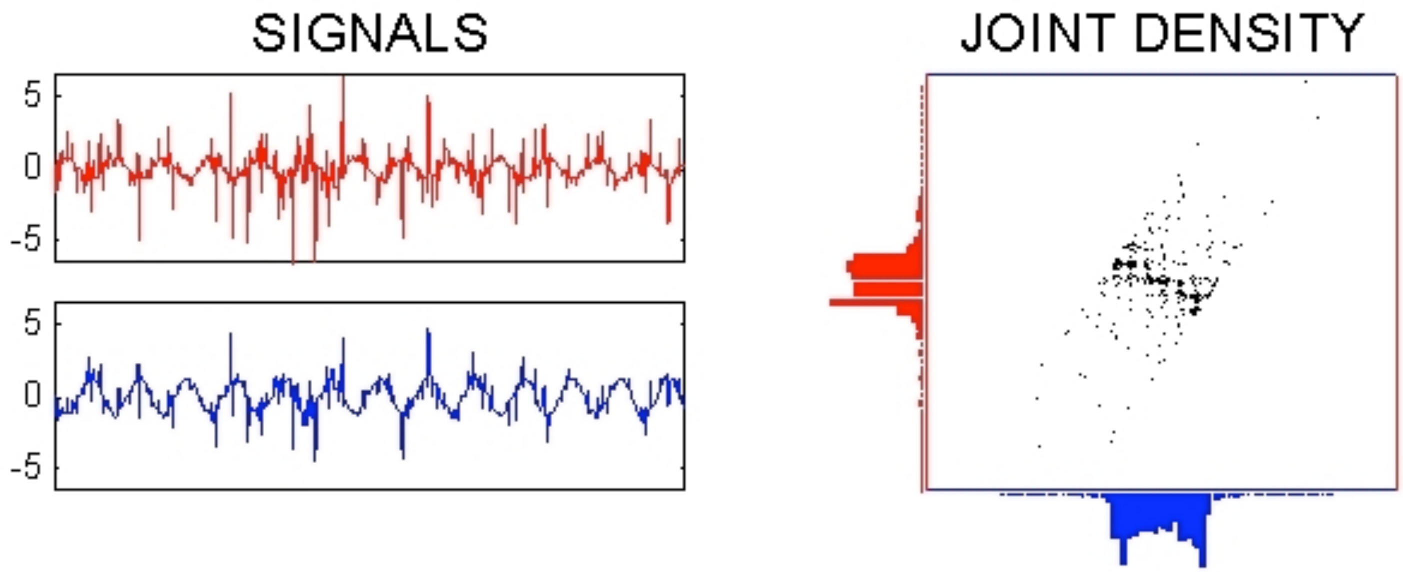
- The independent components are achieved by an appropriate rotation of the whitened signals.
- This involves **maximizing** the non-normal aspects of the marginal densities, since
- A linear mixture of independent random variables is necessarily “more Gaussian” than the original variables
- Maximization can be done incrementally.

Fast ICA Intermediate Steps



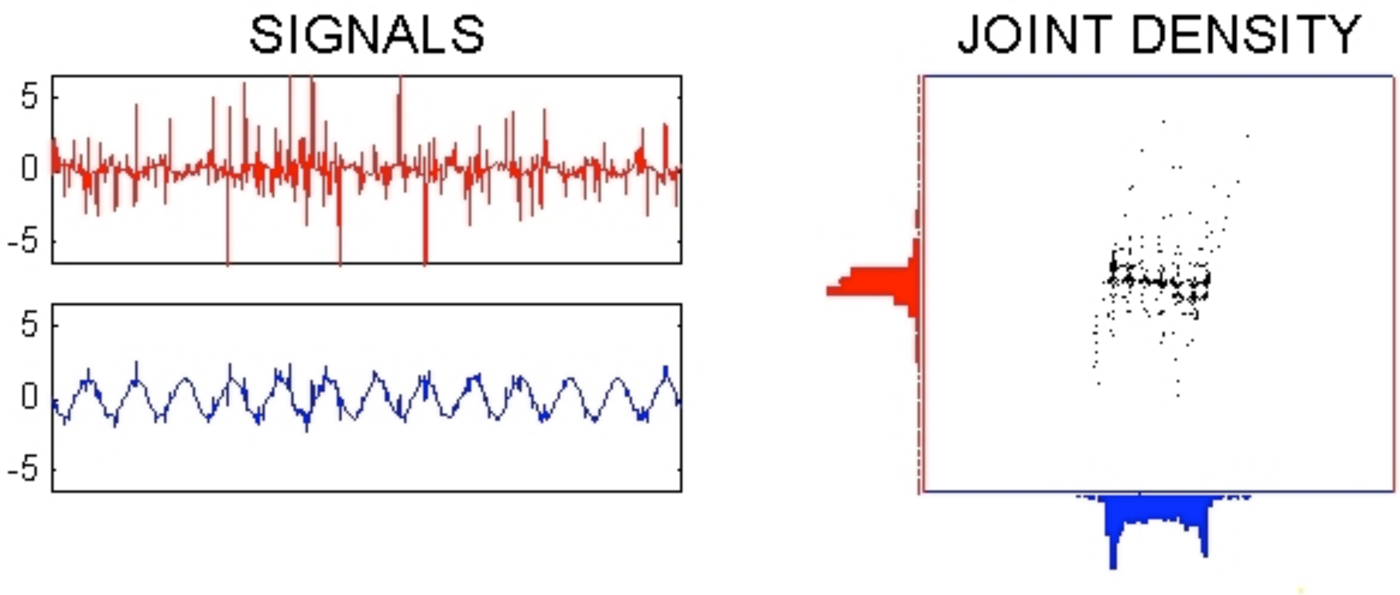
Separated signals after 1 step of FastICA

Fast ICA Intermediate Steps



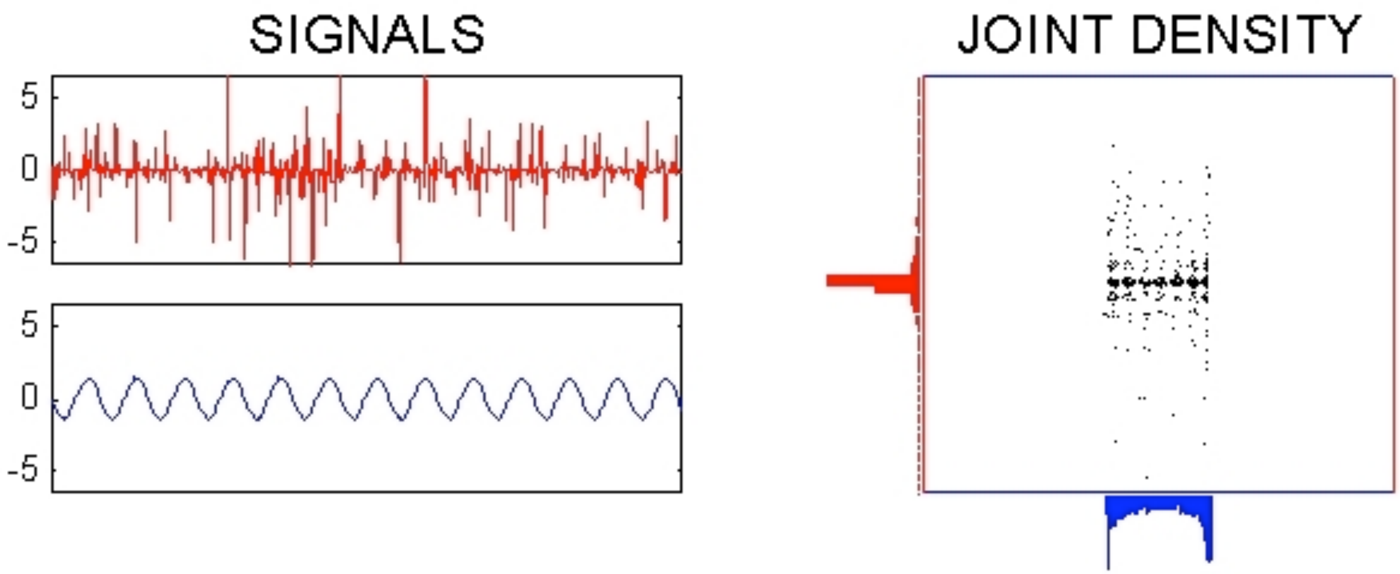
Separated signals after 2 steps of FastICA

Fast ICA Intermediate Steps



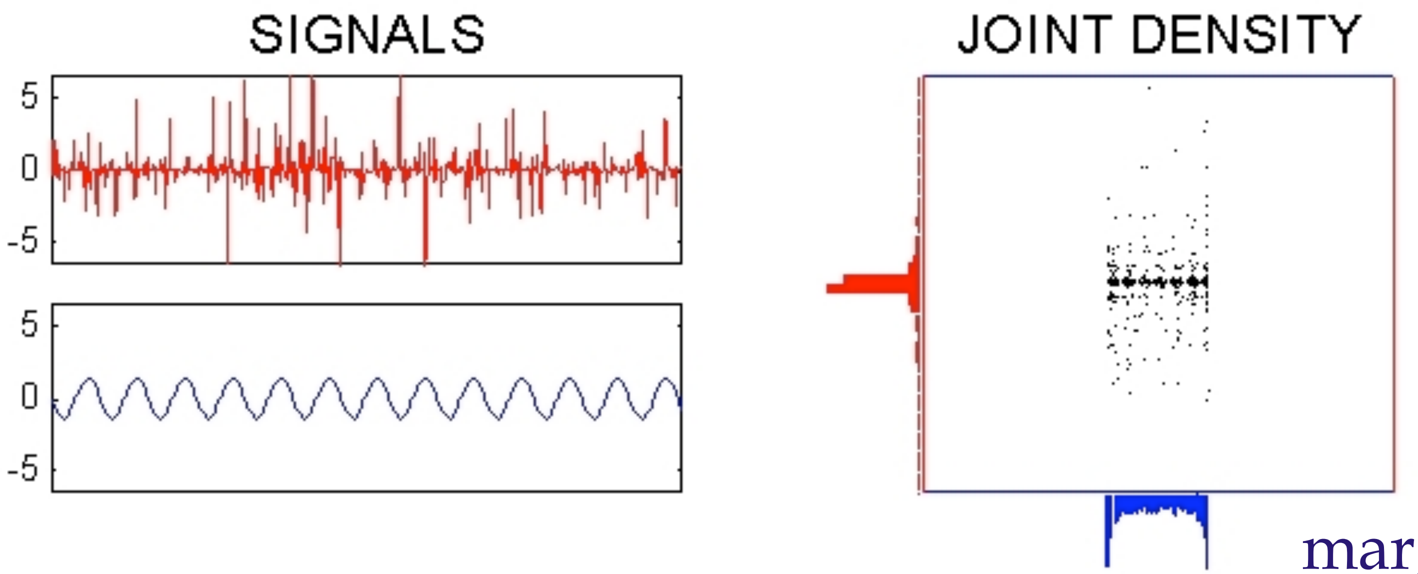
Separated signals after 3 steps of FastICA

Fast ICA Intermediate Steps



Separated signals after 4 steps of FastICA

Separated Signals



marginal
densities

Separated signals after 5 steps of FastICA

Neural ICA Algorithms

- Bell and Sejnowski: “infomax” method, minimizing mutual information, using an iterative formulation, similar to PCA NN:

  $W_{k+1} = W_k + \beta_k[W_k^{-T} + z_k x_k^T]$

  $z(i) = \partial/\partial u(i)\ \partial u(i)/\partial y(i)$

  $u = f(Wx)$

  e.g. f = tansig
- Also related to “maximum likelihood estimation”. Subsequent Bayesian derivation by Kevin Knuth

Matlab Core Code
based on Bell-Sejnowski

```
% Begin gradient ascent on h ...
for iter=1:maxiter
            % Get estimated source signals, y.

            y = x*W; % wt vec in col of W.

            % Get estimated maximum entropy signals Y=cdf(y).

            Y = tanh(y);

            % Find value of function h.
            % h = log(abs(det(W))) + sum( log(eps+1-Y(:).^2) )/N;

            detW = abs(det(W));
            h = ( (1/N)*sum(sum(Y)) + 0.5*log(detW) );

            % Find matrix of gradients @h/@W_ji ...
            g = inv(W') - (2/N)*x'*Y;

            % Update W to increase h ...

            W = W + eta*g;

            % Record h and magnitude of gradient ...

            hs(iter)=h; gs(iter)=norm(g(:));
end;
```

Neural ICA Algorithms

- Bell-Sejnowski was similar to an earlier Herault-Jutten formulation:

$$W = (I+S)^{-1}$$

$$S_{k+1} = S_k + \beta_k g(y_k) h(y_k^T)$$

$$g = t,\ h = t^3;\ g = \text{hardlim},\ h = \text{tansig}$$

Neural ICA Algorithms

- EASI (Equivariant Adaptive Separation via Independence): Cardoso et al

$$W_{k+1} = W_k - \beta_k[y_k y_k^T - I + g(y_k)h(y_k)^T - (y_k)g(y_k)^T]W_k$$

g=t, h=tansig

ICA Image Separation Demo (David Gleich '03)

Original 3 images

Mixture

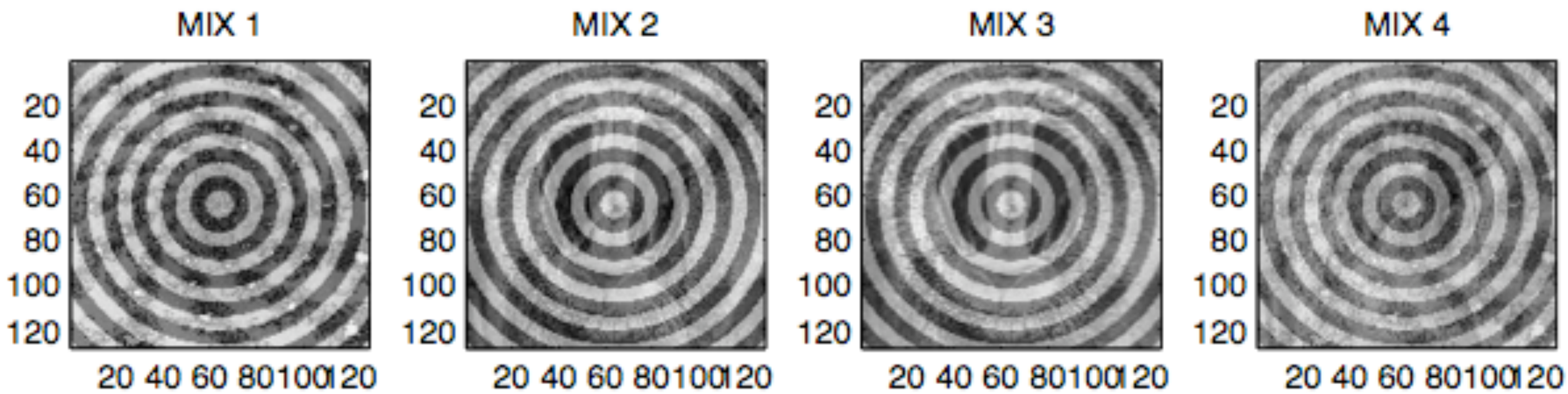
ICA Image Separation Example (David Gleich Gleich '03)

Bell and Sejnowski separation

EASI Algorithm separation

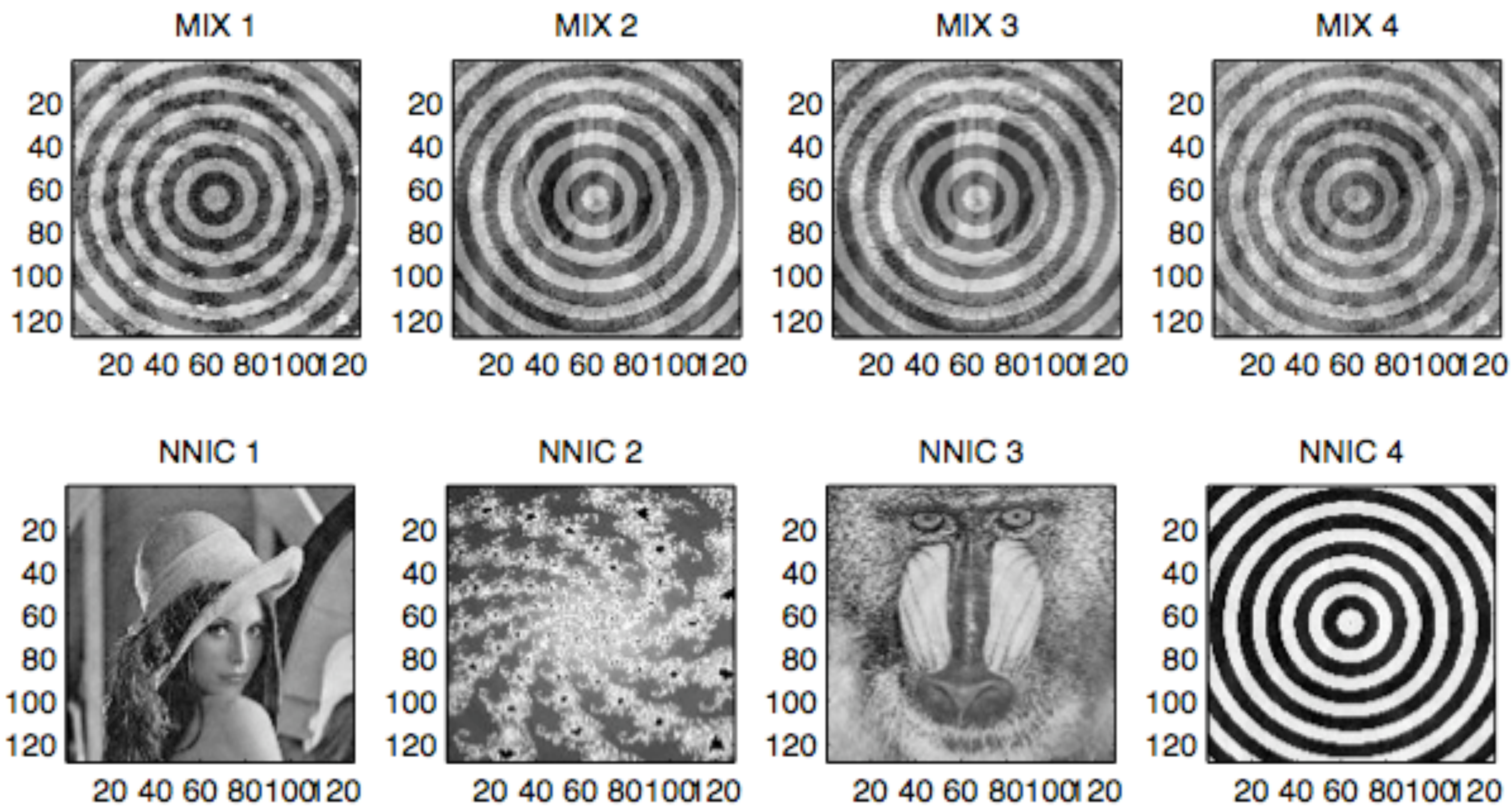
Original images

4-source mixture



4-source separation

Simone Fiori, Journal of Machine Learning Research 6 (2005) 743-781



Amari's Recurrent Neural ICA

- Fully recurrent neural network with self -inhibitory connections.

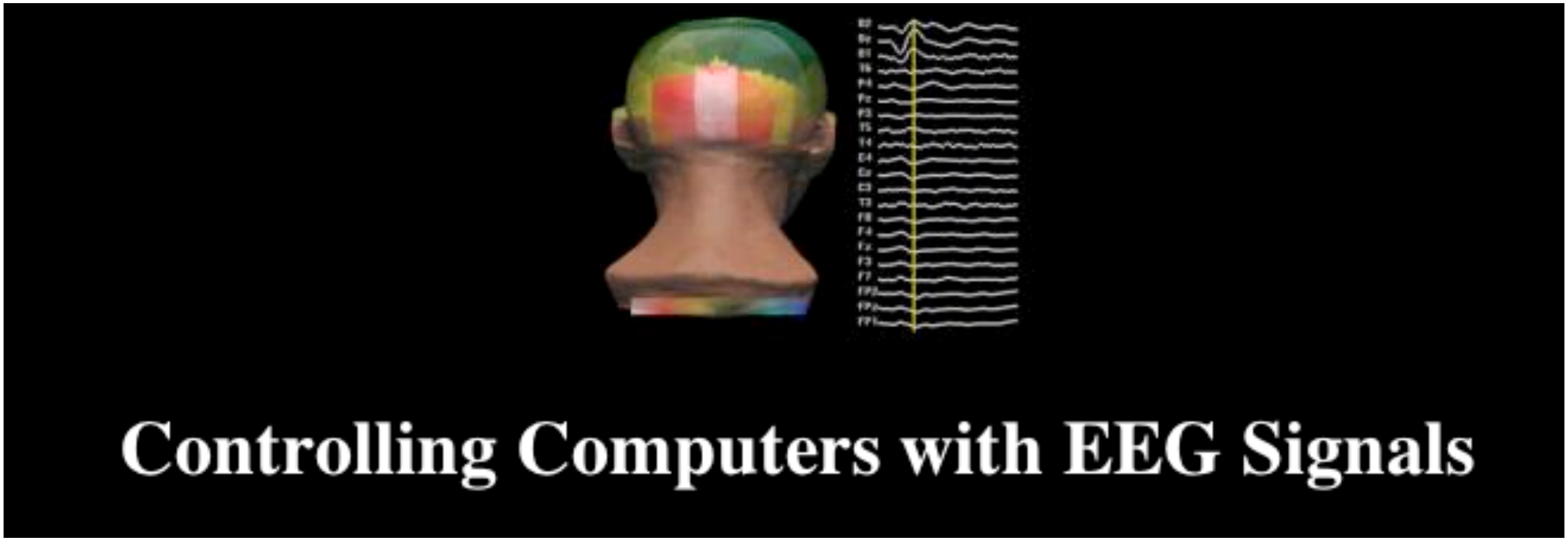
$$\tau_i \frac{dy_i}{dt} + y_i = x_i(t) - \sum_{i=1}^{n} \widehat{w}_{ij}(t) y_j,$$

$$y(t) = (I + \widehat{W}(t))^{-1} x(t),$$

$$y(t) = x(t) - \widehat{W}(t) y(t - \tau),$$

$$\frac{d\widehat{W}}{dt} = -\mu(t)[I + \widehat{W}][\Lambda - f(y(t)) g^T(y(t))].$$

Culpepper/Keller Project using: http://www.cs.hmc.edu/~bjc/research/



ICA was used to achieve a separation among 12 EEG channels, used to discriminate between two or three modes of thought.

Eye-blink EEG removal
(Peterson and Anderson, 1999)

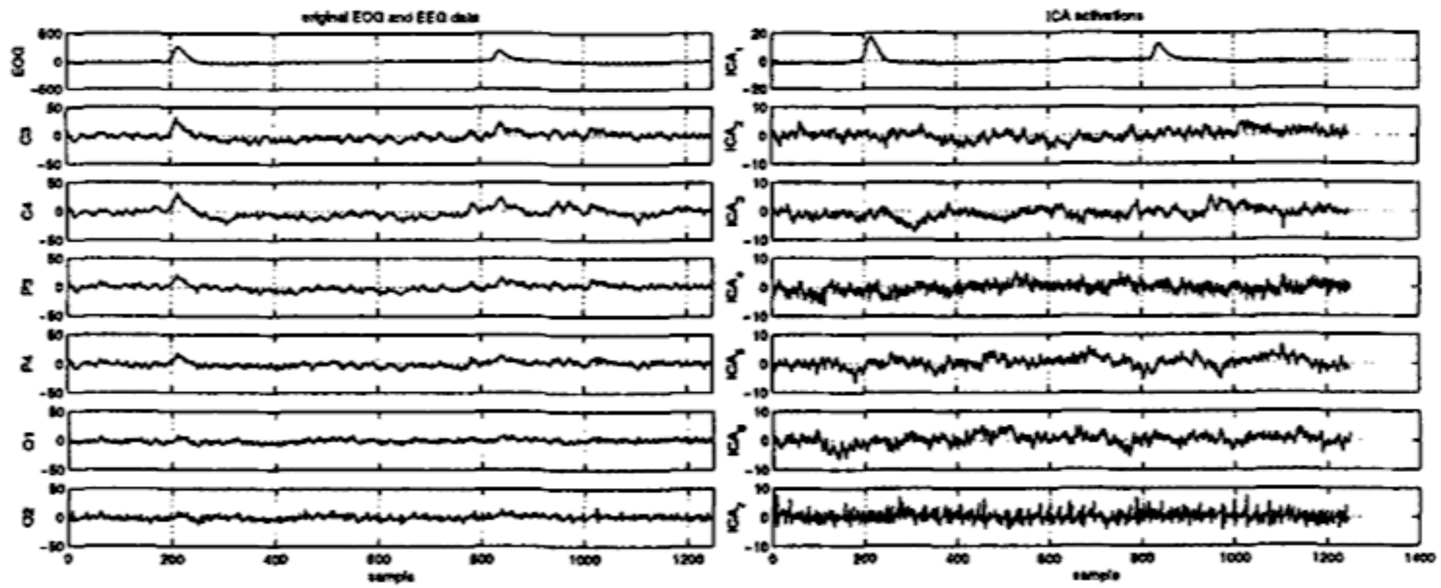


Fig. 1. Eye blink subtraction with ICA

Financial Application

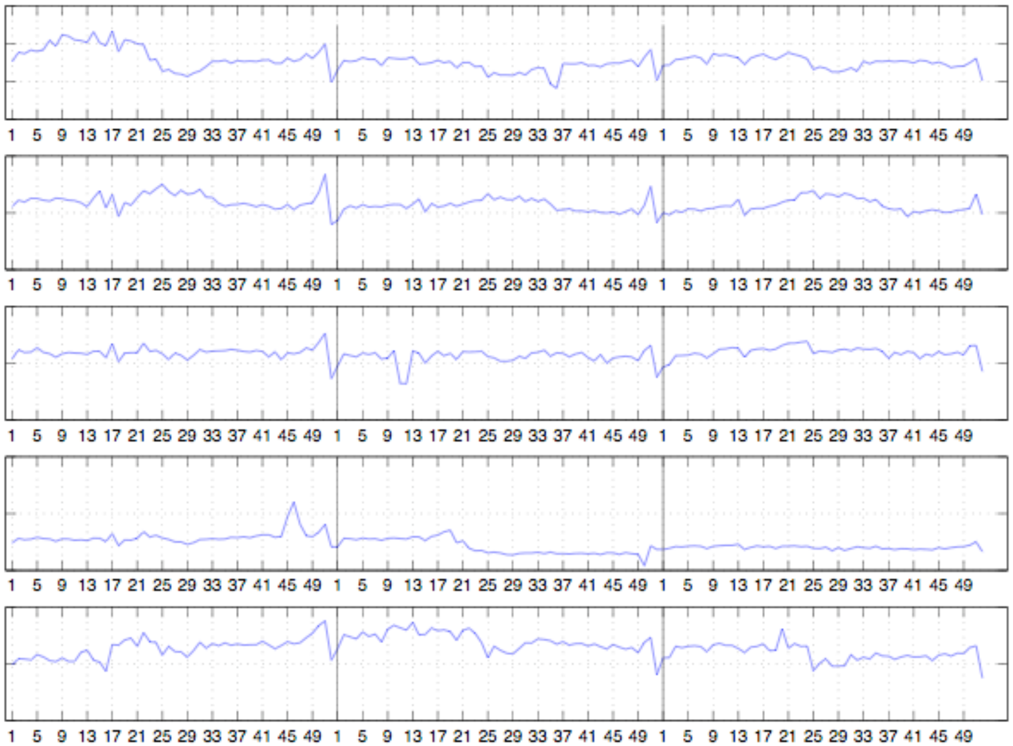


Figure 13: (from Kiviluoto and Oja, 1998). *Five samples of the original cashflow time series (mean removed, normalized to unit standard deviation). Horizontal axis: time in weeks.*

From Aapo Hyvärinen and Erkki Oja
Neural Networks, 13(4-5):411-430, 200

Financial Application

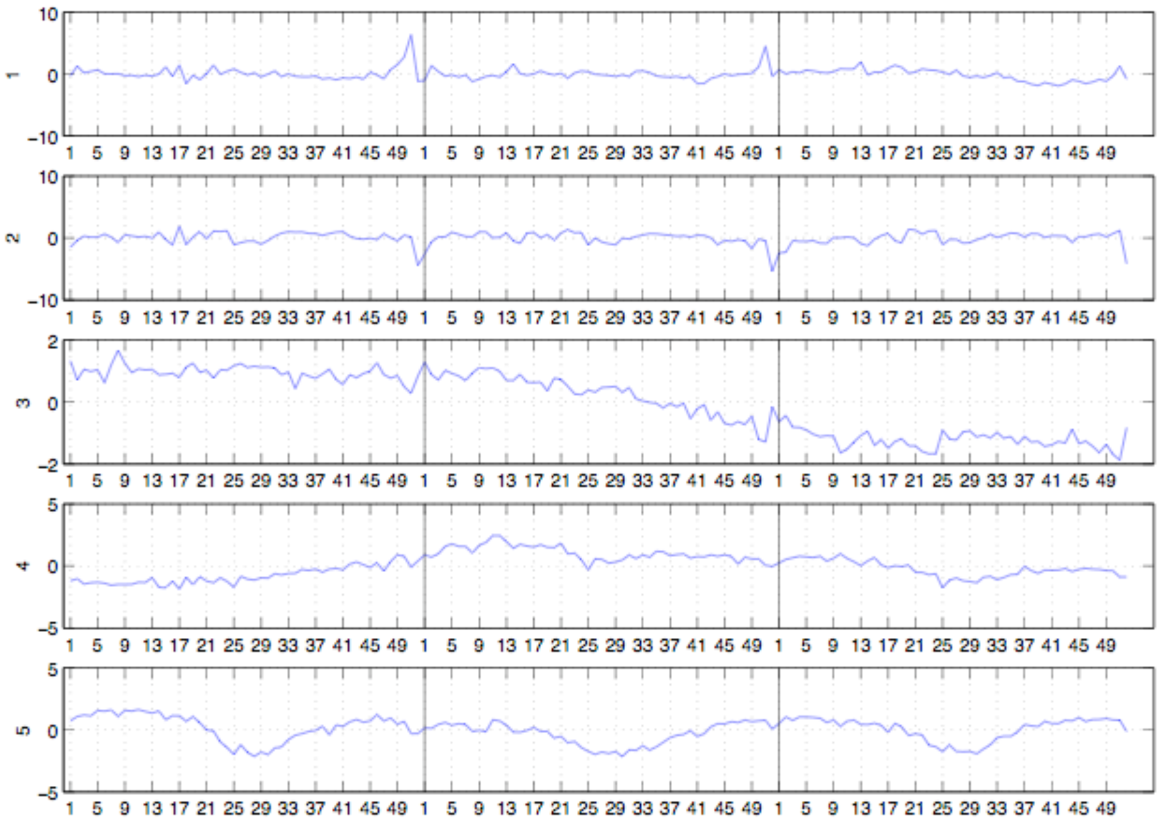


Figure 14: (from Kiviluoto and Oja, 1998). *Four independent components or fundamental factors found from the cashflow data.*

From Aapo Hyvärinen and Erkki Oja
Neural Networks, 13(4-5):411-430, 200

Image Noise Removal App.

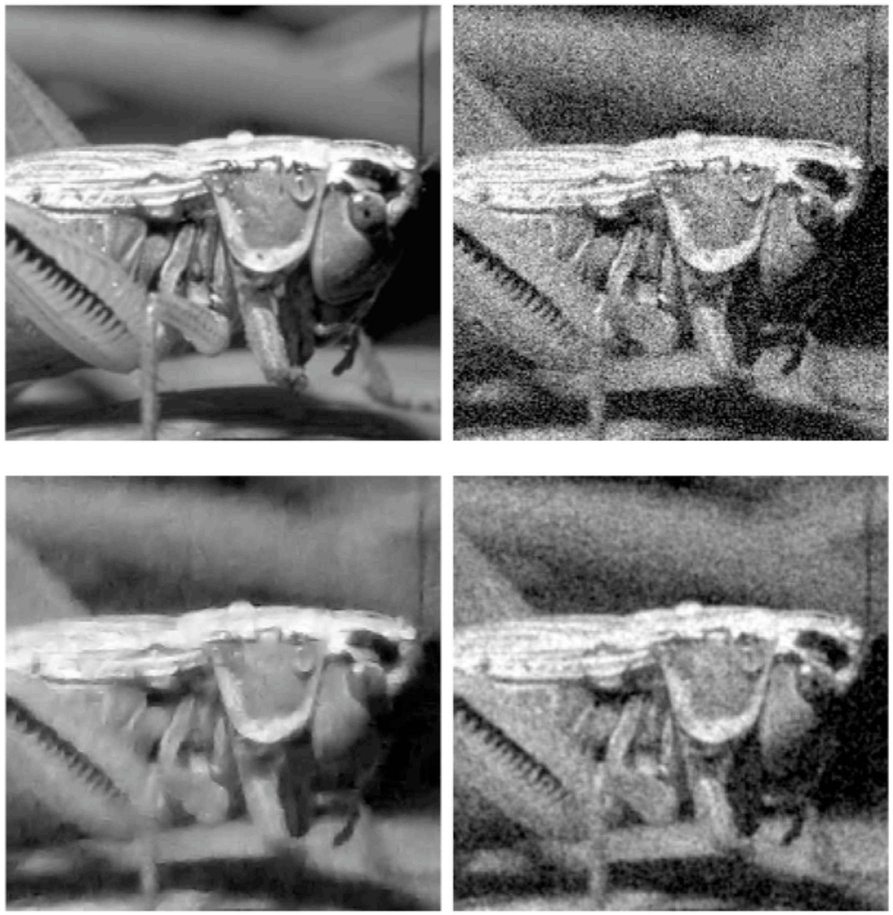
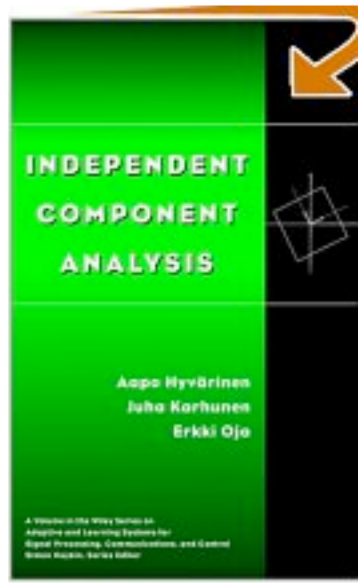


Figure 15: (from Hyvärinen, 1999d). *An experiment in denoising. Upper left: original image. Upper right: original image corrupted with noise; the noise level is 50 %. Lower left: the recovered image after applying sparse code shrinkage. Lower right: for comparison, a wiener filtered image.*

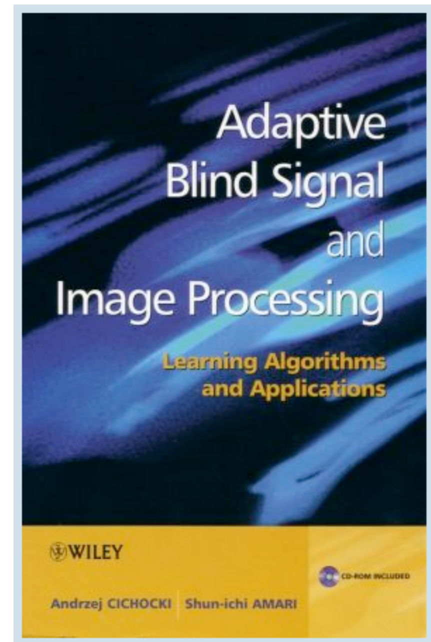
From Aapo Hyvärinen and Erkki Oja
Neural Networks, 13(4-5):411-430, 200

ICA Sources

James V. Stone



Aapo Hyvärinen,



Andrzej Cichocki,
Shun-ichi Amari

ICA Shortcomings

- ICA does not take sequence or structure into account; it is purely statistical.
- It might be possible to do better by considering the ignored information.