CS 4602

Introduction to Machine Learning

Dimensionality reduction

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Roadmap

- Introduction and Basic Concepts
- Regression
- Bayesian Classifiers
- Decision Trees
- Linear Classifier
- Neural Networks
- Deep learning
- Convolutional Neural Networks
- The others
- KNN
- Clustering
- Data Exploration & Dimensionality reduction
- Model Selection and Evaluation

Outline

- Curse of dimensionality
- Linear Dimensionality reduction
  - PCA
  - ICA
- Nonlinear Dimensionality Reduction

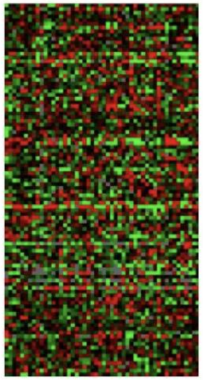
Lots of high-dimensional data...

face images

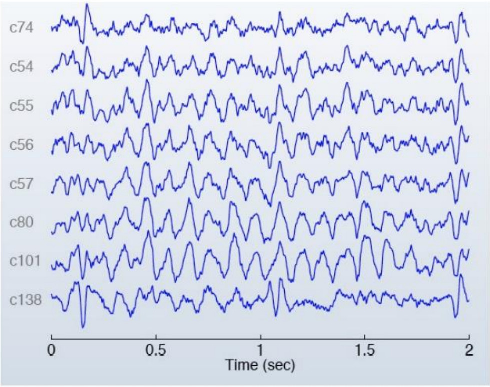
Zambian President Levy Mwanawasa has won a second term in office in an election his challenger Michael Sata accused him of rigging, official results showed on Monday.

According to media reports, a pair of hackers said on Saturday that the Firefox Web browser, commonly perceived as the safer and more customizable alternative to market leader Internet Explorer, is critically flawed. A presentation on the flaw was shown during the ToorCon hacker conference in San Diego.

documents

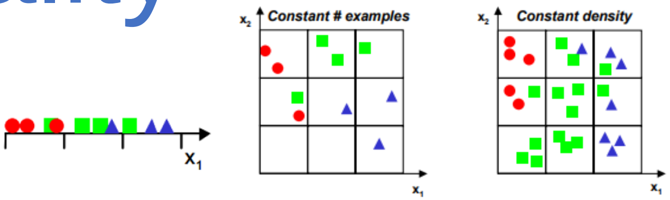


gene expression data

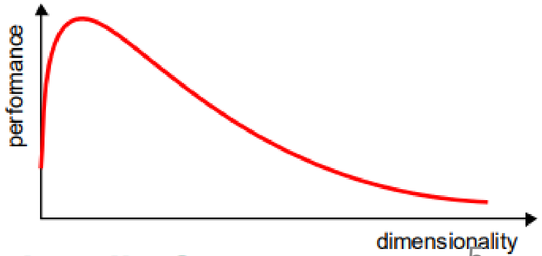


MEG readings

Curse of dimensionality



- The number of examples needed to accurately estimate a function increases exponentially with the dimensionality.
- For a specific sample size, there exists an upper limit of features beyond which the performance of a classifier deteriorates instead of improving.
- As the dimensionality of the training set increases, the likelihood of overfitting also escalates.
- How do we beat the curse of dimensionality?
  - By incorporating prior knowledge
  - By increasing the size of dataset
  - By reducing the dimensionality



Why do dimensionality reduction?

- Computational: compress data $\Rightarrow$ time/space efficiency
- Statistical: fewer dimensions $\Rightarrow$ better generalization
- Visualization: understand structure of data

Feature selection vs extraction

- In the presence of many of features, select the most relevant subset of (weighted) combinations of features.

Feature Selection: $X_1, \ldots, X_m \rightarrow X_{k1}, \ldots, X_{kp}$

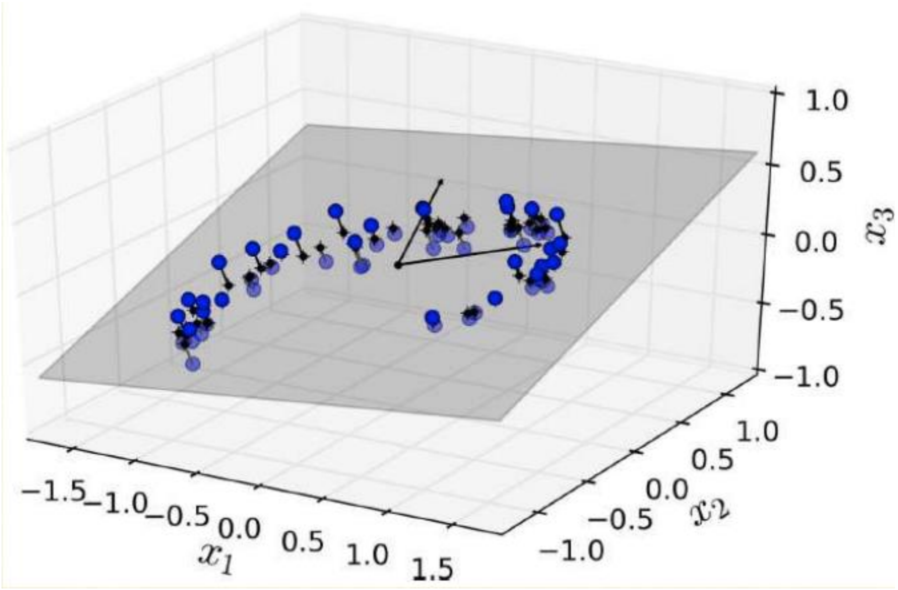
Dimensionality Reduction: $X_1, \ldots, X_m \rightarrow f_1(X_1, \ldots, X_m), \ldots, f_p(X_1, \ldots, X_m)$

- Linear feature extraction

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \\ x_N \end{bmatrix} \xrightarrow{\text{linear feature extraction}} \begin{bmatrix} y_1 \\ y_2 \\ \\ y_M \end{bmatrix} = \begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1N} \\ w_{21} & w_{22} & \cdots & w_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ w_{M1} & w_{M2} & & w_{MN} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \\ x_N \end{bmatrix}$$

Projection

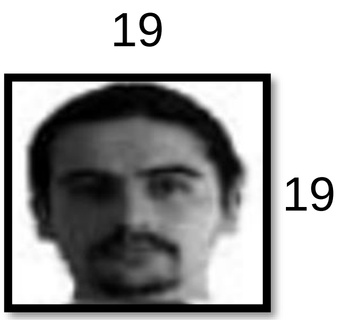
- Most real-world problems do not have training instances spread out across all dimensions



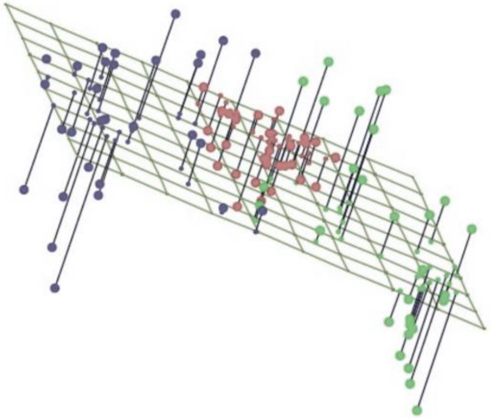
How many features are there?

Which of the feature is almost constant for almost all instances?

Linear dimensionality reduction



Represent each face as a high-dimensional vec$\mathbf{x} \in \mathbb{R}^{361}$



$$\mathbf{x} \in \mathbb{R}^{361}$$

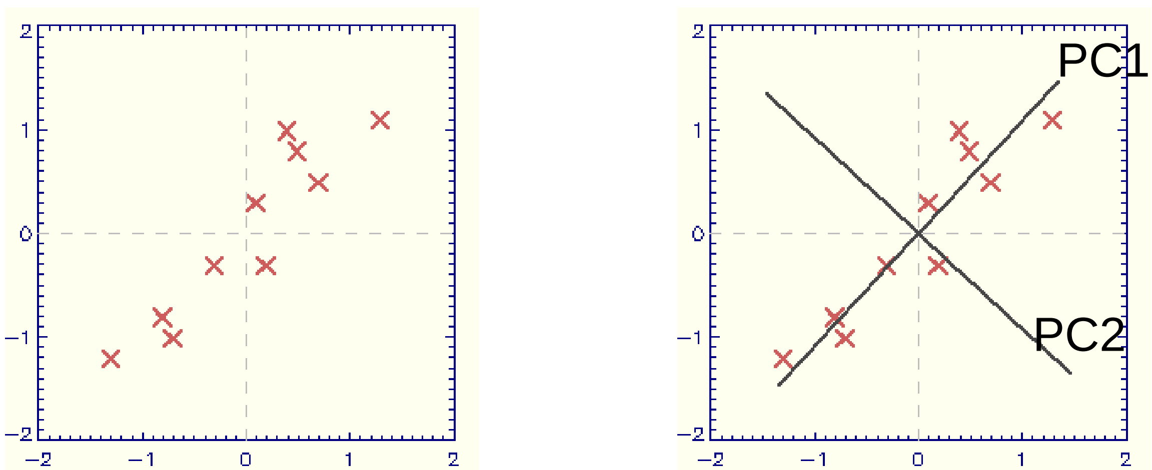
$$\mathbf{z} = \mathbf{U}^\top \mathbf{x}$$

$$\mathbf{z} \in \mathbb{R}^{10}$$

How do we choose U ?

Principal Components Analysis (PCA)

- PCA finds a linear mapping of dataset x to a dataset z of lower dimensionality.



PCA objective 1: reconstruction error

Given n data points in d dimensions: $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$

$$\mathbf{X} = \begin{pmatrix} | & & | \\ \mathbf{x}_1 & \cdots\cdots & \mathbf{x}_n \\ | & & | \end{pmatrix} \in \mathbb{R}^{d \times n}$$

Want to reduce dimensionality from d to k

Choose k directions $\mathbf{u}_1, \ldots, \mathbf{u}_k$

$$\mathbf{U} = \begin{pmatrix} | & & | \\ \mathbf{u}_1 & \cdot\cdot & \mathbf{u}_k \\ | & & | \end{pmatrix} \in \mathbb{R}^{d \times k}$$

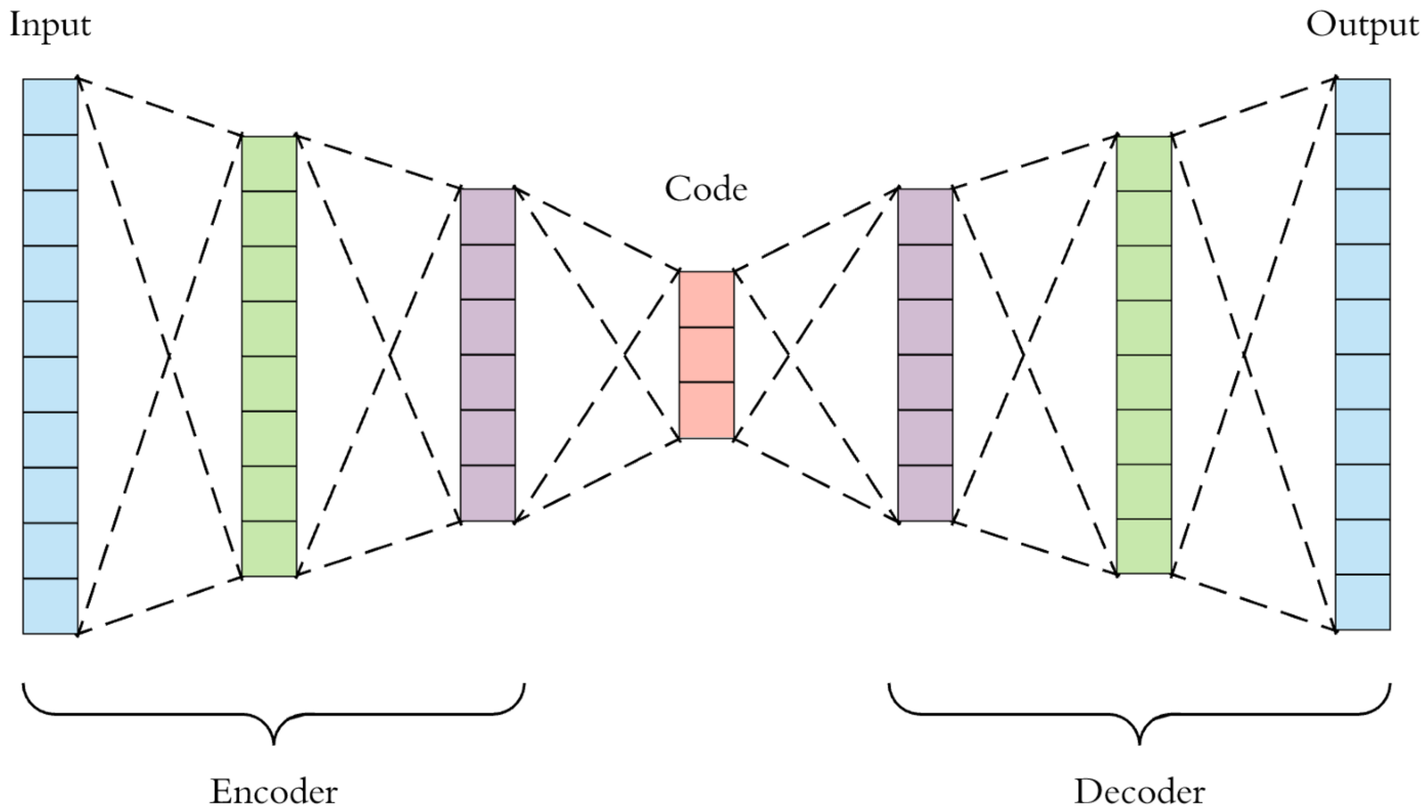
$\mathbf{U}$ serves two functions:

- Encode: $\mathbf{z} = \mathbf{U}^\top \mathbf{x}, \quad z_j = \mathbf{u}_j^\top \mathbf{x}$
- Decode: $\tilde{\mathbf{x}} = \mathbf{U}\mathbf{z} = \sum_{j=1}^{k} z_j \mathbf{u}_j$

Want reconstruction error $\|\mathbf{x} - \tilde{\mathbf{x}}\|$ to be small

Objective: minimize total squared reconstruction error $\min_{\mathbf{U} \in \mathbb{R}^{d \times k}} \sum_{i=1}^{n} \|\mathbf{x}_i - \mathbf{U}\mathbf{U}^\top \mathbf{x}_i\|^2$

Autoencoder!



PCA objective 2: projected variance

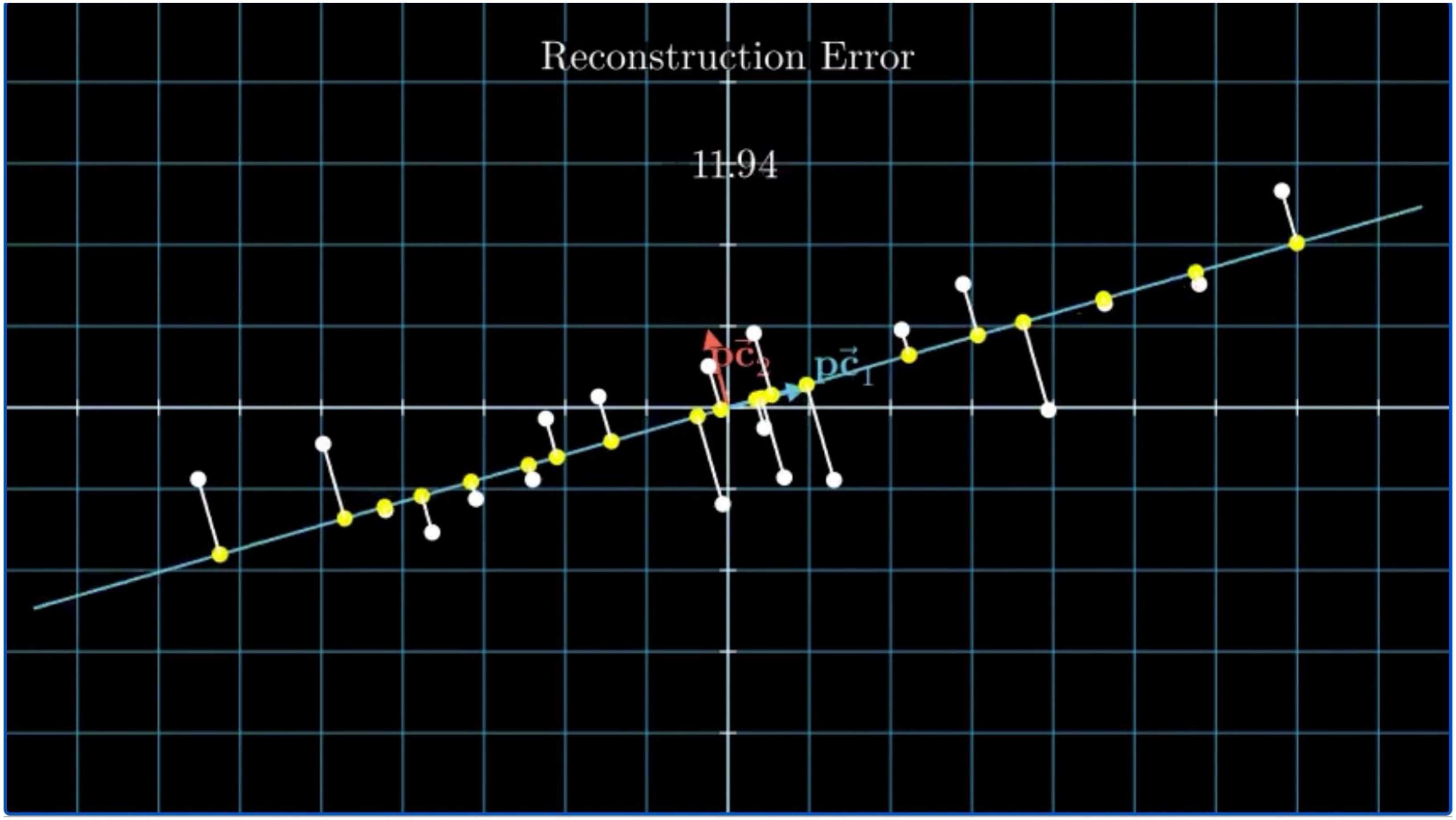
$$\max_{\mathbf{U}\in\mathbb{R}^{d\times k},\mathbf{U}^\top\mathbf{U}=I} \hat{\mathbb{E}}[\|\mathbf{U}^\top\mathbf{x}\|^2]$$

Equivalence in objective 1 & 2

Intuition:

variance of data = captured variance + reconstruction error

fixed $\uparrow$ $\downarrow$



From 3blue1brown

Covariance

- Variance and Covariance:
  - Measure of the “spread” of a set of points around their mean
- Variance:
  - Measure of the deviation from the mean for points in one dimension
- Covariance:
  - Measure of how much each of the dimensions vary from the mean with respect to each other
  - Covariance sees if there is a relation between two dimensions
  - Covariance between one dimension is the variance

Covariance

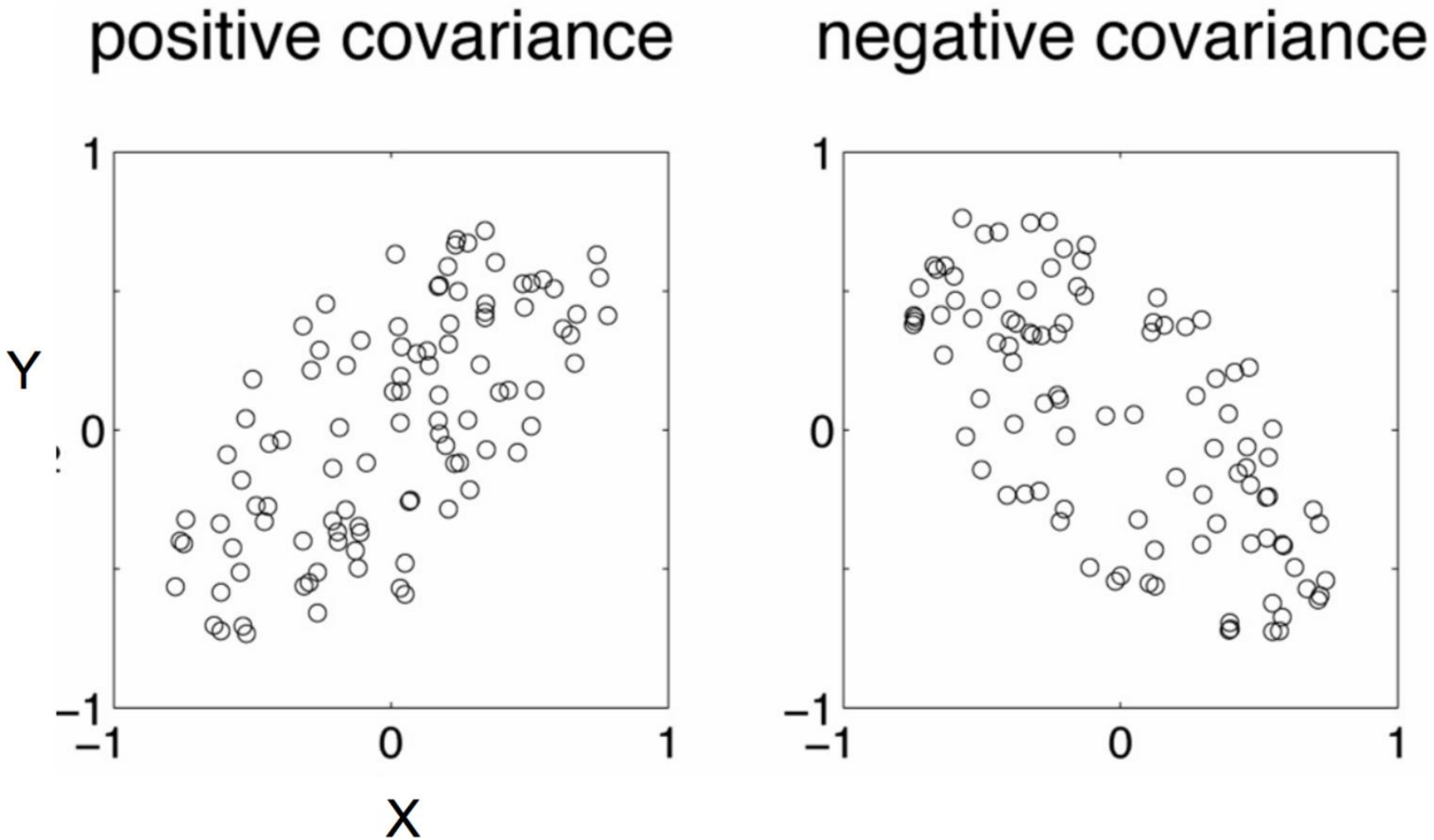
- Used to find relationships between dimensions in high dimensional data sets

$$\mathrm{cov}(X_i, X_j) = \mathrm{E}[(X_i - \mu_i)(X_j - \mu_j)]$$

- Covariance Matrix

$$\Sigma = \begin{bmatrix} \mathrm{E}[(X_1-\mu_1)(X_1-\mu_1)] & \mathrm{E}[(X_1-\mu_1)(X_2-\mu_2)] & \cdots & \mathrm{E}[(X_1-\mu_1)(X_n-\mu_n)] \\ \mathrm{E}[(X_2-\mu_2)(X_1-\mu_1)] & \mathrm{E}[(X_2-\mu_2)(X_2-\mu_2)] & \cdots & \mathrm{E}[(X_2-\mu_2)(X_n-\mu_n)] \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{E}[(X_n-\mu_n)(X_1-\mu_1)] & \mathrm{E}[(X_n-\mu_n)(X_2-\mu_2)] & \cdots & \mathrm{E}[(X_n-\mu_n)(X_n-\mu_n)] \end{bmatrix}.$$

$$\boxed{\mathbf{COR(X,\ Y)} = \frac{\mathbf{COV(X,\ Y)}}{\sqrt{\mathbf{VAR(X)VAR(Y)}}}}$$



Positive: Both dimensions increase together

Negative: While one increase the other decrease

PCA - Steps

- Suppose we are given $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n$ d x 1 vectors

Step 1: compute sample mean

$$\bar{\mathbf{x}} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i$$

Step 2: subtract sample mean (i.e., center data at zero)

$$\Phi_i = \mathbf{x}_i - \bar{\mathbf{x}}$$

Step 3: compute the sample covariance matrix Σ_x

$$\Sigma_{\mathbf{x}} = \frac{1}{n}\sum_{i=1}^{n}\Phi_i \Phi_i^T \quad = \frac{1}{n}AA^T$$

, where $A=[\Phi_1\ \Phi_2\ ...\ \Phi_n]$ (d x n matrix)

PCA - Steps

Step 4: compute the eigenvalues/eigenvectors of Σ_x

$$\Sigma_x u_i = \lambda_i u_i$$

we assume

eigenvalues $\lambda_1 > \lambda_2 > \ldots > \lambda_d$ and $u_1, u_2, \ldots, u_d$ are the corresponding eigenvectors

Since Σ_x is symmetric, $<u_1,u_2,\ldots,u_d>$ form an orthogonal basis in R^d, therefore:

$$\mathbf{x} - \bar{\mathbf{x}} = \sum_{i=1}^{d} \boldsymbol{z}_i \, \boldsymbol{u}_i = \boldsymbol{z}_1 \boldsymbol{u}_1 + \boldsymbol{z}_2 \boldsymbol{u}_2 + \ldots + \boldsymbol{z}_d \boldsymbol{u}_d$$

$$\boldsymbol{z}_i = \frac{(\mathbf{x} - \overline{\mathbf{x}})^{\mathrm{T}} \boldsymbol{u}_i}{\boldsymbol{u}_i^{\mathrm{T}} \boldsymbol{u}_i} = (\mathbf{x} - \overline{\mathbf{x}})^T \boldsymbol{u}_i \text{ if } ||\boldsymbol{u}_i|| = 1$$

Note : most software packages normalize $\mathbf{u}_i$ to unit length to simplify calculations

PCA - Steps

Step 5: <u>dimensionality reduction step</u> – approximate **x** using only the first K eigenvectors (K<d) (i.e., corresponding to the K largest eigenvalues where K is a parameter):

$$\mathbf{x} - \bar{\mathbf{x}} = \sum_{i=1}^{d} \boldsymbol{z}_i\, \boldsymbol{u}_i = \boldsymbol{z}_1 \boldsymbol{u}_1 + \boldsymbol{z}_2 \boldsymbol{u}_2 + \ldots + \boldsymbol{z}_d \boldsymbol{u}_d$$

approximate using first K terms

$$\hat{\mathbf{x}} - \bar{\mathbf{x}} = \sum_{i=1}^{K} \boldsymbol{z}_i\, \boldsymbol{u}_i = \boldsymbol{z}_1 \boldsymbol{u}_1 + \boldsymbol{z}_2 \boldsymbol{u}_2 + \ldots + \boldsymbol{z}_d \boldsymbol{u}_K$$

or

$$(\hat{\mathbf{x}} - \bar{\mathbf{x}}) = \mathrm{U} \begin{bmatrix} \boldsymbol{z}_1 \\ \boldsymbol{z}_2 \\ \cdot \\ \cdot \\ \boldsymbol{z}_K \end{bmatrix}$$

$$\text{where } \mathrm{U} = [\boldsymbol{u}_1 \boldsymbol{u}_2 \ldots \boldsymbol{u}_K]$$

i.e., the columns of U are the the first K eigenvectors of Σ_x

PCA – Linear Transformation

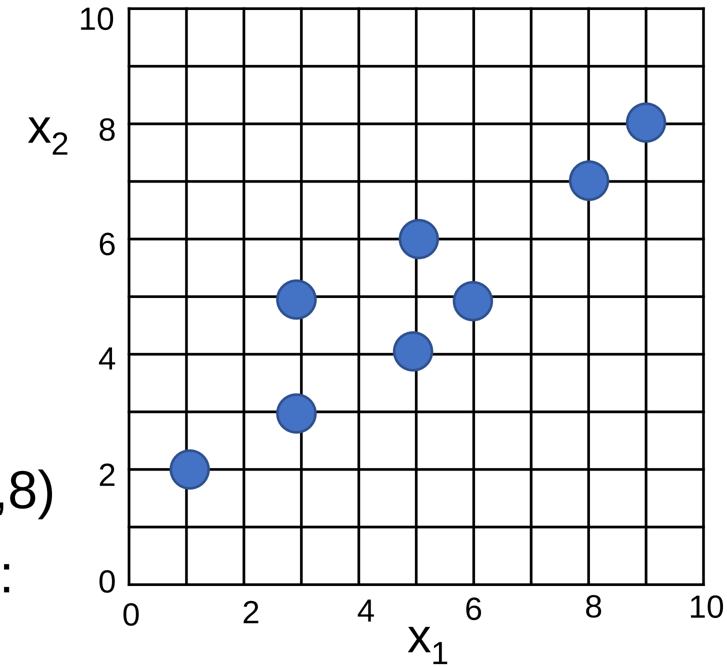
- The linear transformation $R^d \rightarrow R^K$ which performs the dimensionality reduction is:

$$\mathbf{y} = \mathbf{U}^{\mathrm{T}}\mathbf{x} \ \in R^K \text{ where } K<d$$

$$\begin{bmatrix} \boldsymbol{z}_1 \\ \boldsymbol{z}_2 \\ \cdot \\ \cdot \\ \boldsymbol{z}_K \end{bmatrix} = \mathrm{U}^{\mathrm{T}}(\hat{\mathbf{x}} - \bar{\mathbf{x}}) = \begin{bmatrix} \boldsymbol{u}_1^{\mathbf{T}} \\ \boldsymbol{u}_2^{\mathbf{T}} \\ \cdot \\ \cdot \\ \boldsymbol{u}_K^{\mathbf{T}} \end{bmatrix} (\hat{\mathbf{x}} - \bar{\mathbf{x}})$$

i.e., the rows of U^T are the first K eigenvectors of Σ_x

Example



- Compute the PCA for dataset

(1,2),(3,3),(3,5),(5,4),(5,6),(6,5),(8,7),(9,8)

- Compute the sample covariance matrix is:

What do they look like?

$$\Sigma_x = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i - \hat{\boldsymbol{\mu}})(\mathbf{x}_i - \hat{\boldsymbol{\mu}})^{\mathrm{T}} \qquad \Sigma_x = \begin{bmatrix} 6.25 & 4.25 \\ 4.25 & 3.5 \end{bmatrix}$$

- The eigenvalues can be computed by finding the roots of the characteristic polynomial:

$$\Sigma_x v = \lambda v \Rightarrow |\Sigma_x - \lambda I| = 0$$
$$\Rightarrow \begin{vmatrix} 6.25-\lambda & 4.25 \\ 4.25 & 3.5-\lambda \end{vmatrix} = 0$$
$$\Rightarrow \boldsymbol{\lambda_1 = 9.34; \lambda_2 = 0.41}$$

Example (cont'd)

- The eigenvectors are the solutions of the systems:

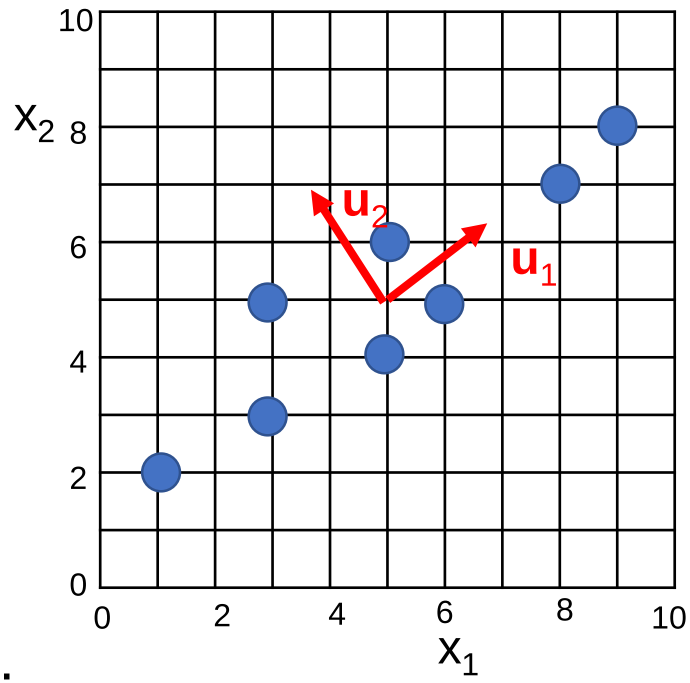
$$\boldsymbol{\Sigma}_{\mathbf{x}}\boldsymbol{u}_i = \lambda_i \boldsymbol{u}_i$$

$$\begin{bmatrix} 6.25 & 4.25 \\ 4.25 & 3.5 \end{bmatrix} \begin{bmatrix} u_{11} \\ u_{12} \end{bmatrix} = 9.34 \begin{bmatrix} u_{11} \\ u_{12} \end{bmatrix}$$

$$\begin{bmatrix} 6.25 & 4.25 \\ 4.25 & 3.5 \end{bmatrix} \begin{bmatrix} u_{21} \\ u_{22} \end{bmatrix} = 0.41 \begin{bmatrix} u_{21} \\ u_{22} \end{bmatrix}$$

$$\boldsymbol{u}_1 = \begin{bmatrix} u_{11} \\ u_{12} \end{bmatrix} = \begin{bmatrix} 0.81 \\ 0.59 \end{bmatrix}$$

$$\boldsymbol{u}_2 = \begin{bmatrix} u_{21} \\ u_{22} \end{bmatrix} = \begin{bmatrix} -0.59 \\ 0.81 \end{bmatrix}$$



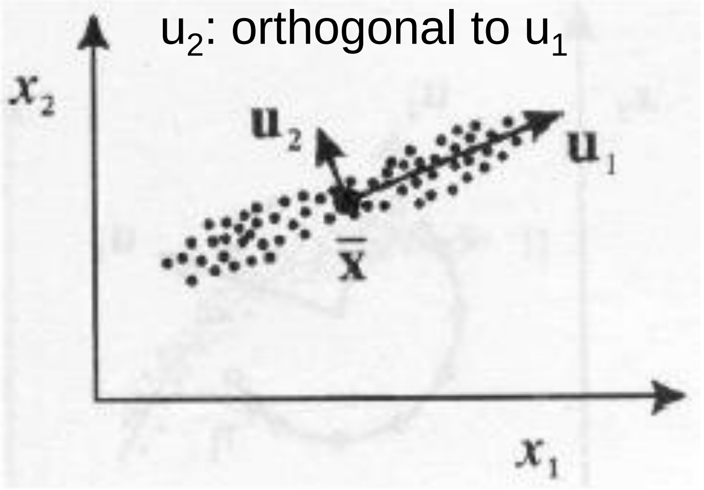
- Normalize the eigenvectors to unit-length.

Note: if u_i is a solution, then (cu_i) is also a solution where c is any constant.

Geometric interpretation

- PCA chooses the eigenvectors of the covariance matrix corresponding to the largest eigenvalues.
- The eigenvalues correspond to the variance of the data along the eigenvector directions.
- Therefore, PCA projects the data along the directions where the data varies most!

u_1: direction of max variance
u_2: orthogonal to u_1



How do we choose K

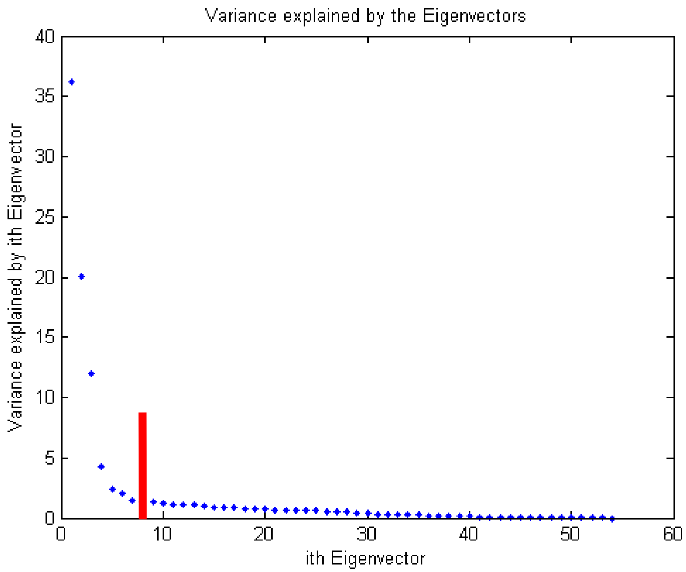
- Similar to question of *"How many clusters?"*
- *K* is typically chosen based on how much information (variance) we want to preserve:

$$\frac{\sum_{i=1}^{K} \lambda_i}{\sum_{i=1}^{N} \lambda_i} > T \quad where\ T\ is\ a\ threshold\ (e.g., 0.9)$$

- If T=0.9, for example, we say that we "preserve" 90% of the information (variance) in the data.
- If K=N, then we "preserve" 100% of the information in the data (i.e., just a change of basis)

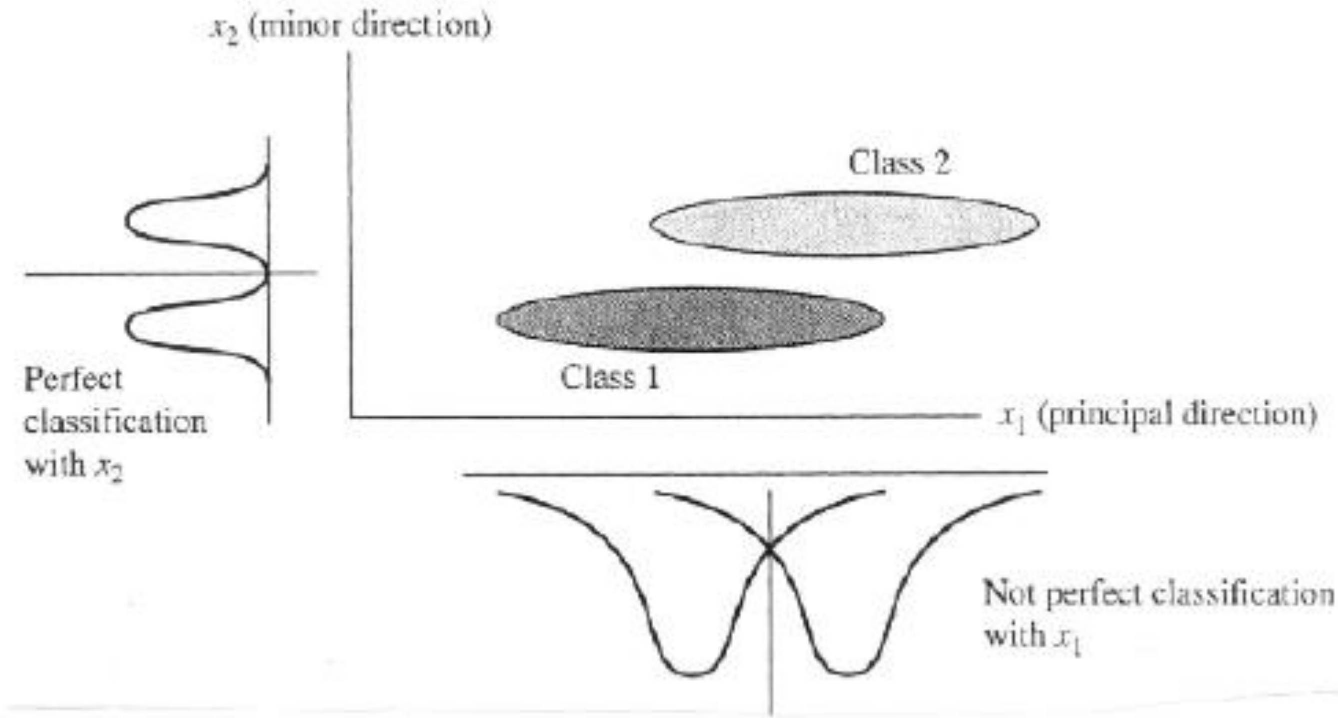
How do we choose K

- Check the distribution of eigenvalues
- Take enough eigenvectors to cover 80-90% of the variance

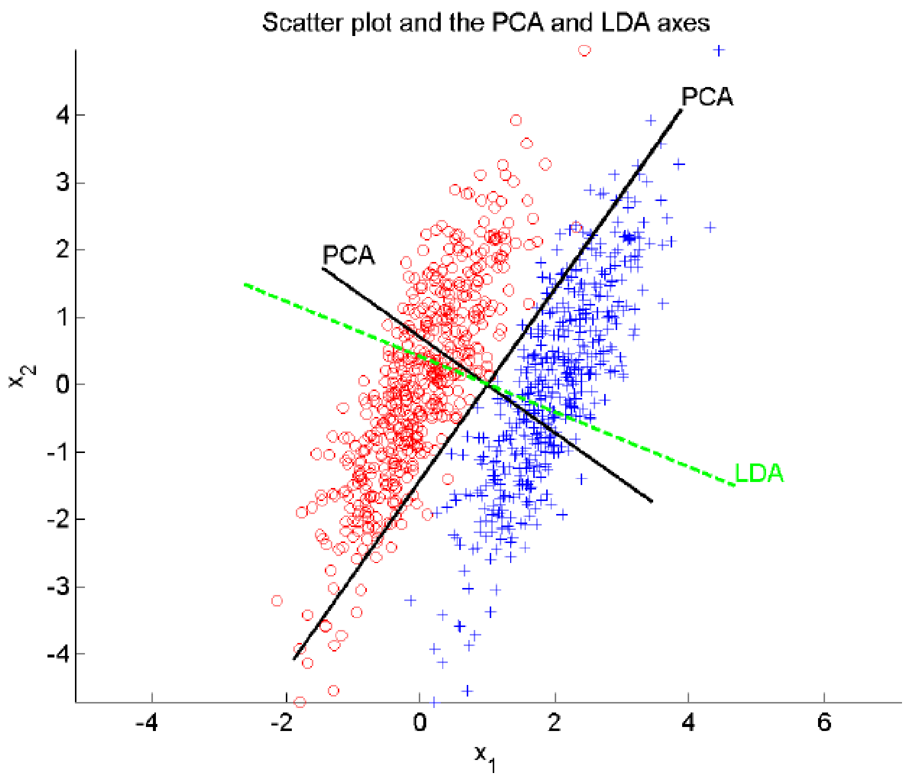


Limitations

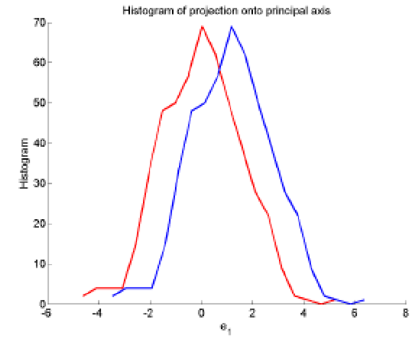
- PCA is not always an optimal dimensionality-reduction technique for classification purposes.



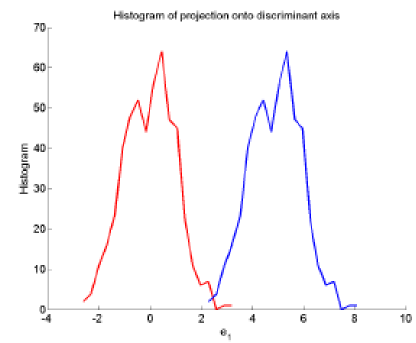
PCA vs. LDA



(a) Scatter plot.



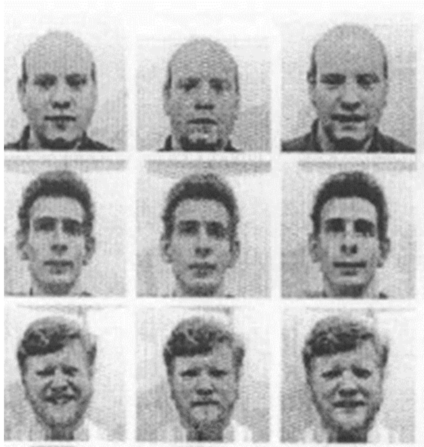
(b) Projection onto the first PCA axis.

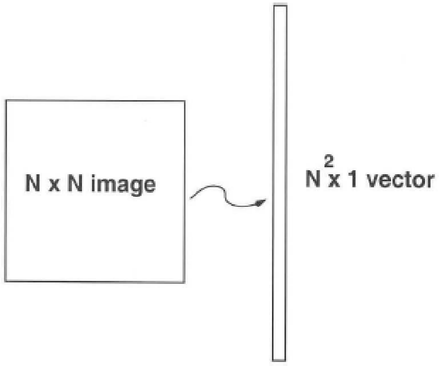


(c) Projection onto the first LDA axis.

Application to Images

- The goal is to represent images in a space of lower dimensionality using PCA.
  - Useful for various applications, e.g., face recognition, image compression, etc.
- Given M images of size N x N, first represent each image as a 1D vector (i.e., by stacking the rows together).
  - Note that for face recognition, faces must be centered and of the same size.





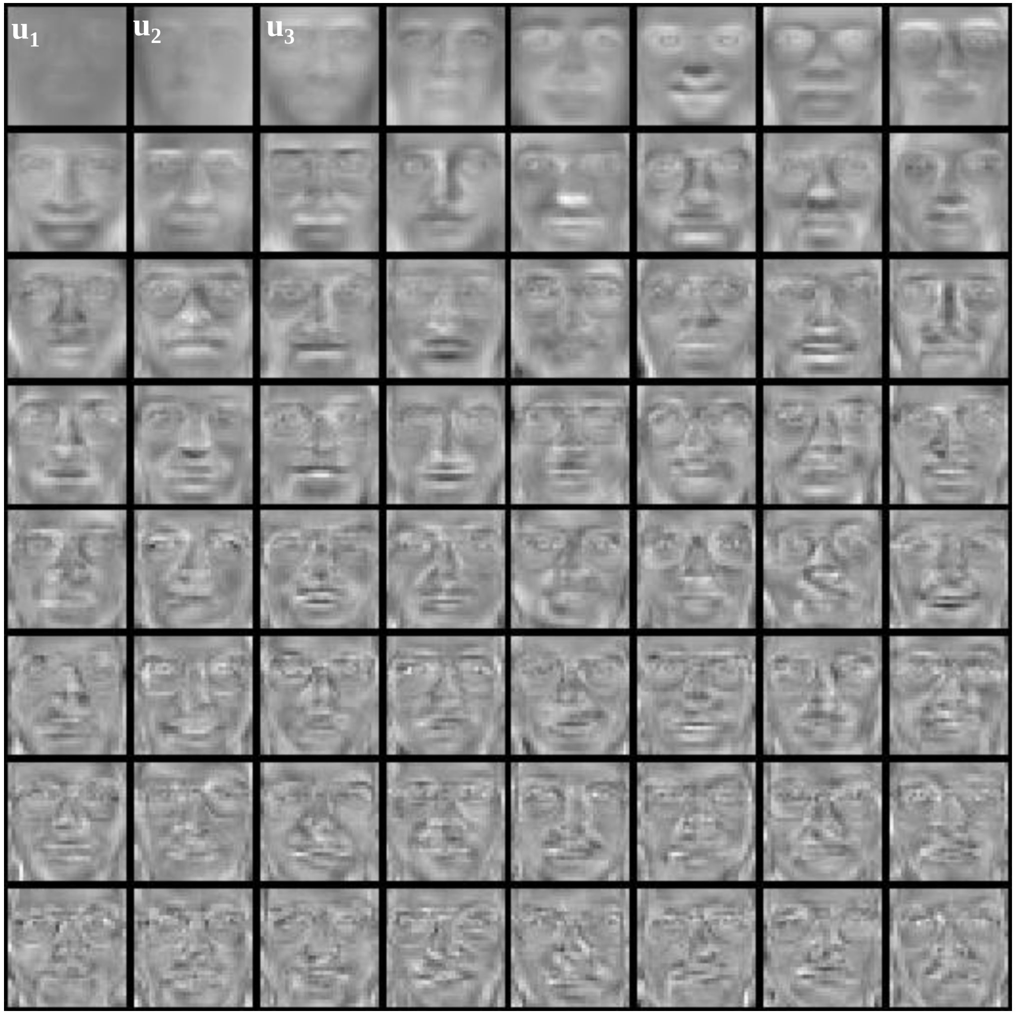
Example: face recognition

Dataset

Mean face: $\bar{\mathbf{x}}$

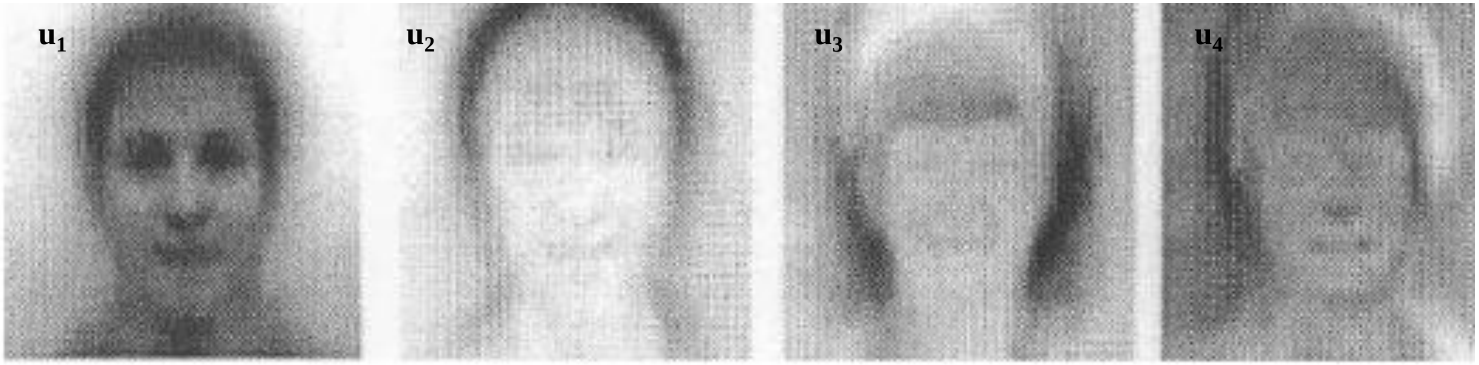
Top eigenvectors: $\mathbf{u}_1,\ldots\mathbf{u}_k$

(visualized as images - eigenfaces)

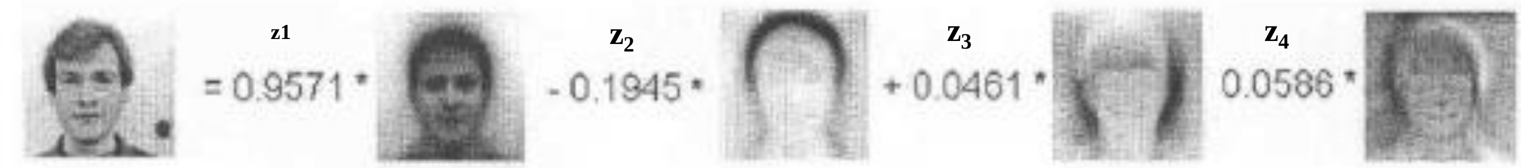


Example (cont'd)

- Interpretation: represent a face in terms of eigenfaces



$$\hat{\mathbf{x}} = \sum_{i=1}^{K} z_i\, u_i = z_1 u_1 + z_2 u_2 + \ldots + z_K u_K + \bar{\mathbf{x}} \qquad Z = \begin{bmatrix} z_1 \\ z_2 \\ \cdot \\ \cdot \\ z_K \end{bmatrix}$$



$+\overline{\mathbf{x}}$

Experiments in the original Eigenface paper presented the following results: an average of 96% with light variation, 85% with orientation variation, and 64% with size variation. (Turk & Pentland 1991)

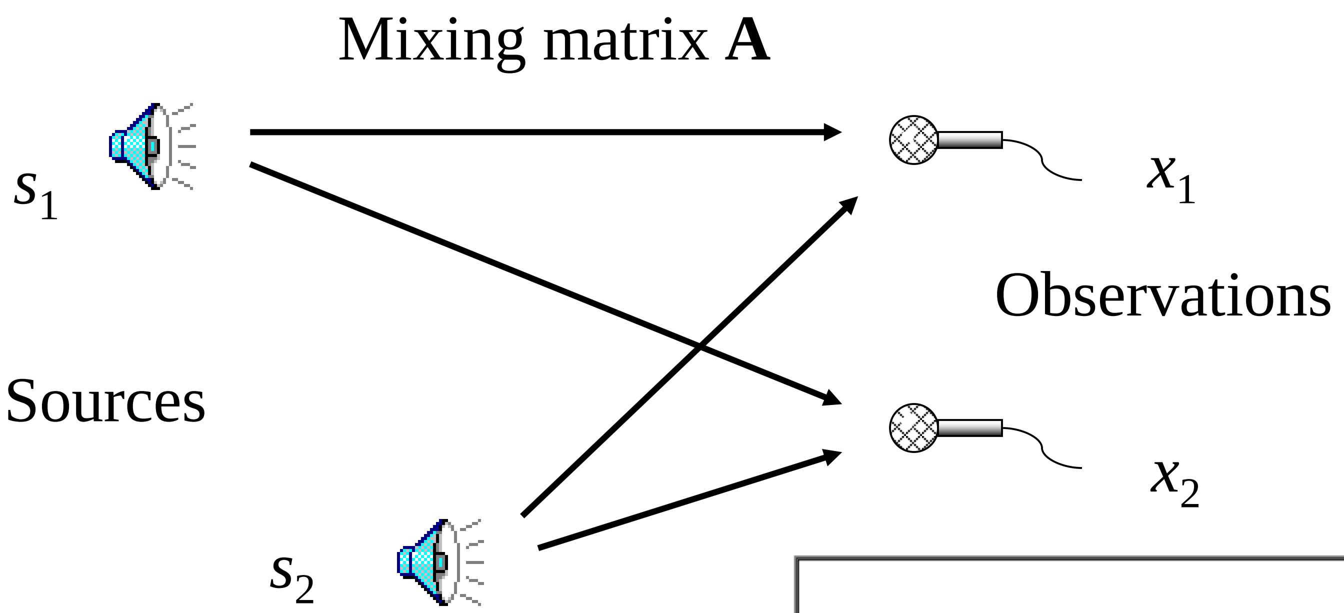
Independent Component Analysis (ICA)

Blind Signal Separation (BSS) or Independent Component Analysis (ICA) is the identification & separation of mixtures of sources

- Applications include:
  - Audio Processing
  - Biomedical signals
  - Finance
- While PCA seeks directions that represents data best in a $\boldsymbol{\Sigma|x_0 - x|^2}$ sense, ICA seeks such directions that are most independent from each other.

Often used on Time Series separation of Multiple Targets

The “Cocktail Party” Problem



n sources, m=*n* observations

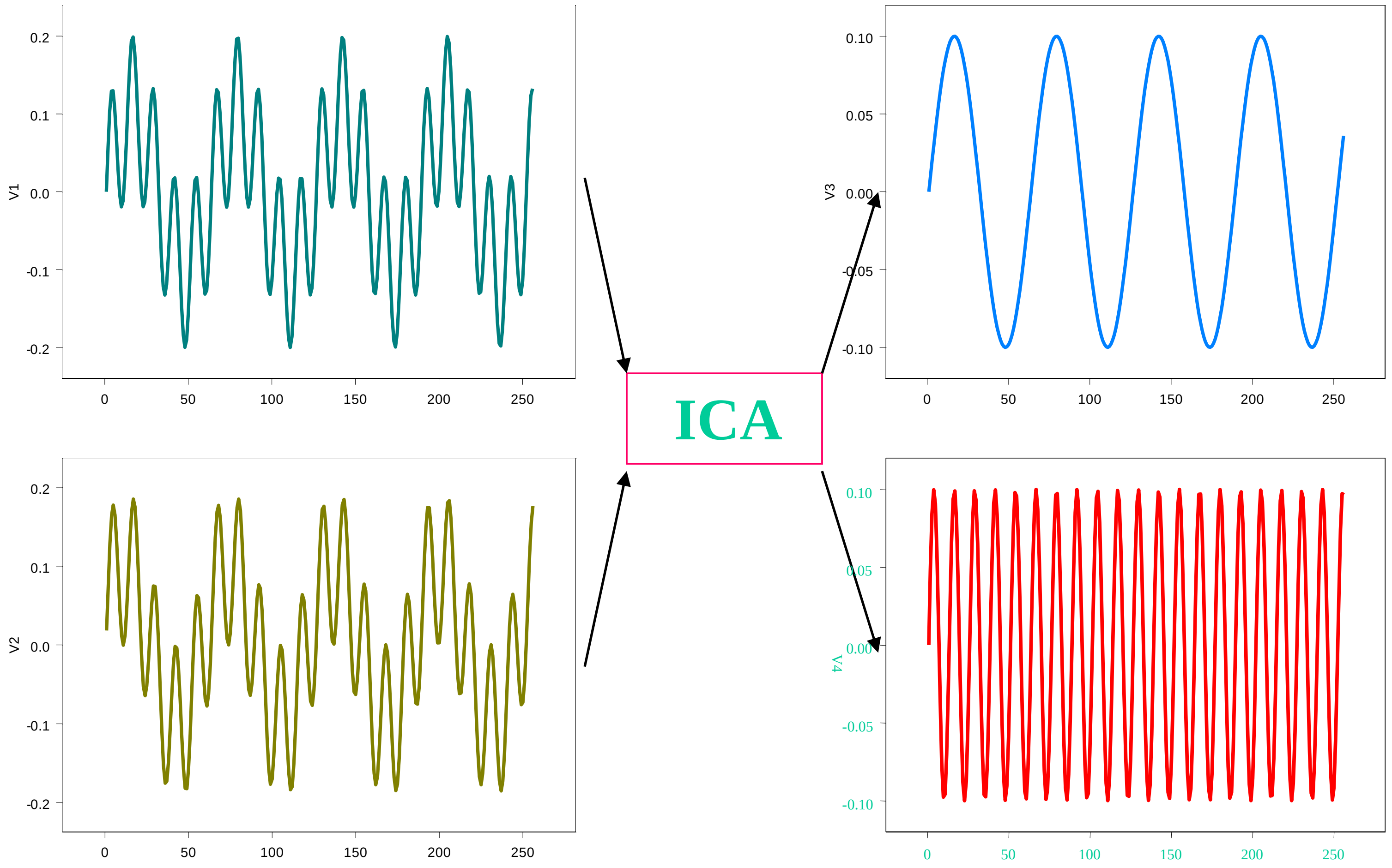
$$\boxed{X=AS}$$

“observations” “mixing matrix” “sources”

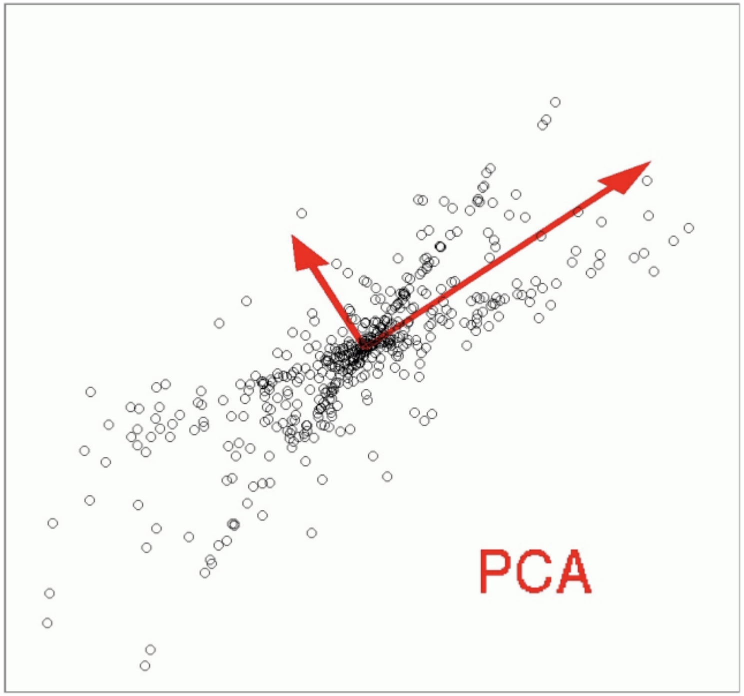
ICA estimation

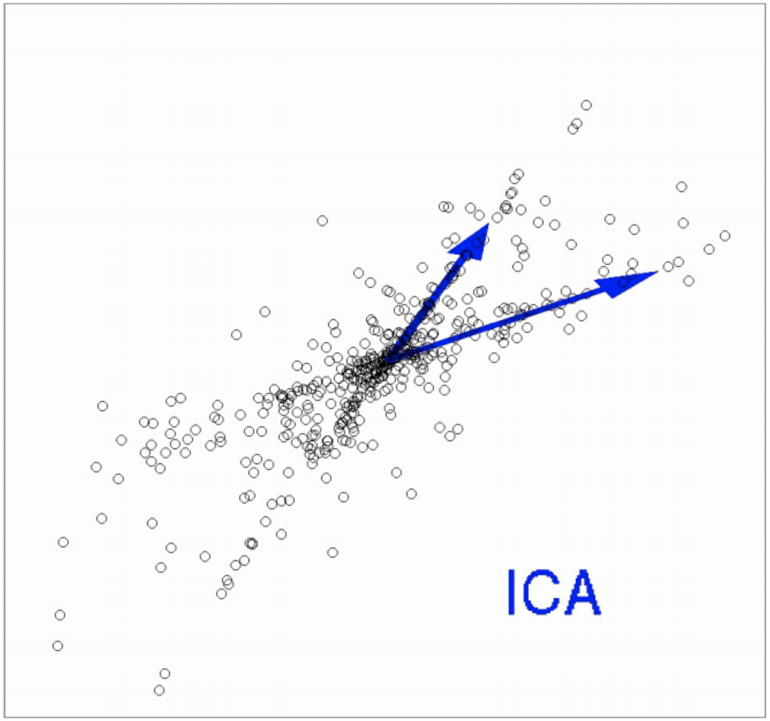
Observing signals

Original source signal



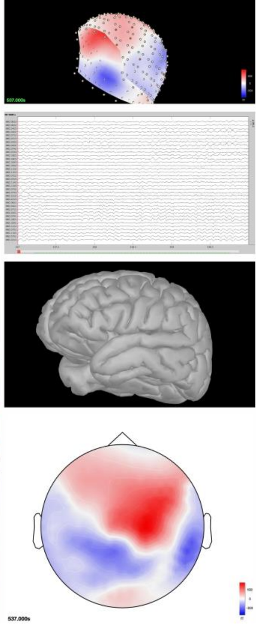
ICA vs PCA





- PCA vectors are orthogonal
- ICA vectors are not orthogonal

Application: Signal processing



- Data: MEG data
  - Eye artifacts:
    - ask person to “blink” and to make “horizontal saccades”
  - Muscle artifacts:
    - Asked to bite teeth for as long as 20 seconds.
  - Other artifact:
    - Cardiac cycle
- Subset: 12 subset of MEG signals $x_i(t)$

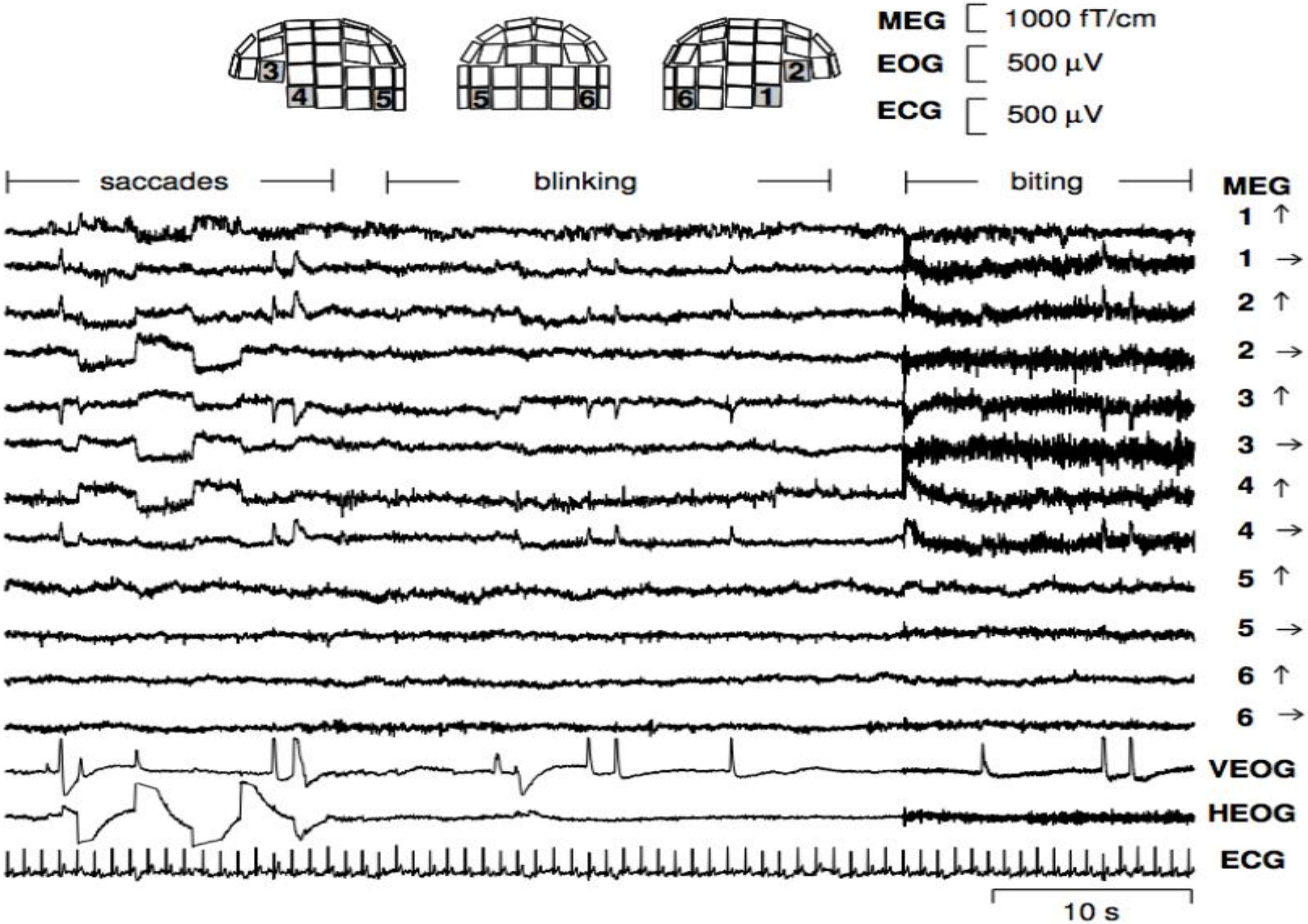
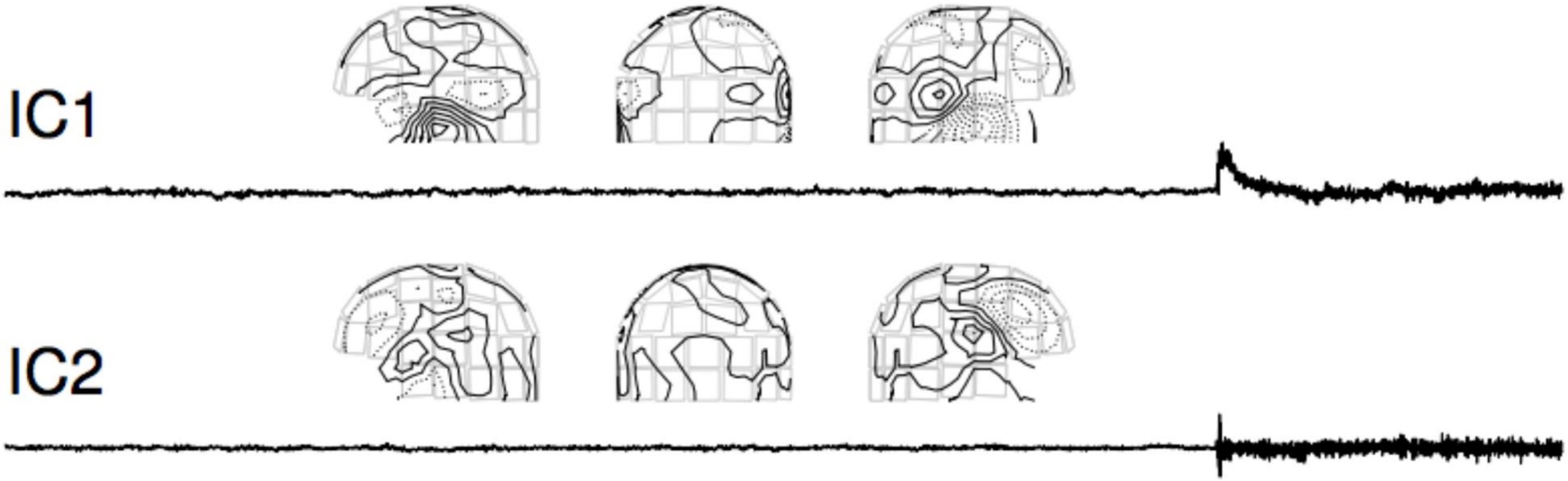


Figure: Samples of MEG signals, showing artifacts produced by blinking, saccades, biting and cardiac cycle. For each of the 6 positions shown, the two orthogonal directions of the sensors are plotted.

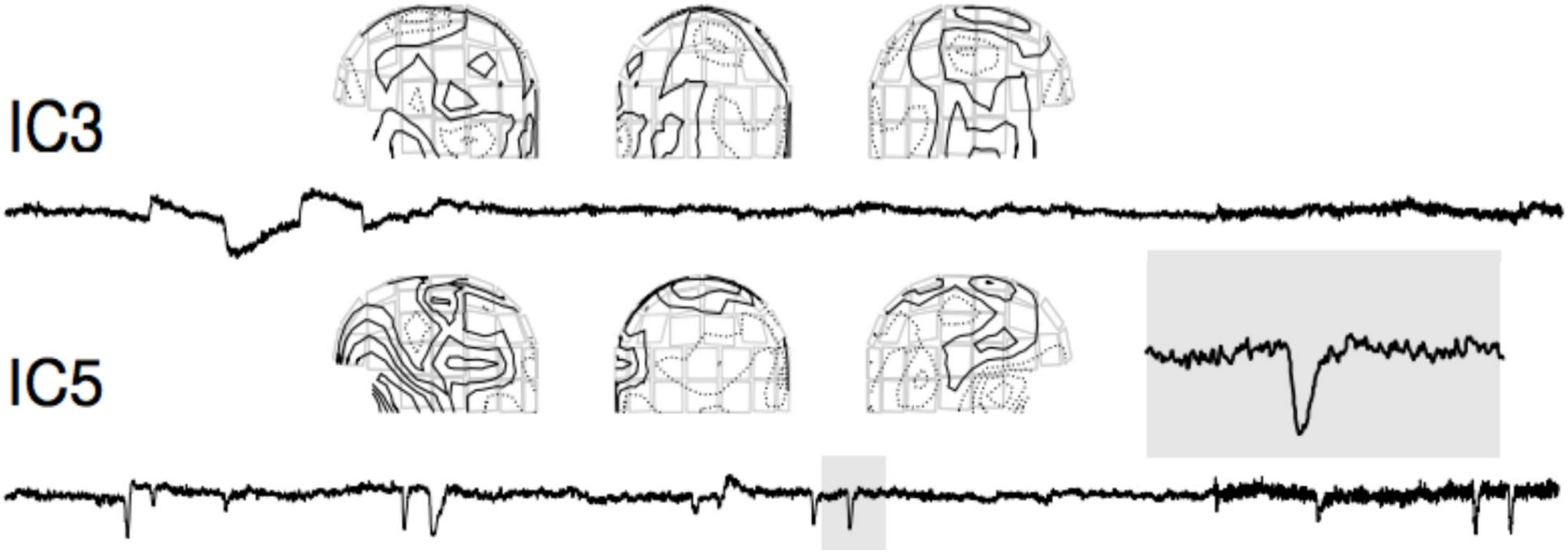
MEG application

There are 9 ICA found from the recorded data



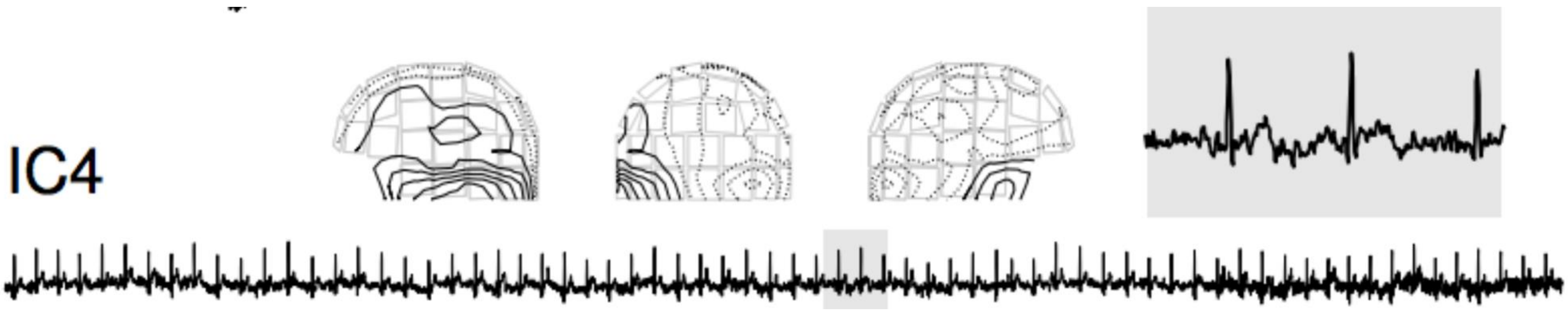
➔ Clearly due to the muscular activity originated for the biting

MEG application



➔ Showing Horizontal eye movement IC3 and the eye blinks IC5

MEG application

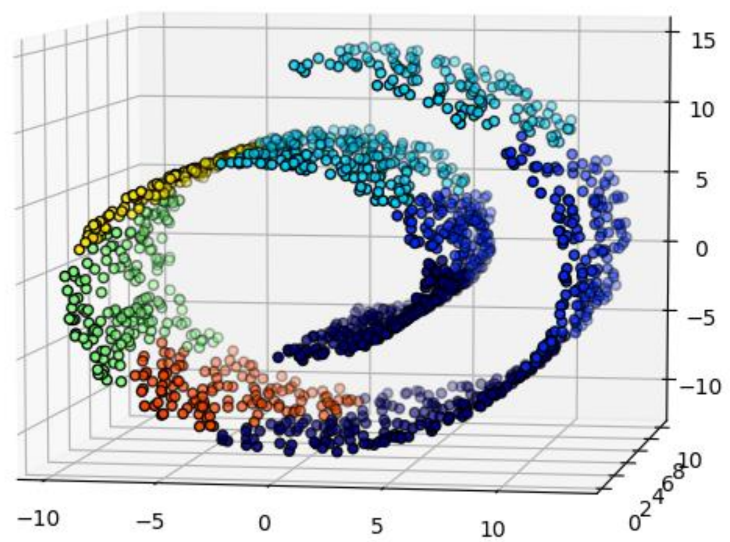


➔IC4 is clearly extracted to represents the cardiac artifact.

MEG Signal = ~~IC1~~ + ~~IC2~~ + ~~IC3~~ + ~~IC4~~ + ~~IC5~~ + IC6 + IC7 + IC8 + IC9

From **Linear** to **Nonlinear**

- Is projection always good?
  - Not really! Example: Swiss roll toy dataset
  - **Nonlinear** methods should be considered
    - MDS
    - ISOMAP
    - LLE
    - t-SNE



Questions?