18-661 Introduction to Machine Learning

Dimensionality Reduction

Fall 2020

ECE – Carnegie Mellon University

Announcements

- HW 6 is due on 11/19.

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- HW 7 (last homework) will be released tomorrow.

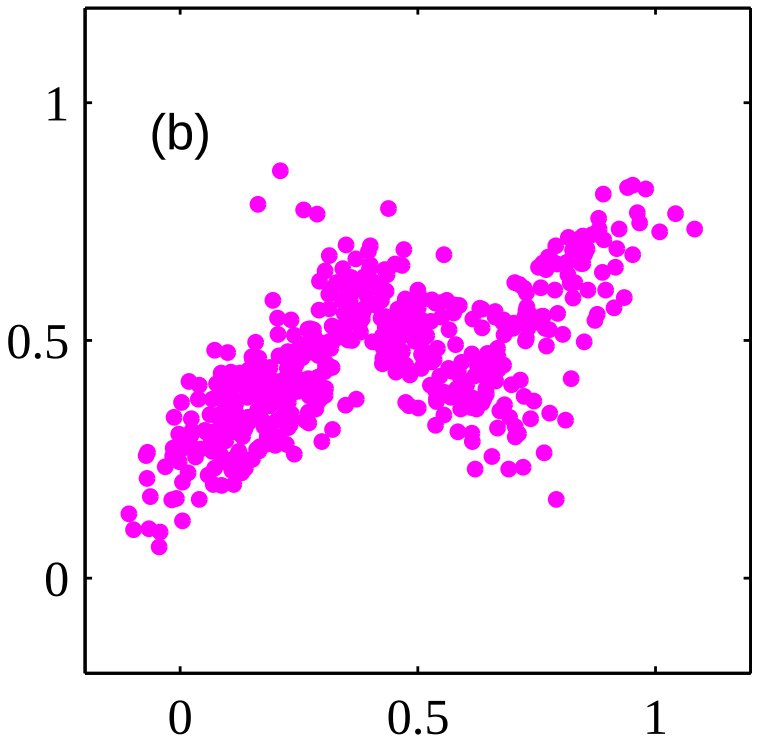
Outline

1. Recap: Gaussian Mixture Models
2. Principal Component Analysis (PCA)
3. Independent Component Analysis (ICA)

Recap: Gaussian Mixture Models

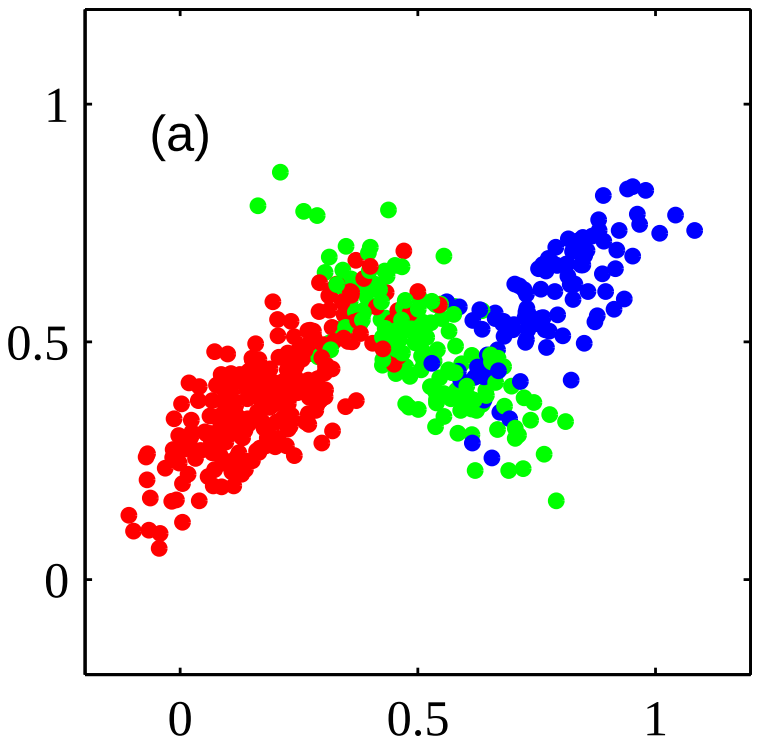
Probabilistic interpretation of clustering?

How can we model $p(\boldsymbol{x})$ to reflect our intuition that points stay close to their cluster centers?



- Points seem to form 3 clusters
- We cannot model $p(\boldsymbol{x})$ with simple and known distributions
- E.g., the data is not a Gaussian b/c we have 3 distinct concentrated regions...

Gaussian mixture models: Intuition



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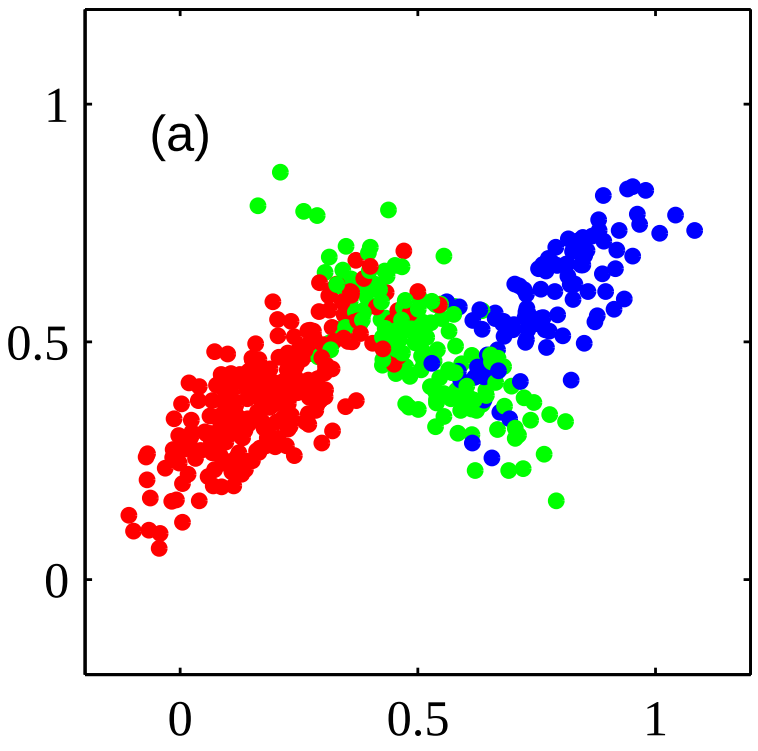

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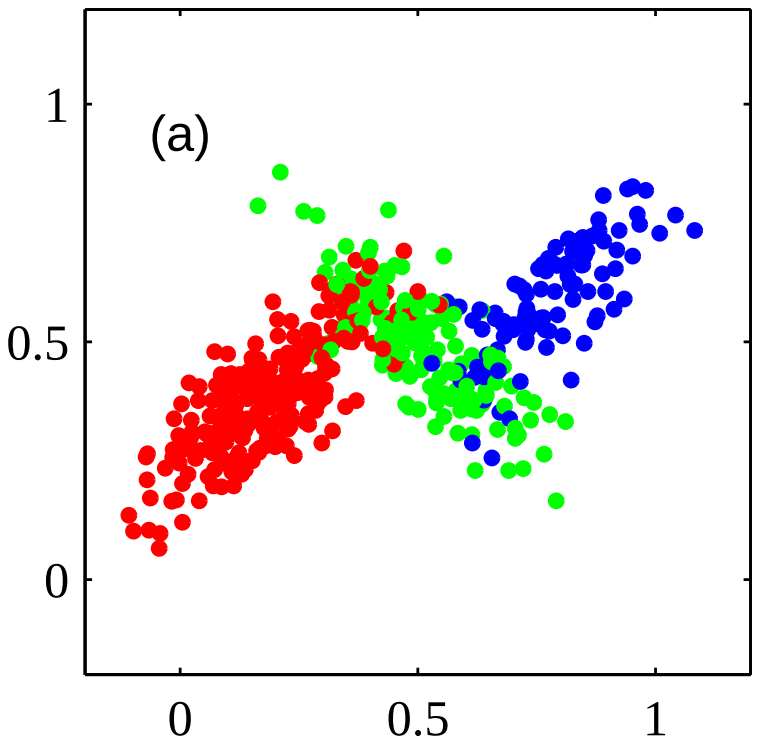

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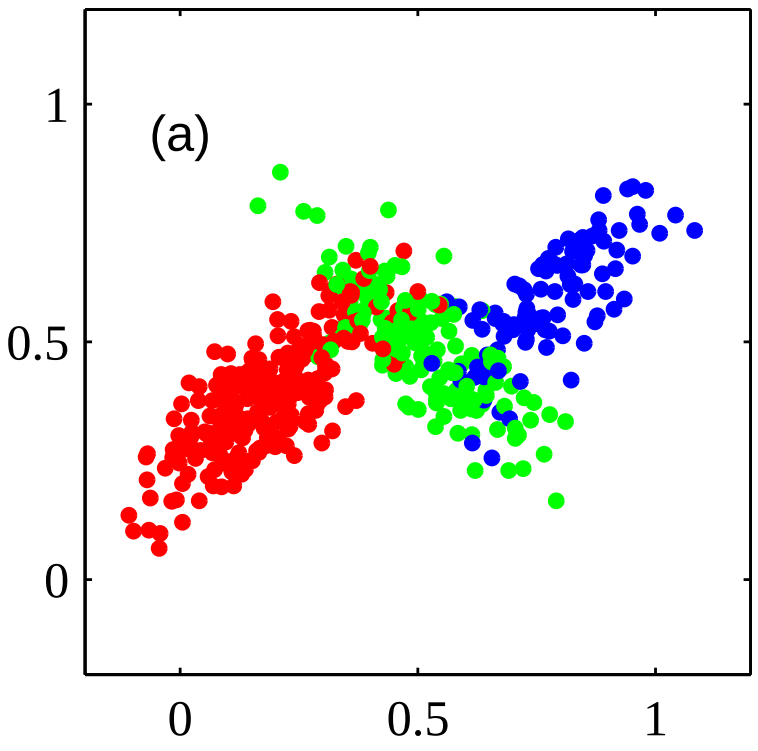

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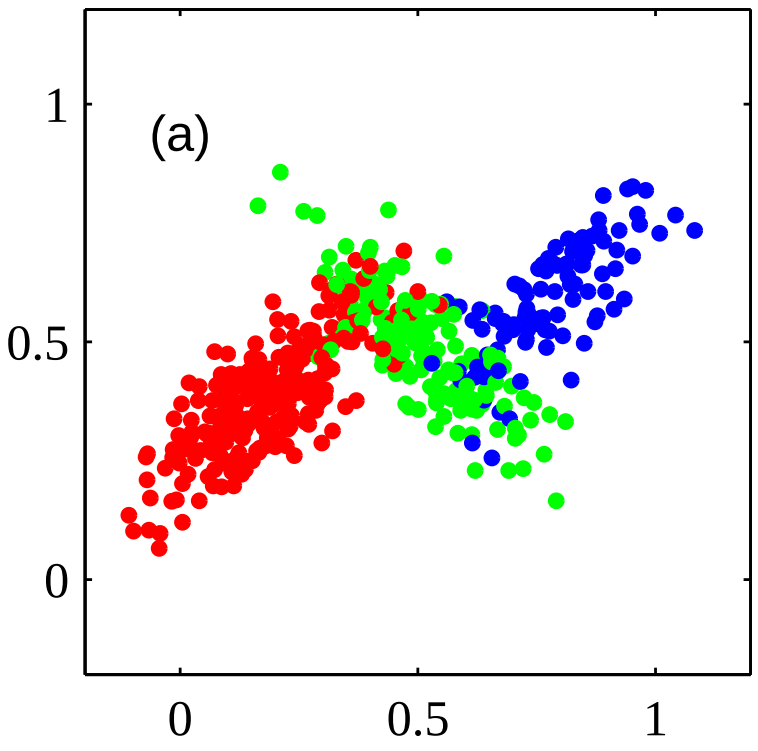

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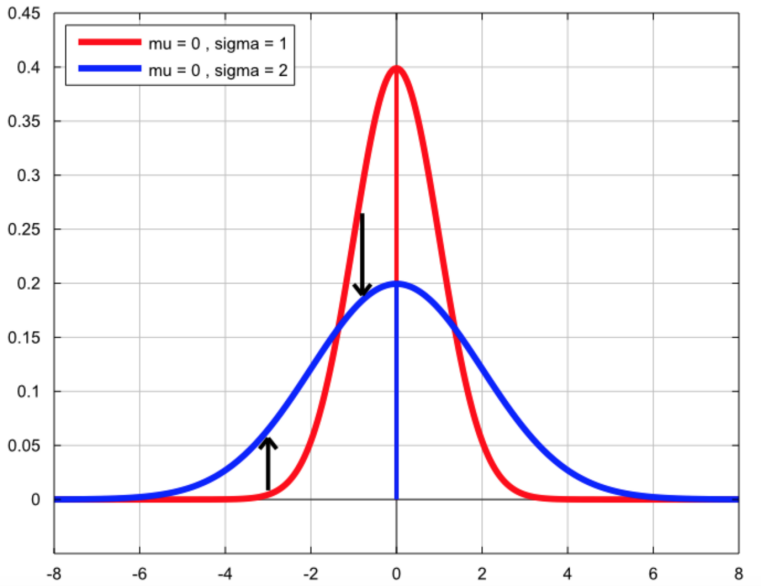
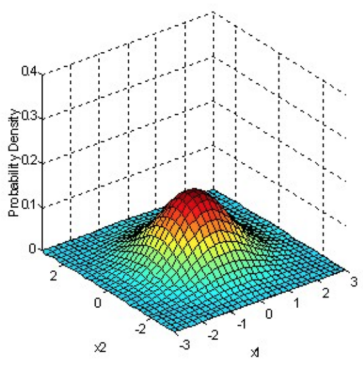
- Can use Gaussians — Gaussian mixture models (GMMs)
- *However*, we don't know *cluster assignments* (label), *parameters* of Gaussians, or *mixture components*!
- Must learn these values from *unlabeled* data $\mathcal{D} = \{\boldsymbol{x}_n\}_{n=1}^N$

Recall: Gaussian (normal) distributions

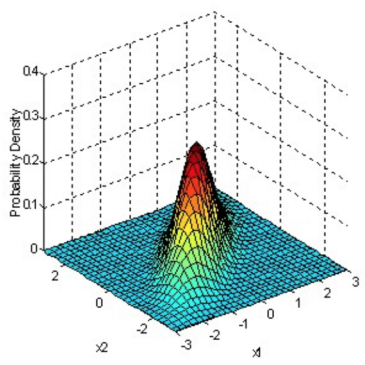
$$\mathbf{x} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \qquad f(\boldsymbol{x}) = \frac{\exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}))}{\sqrt{(2\pi)^n |\boldsymbol{\Sigma}|}}$$



$\boldsymbol{\mu} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \boldsymbol{\Sigma} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$



$\boldsymbol{\mu} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \boldsymbol{\Sigma} = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}$



Gaussian mixture models: Formal definition

GMM has the following density function for $\boldsymbol{x}$

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \omega_k N(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

- K: number of Gaussians — they are called mixture components
- $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}_k$: mean and covariance matrix of k-th component
- ω_k: mixture weights (or priors) represent how much each component contributes to final distribution. They satisfy 2 properties:

$$\forall\ k,\ \omega_k > 0, \quad \text{and} \quad \sum_k \omega_k = 1$$

These properties ensure $p(\boldsymbol{x})$ is in fact a probability density function.

GMM as the marginal distribution of a joint distribution

Consider the following joint distribution

$$p(\boldsymbol{x}, z) = p(z)p(\boldsymbol{x}|z)$$

where z is a discrete random variable taking values between 1 and K.

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Then, the marginal distribution of $\boldsymbol{x}$ is

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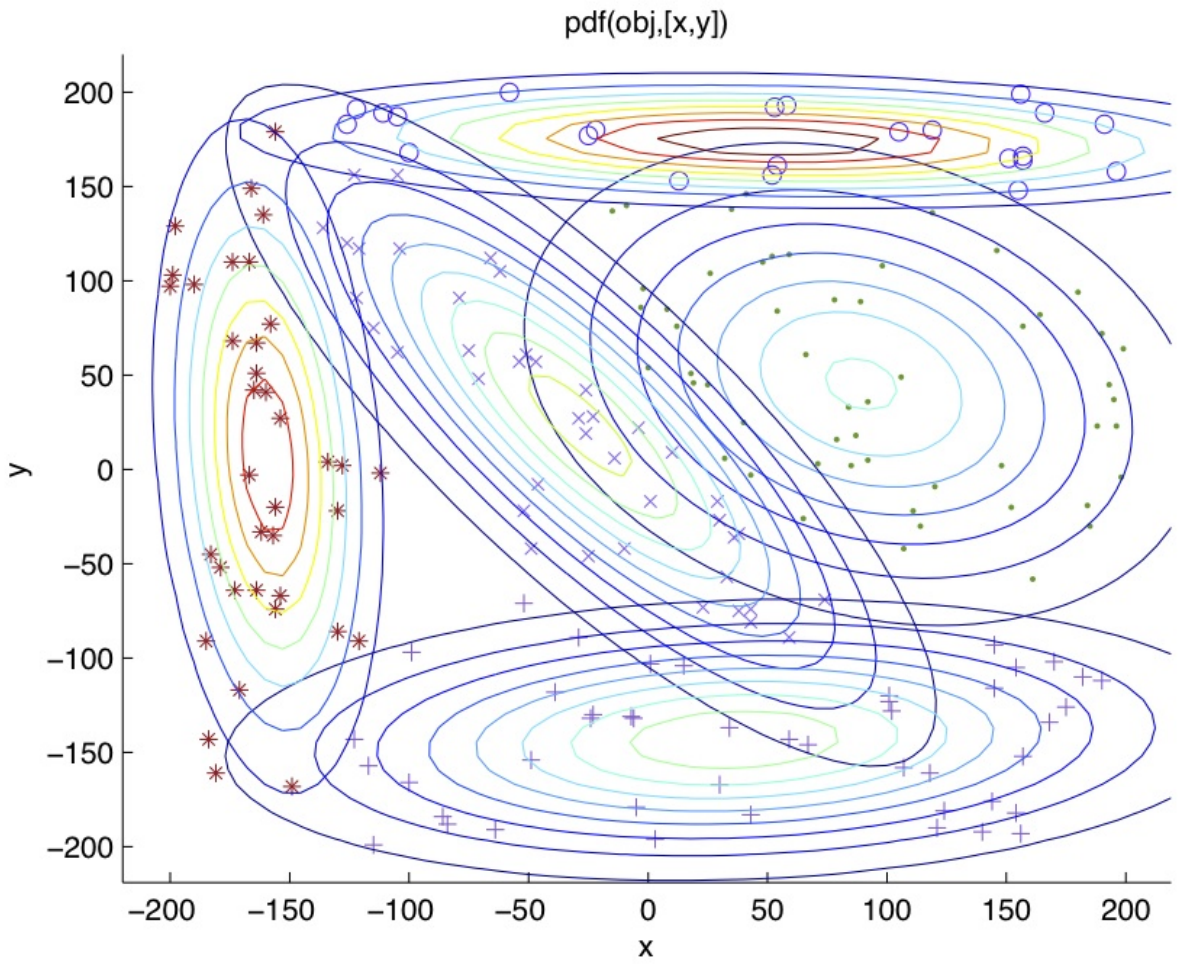
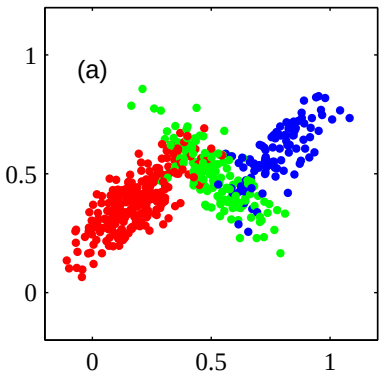
Namely, the Gaussian mixture model

Gaussian mixture model for clustering



GMMs: Example



The conditional distribution between $\boldsymbol{x}$ and z (representing color) are

$$p(\boldsymbol{x}|z = red) = N(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$$
$$p(\boldsymbol{x}|z = blue) = N(\boldsymbol{x}|\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)$$
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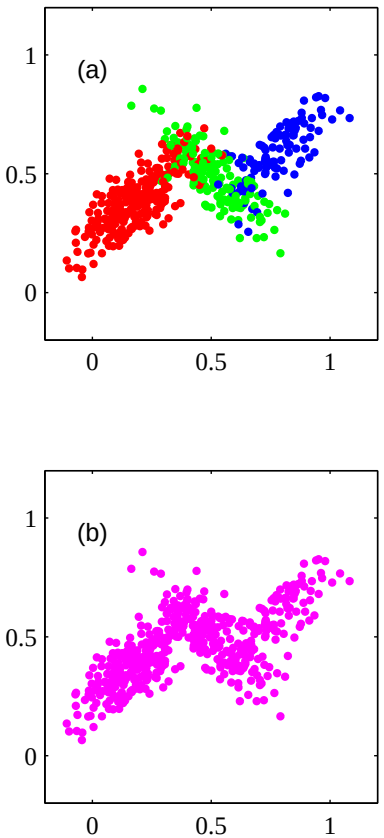

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The marginal distribution is thus

$$\begin{aligned} p(\boldsymbol{x}) = & \, p(z = red)N(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \\ & + p(z = blue)N(\boldsymbol{x}|\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \\ & + p(z = green)N(\boldsymbol{x}|\boldsymbol{\mu}_3, \boldsymbol{\Sigma}_3) \end{aligned}$$

Parameter estimation for Gaussian mixture models

The parameters in GMMs are:

$$\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^{K}$$

Let's first consider the (unrealistic) case where *we know the labels* z.

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Define $\mathcal{D}' = \{\boldsymbol{x}_n, z_n\}_{n=1}^{N}$, $\mathcal{D} = \{\boldsymbol{x}_n\}_{n=1}^{N}$

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Given $\mathcal{D}'$, the maximum likelihood estimation of the $\boldsymbol{\theta}$ is given by

$$\boldsymbol{\theta} = \arg\max \sum_n \log p(\boldsymbol{x}_n, z_n)$$

Parameter estimation for GMMs: Complete data

The complete likelihood is decomposable across the labels:

$$\sum_n \log p(\boldsymbol{x}_n, z_n) = \sum_n \log p(z_n) p(\boldsymbol{x}_n | z_n) = \sum_k \sum_{n:z_n=k} \log p(z_n) p(\boldsymbol{x}_n | z_n)$$

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In the complete setting, the r_{nk} just add to the notation, but later we will 'relax' these variables and allow them to take on fractional values.

Parameter estimation for GMMs: Complete data

The MLE is:

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Parameter estimation for GMMs: Incomplete data

GMM Parameters

$$\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^{K}$$

Incomplete Data

Our data contains observed and unobserved data, and hence is incomplete:

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The objective function is called the *incomplete* log-likelihood.

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&= \frac{N(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \times \omega_k}{\sum_{k'=1}^K N(\boldsymbol{x}_n|\boldsymbol{\mu}_{k'}, \boldsymbol{\Sigma}_{k'}) \times \omega_{k'}}
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M-Step: If we solve for the MLE of $\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$ given soft r_{nk}s, we get the same expressions as before!

$$\omega_k = \frac{\sum_n r_{nk}}{\sum_k \sum_n r_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n r_{nk}} \sum_n r_{nk} \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n r_{nk}} \sum_n r_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top$$

But remember, we're 'cheating' by using $\boldsymbol{\theta}$ to compute r_{nk}!

EM procedure for GMM

Alternate between estimating r_{nk} and estimating parameters θ

- Step 0: Initialize θ with some values (random or otherwise)
- Step 1: E-Step: Set $r_{nk} = p(z_n = k|\boldsymbol{x}_n)$ with the current values of θ using Bayes Rule
- Step 2: M-Step: Update θ using the r_{nk}s from Step 2 using MLE
- Step 3: Go back to Step 1.

At the end convert r_{nk} back to binary by setting the largest r_{nk} for point x_n to 1 and others to 0.

GMMs and K-means

GMMs provide probabilistic interpretation for K-means

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GMMs reduce to K-means under the following assumptions (in which case EM for GMM parameter estimation simplifies to K-means):

- Assume all Gaussians have $\sigma^2 \boldsymbol{I}$ covariance matrices
- Further assume $\sigma \to 0$, so we only need to estimate $\boldsymbol{\mu}_k$, i.e., means

K-means is often called "hard" GMM or GMMs is called "soft" K-means

The posterior r_{nk} provides a probabilistic assignment for $\boldsymbol{x}_n$ to cluster k

GMMs vs. k-means

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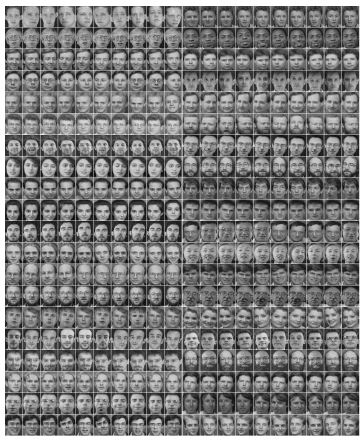
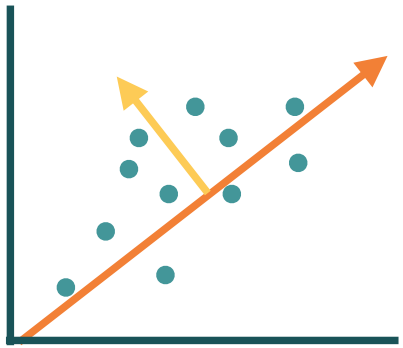
- GMMs can be more accurate, as they model more information (soft clustering, variance), but can be more expensive to compute
- Both methods have a similar set of practical issues (having to select k, the distance, and the initialization)

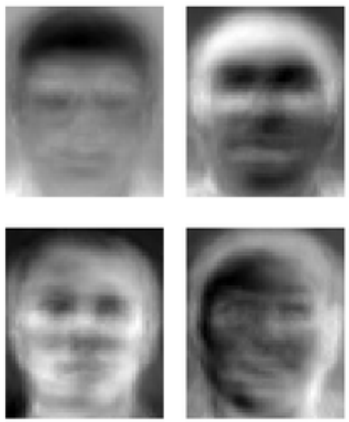
Principal Component Analysis (PCA)

Task 4: Embedding

How to reduce size of dataset?







input: large dataset $\{x\}$ **find**: sources of variation **return**: representation $\{z\}$

Topics: Dimensionality Reduction, PCA

High-dimensional Data

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- But in practice we often measure redundant signals, e.g., US and European shoe sizes
- We also represent data via the method by which it was gathered, e.g., pixel representation of brain imaging data

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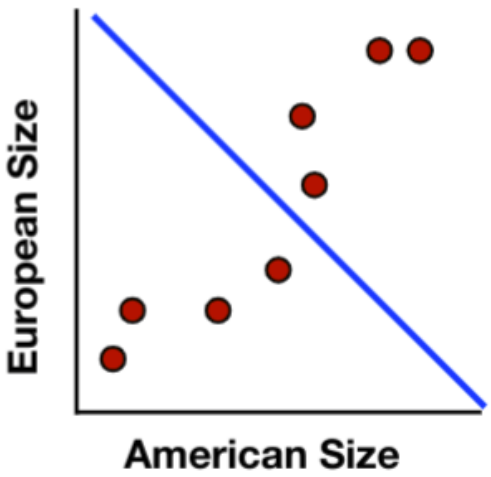
How do we define "better"?

Dimensionality Reduction (Eg. Shoe Size)



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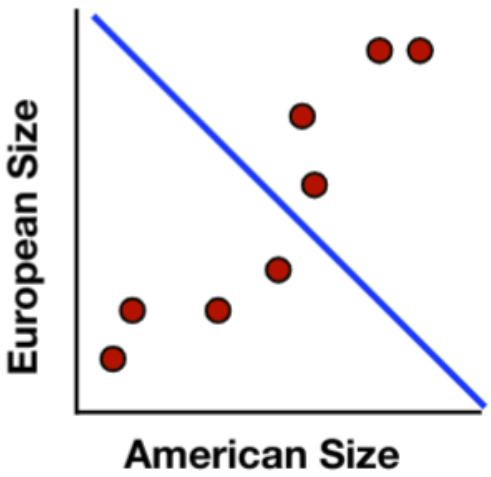

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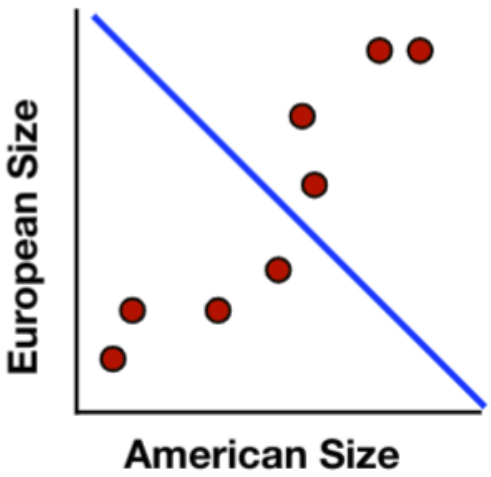

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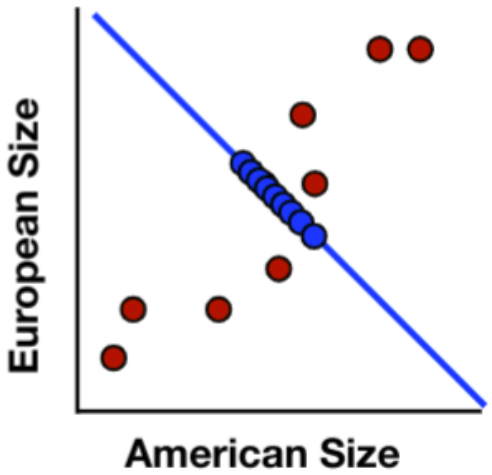

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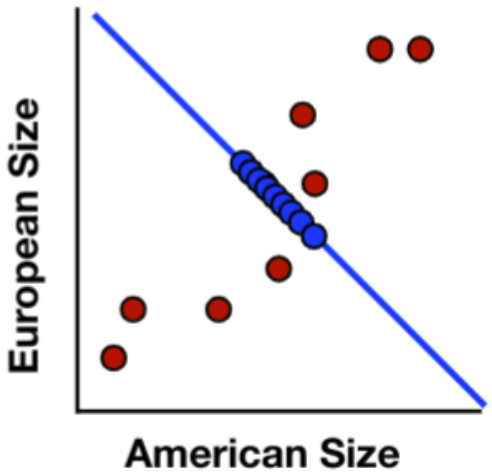

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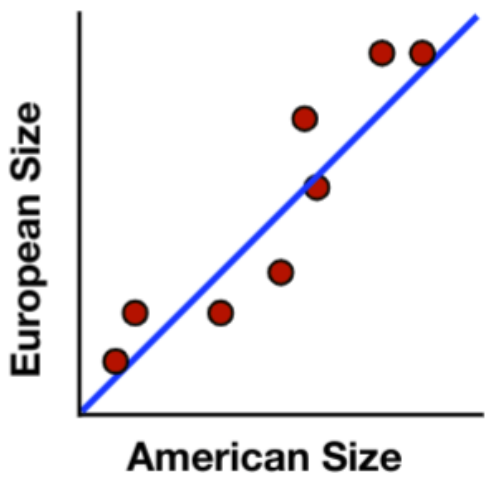

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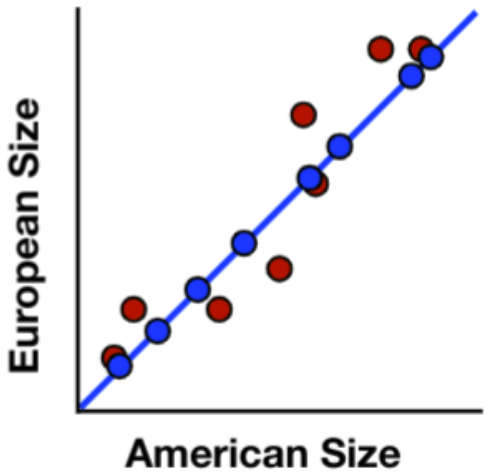

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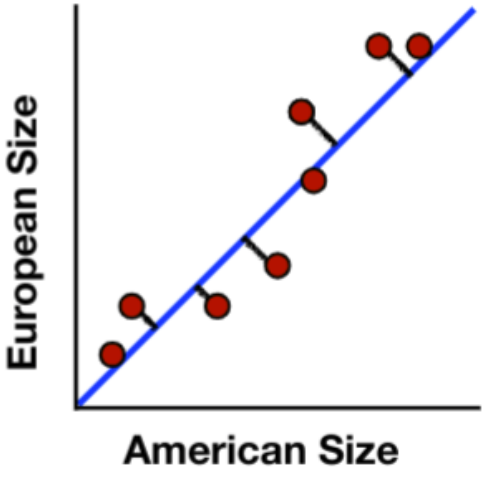
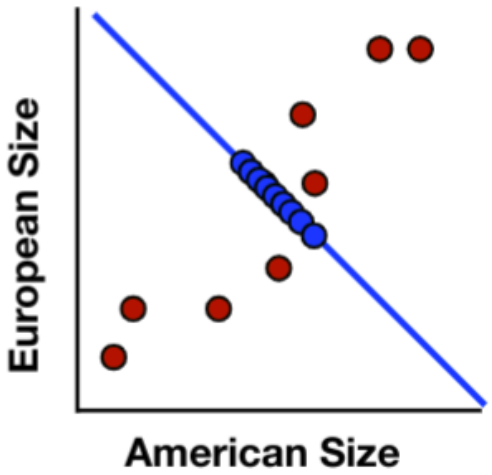
Goal: Minimize Reconstruction Error





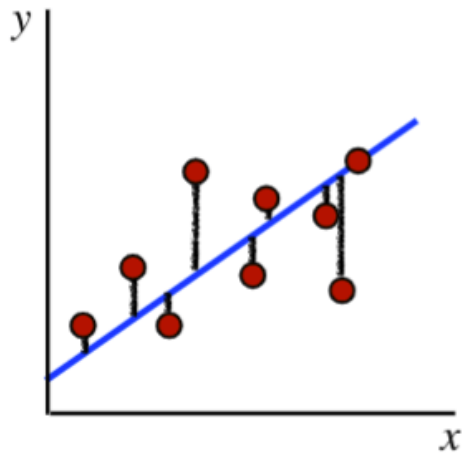
Minimize Euclidean distances between original points and their projections

PCA solution solves this problem!

Goal: Minimize Reconstruction Error

Linear Regression

Predict y from x. Evaluate predictions (represented by blue line) by vertical distances between points and the line.



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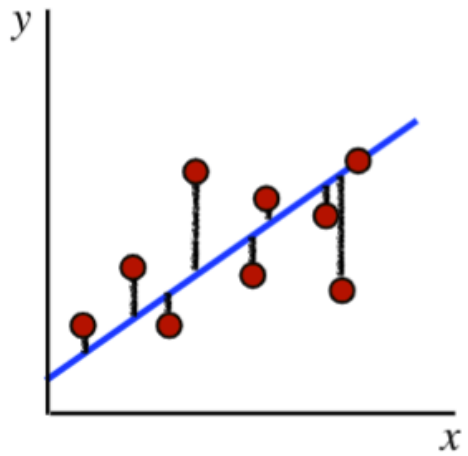
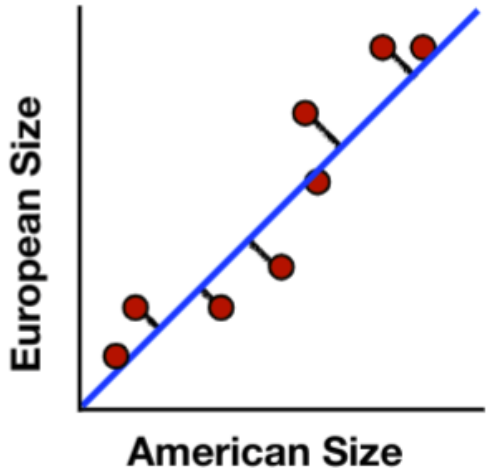


PCA

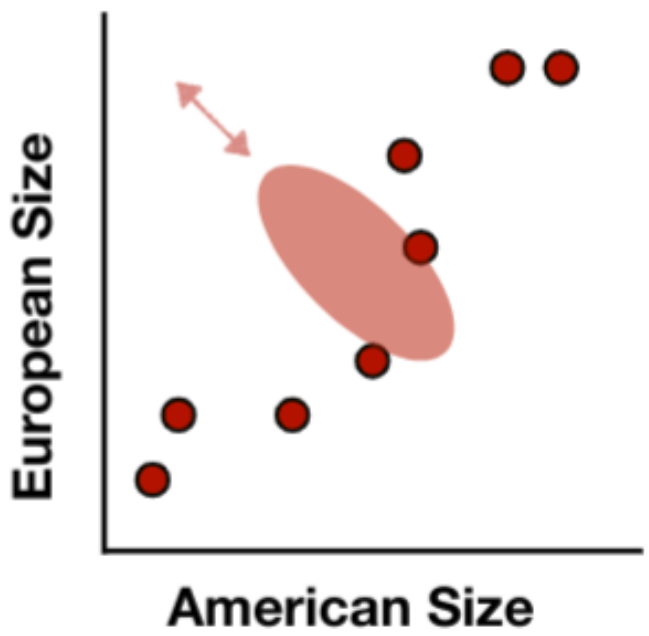
Reconstruct 2D data via 2D data with single degree of freedom. Evaluate reconstructions (represented by blue line) by Euclidean distances.



The distinction is even more apparent with high-dimensional data.

Goal: Maximize Variance and Minimize Feature-Correlation

- To identify patterns we want to study variation across observations
- Can we do "better", i.e., find a compact representation that captures variation?



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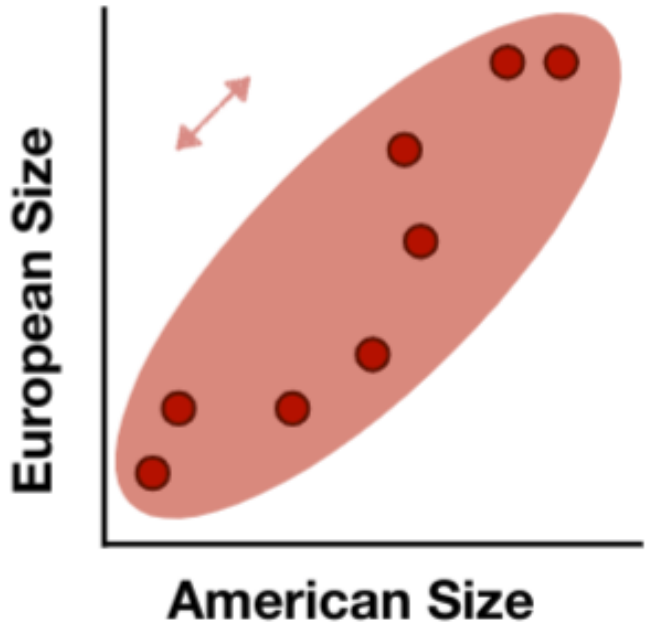

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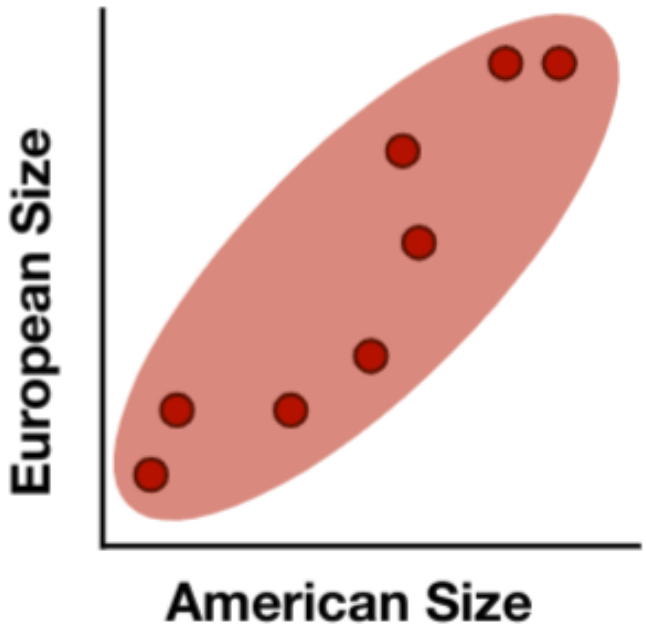
- PCA solution finds directions of maximal variance that are orthogonal to each other



PCA Formulation

- $\mathbf{X}$ is $n \times d$ (raw data, each row is a data point)
- $\mathbf{P}$ is $d \times k$ (columns are k principal components)
- $\mathbf{Z} = \mathbf{XP}$ is $n \times k$ (reduced representation, PCA "scores")
- Linearity assumption ($\mathbf{Z} = \mathbf{XP}$) simplifies problem

$$\begin{bmatrix} \\ \mathbf{Z} \\ \\ \end{bmatrix} = \begin{bmatrix} \\ \mathbf{X} \\ \\ \end{bmatrix} \begin{bmatrix} \\ \mathbf{P} \\ \\ \end{bmatrix}$$

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- Projecting each row of X along the column vectors of $\mathbf{P}$
- How do we design the matrix $\mathbf{P}$?

Step 1: Zero-Center All the Features

Given n training points with d features:

- $\mathbf{X} \in \mathbb{R}^{n \times d}$: matrix storing points
- $\mathbf{x}_j^{(i)}$: j^{th} feature value for i^{th} point
- μ_j: mean of j^{th} feature
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From now on, assume that all columns of X are zero-centered

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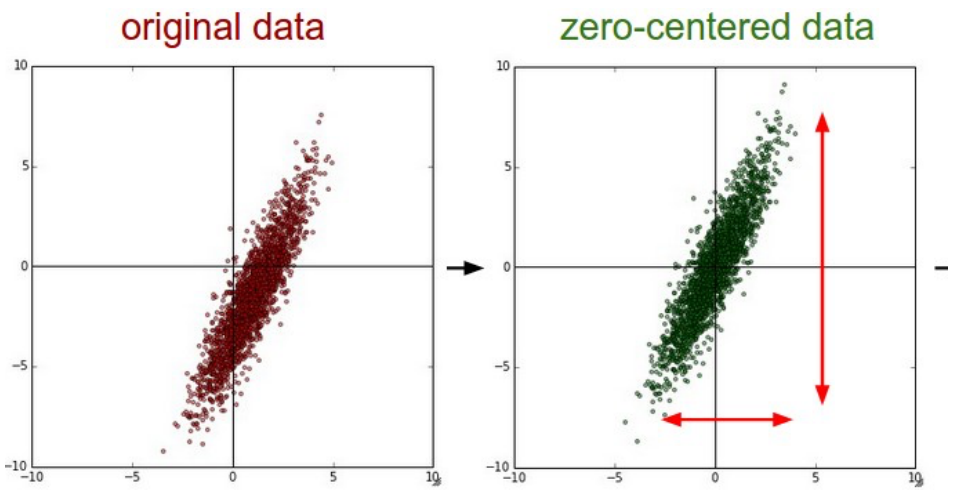

Variance and Co-variance of the Features

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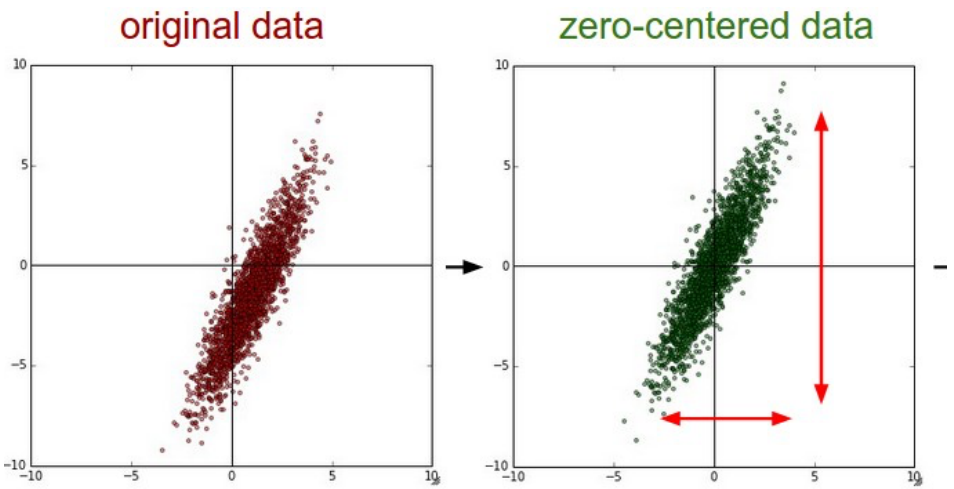

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- What is the covariance matrix in terms of mean-removed samples?

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Idea: Eigen-value decomposition of $\mathbf{C_X}$

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- Eigen-values of $\mathbf{C_X}$ are ordered $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d$
- $\mathbf{Q}$ is an matrix of d orthonormal eigen-vectors $\mathbf{v}_i$ of $\mathbf{C_X}$

Recall: Orthogonal and Orthonormal Vectors

Orthogonal vectors are **perpendicular** to each other

- Equivalently, their dot product equals zero
- $\mathbf{a}^T\mathbf{b} = 0$ and $\mathbf{d}^T\mathbf{b} = 0$, but $\mathbf{c}$ isn't orthogonal to others

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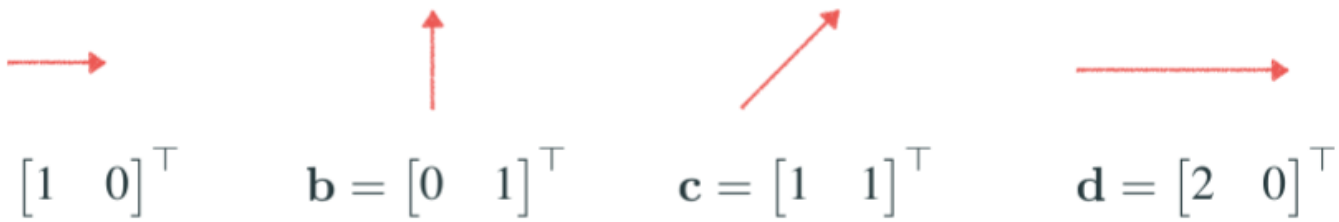

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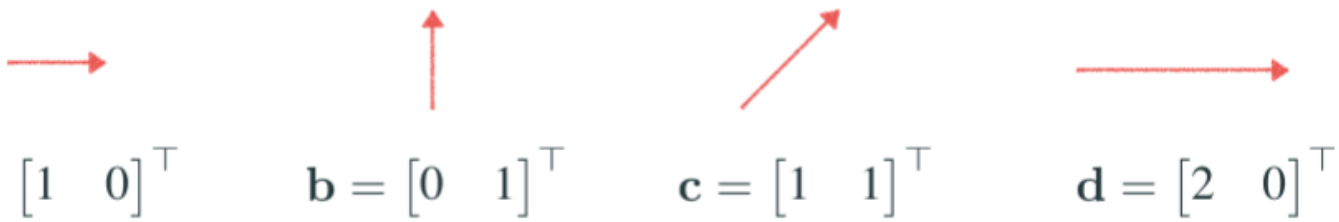

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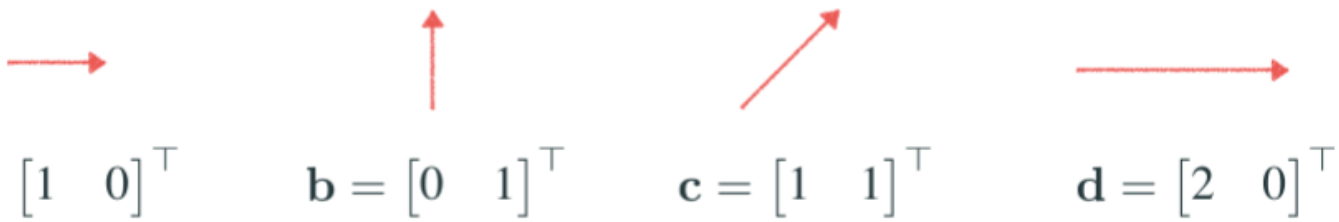

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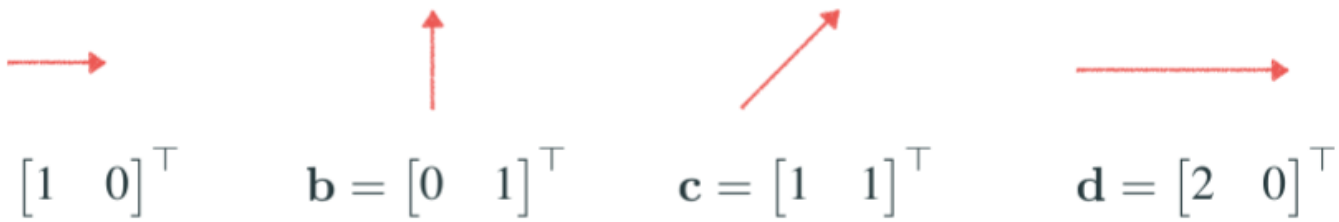

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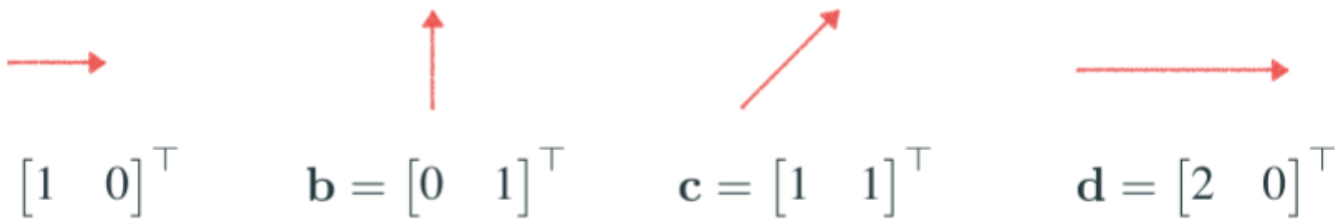

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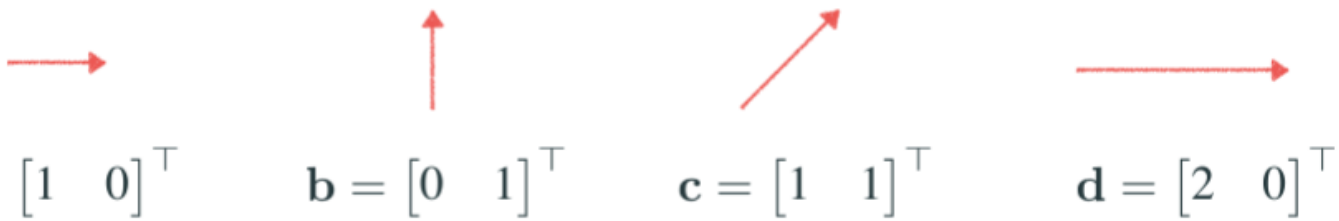

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If $\mathbf{Q}$ is an orthonormal matrix, then $\mathbf{Q}^T = \mathbf{Q}^{-1}$

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- The covariance matrix $\mathbf{C_X}$ is symmetric, positive semi-definite and it can be decomposed as follows

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- Capture the k directions of maximum variance.

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Suppose the covariance of X is

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Thus $\mathbf{P} = [\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}]^T$

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Can choose k such that we retain some fraction of the variance, eg. 95%

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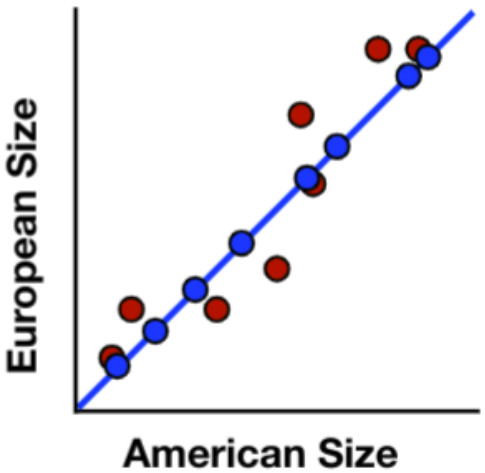

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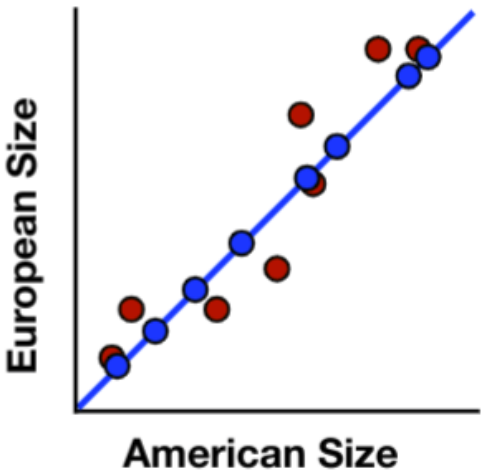

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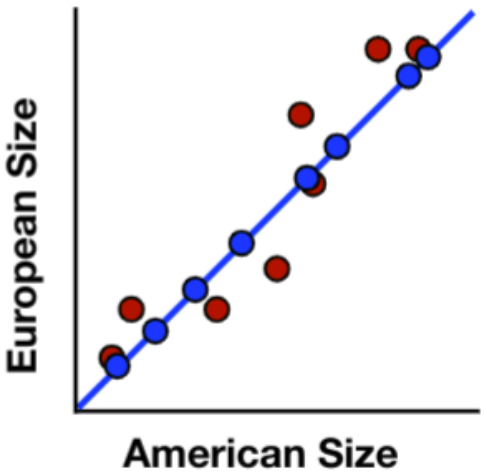

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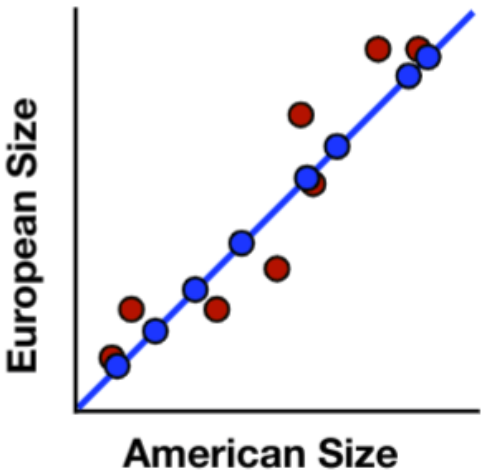

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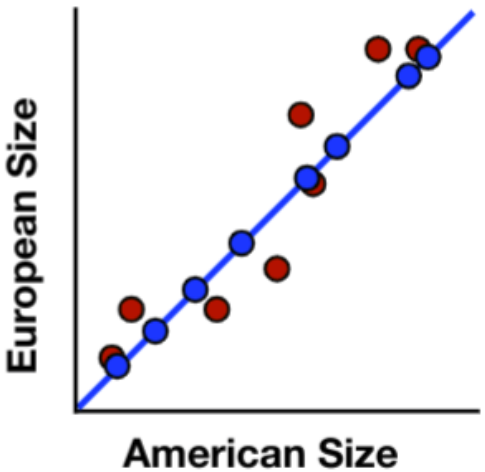

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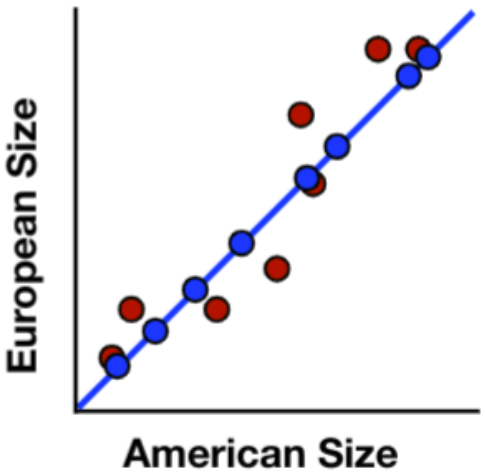
4. Return $\mathbf{v}_1$



Why does Eigen-value Decomposition Maximize Variance?

Consider PCA with $k = 1$

- $\mathbf{z} = \mathbf{X}\mathbf{p}$ is $n \times 1$
- $\mathbf{p}$ is $d \times 1$ (first principal component)

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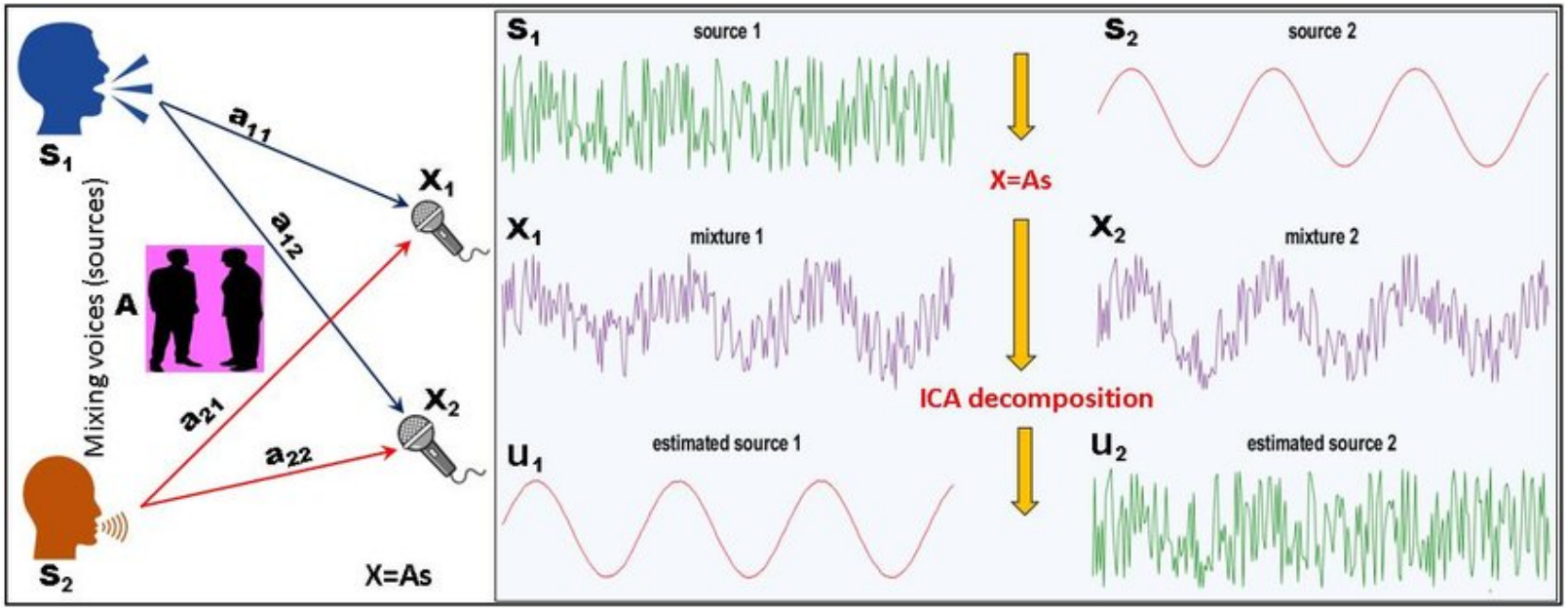
- Goal: $\max_{\mathbf{p}} \sigma_{\mathbf{z}}^2$ where $||\mathbf{p}||_2 = 1$
- The top eigenvector $\mathbf{v}_1$ is known to achieve the optimum for any symmetric matrix $\mathbf{C}_{\mathbf{X}}$

Independent Component Analysis (ICA)

The Cocktail Party Problem



- PCA tries to find an orthogonal representation of the mixed data.

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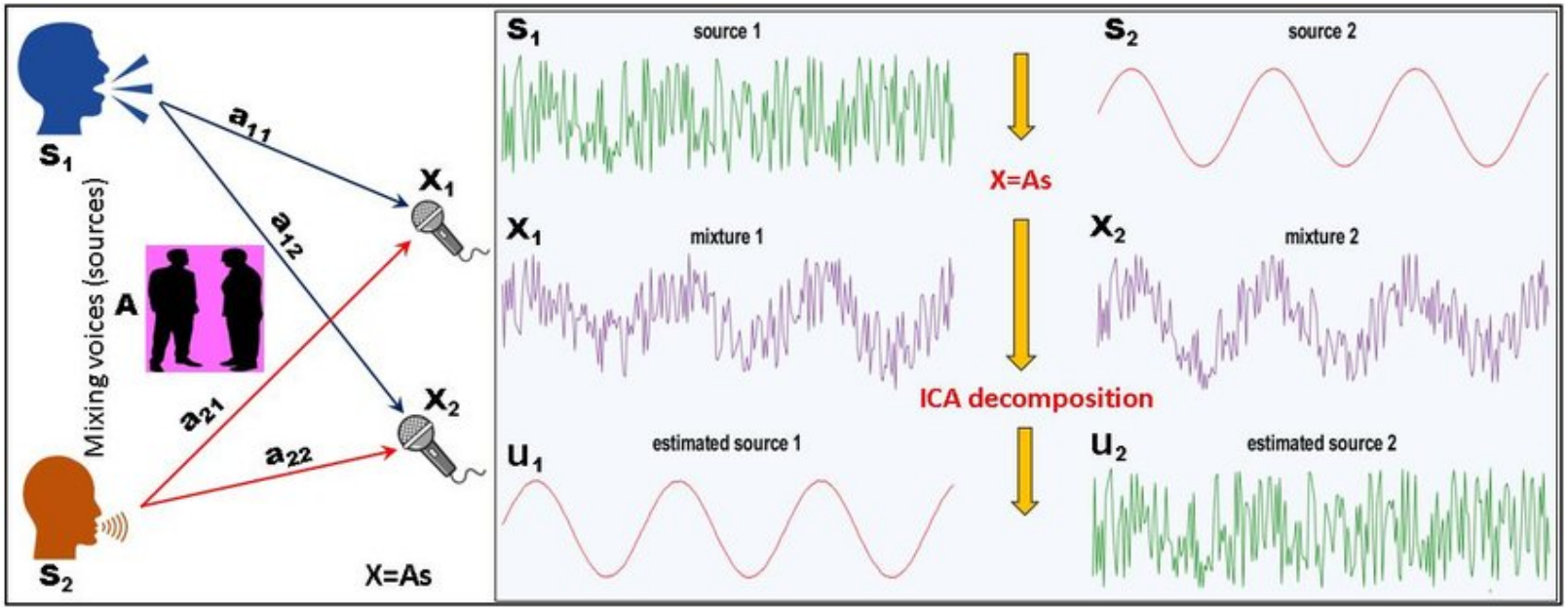
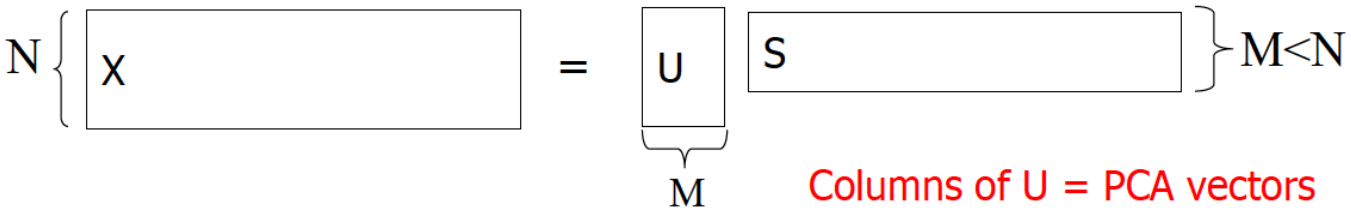


- PCA tries to find an orthogonal representation of the mixed data.
- ICA tries to disentangle the data sources.

How Does ICA Work?

Both ICA and PCA linearly transform the original data with matrix factorization.

PCA compresses data with low-rank matrix factorization



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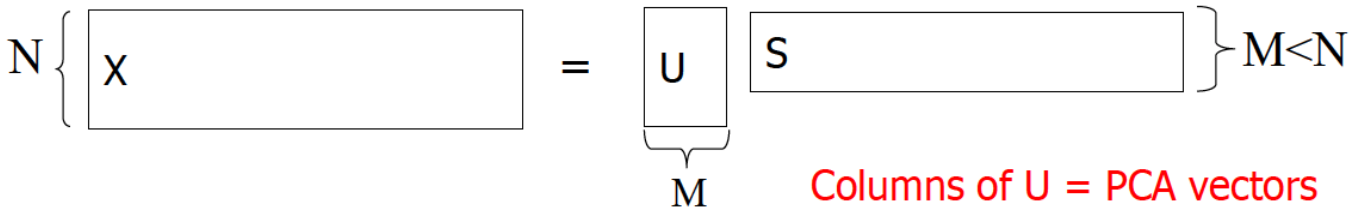
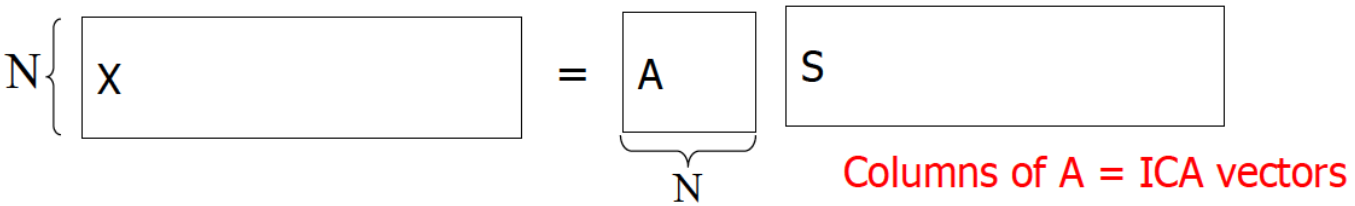


ICA removes dependencies between data with full-rank matrix factorization



Comparing PCA and ICA

Let $\mathbf{S}$ denote our original data. It can be transformed to a new set of features $\mathbf{X}$:

$$\text{PCA} : \mathbf{X} \approx \mathbf{US},\ \mathbf{U}^T\mathbf{U} = \mathbf{I}$$

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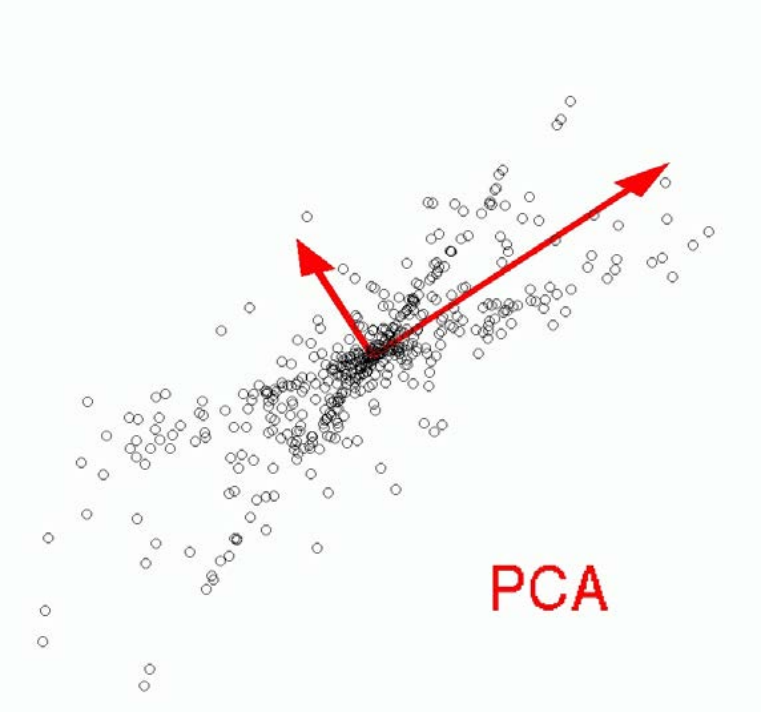
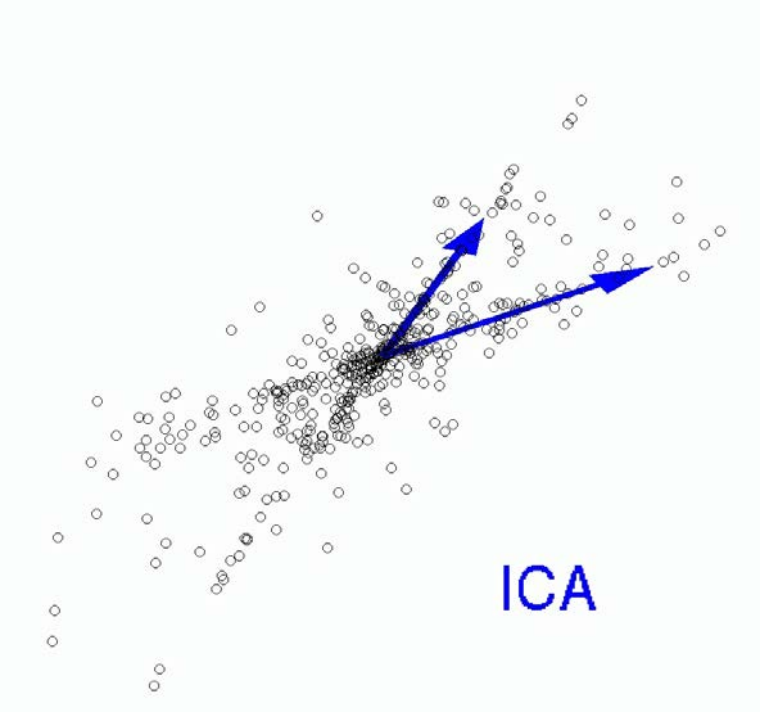
- PCA allows you to rank the importance of the new features. ICA does not.

ICA vs. PCA





Applications of ICA

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  - Medical signal processing: fMRI, ECG, EEG
  - Modeling of the visual cortex, hippocampus
  - Time series analysis
  - Financial applications

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