Data Analysis and Information Exploitation (ADEI)

Bachelor Degree in Informatics Engineering
Information System Track

FIB-ADEI – 6 ECTS - Course 2021-22

BarcelonaTech - UPC

UNIT 3. KNOWLEGDE DISCOVERY

Lecturer in charge : Josep Franquet (DEIO)

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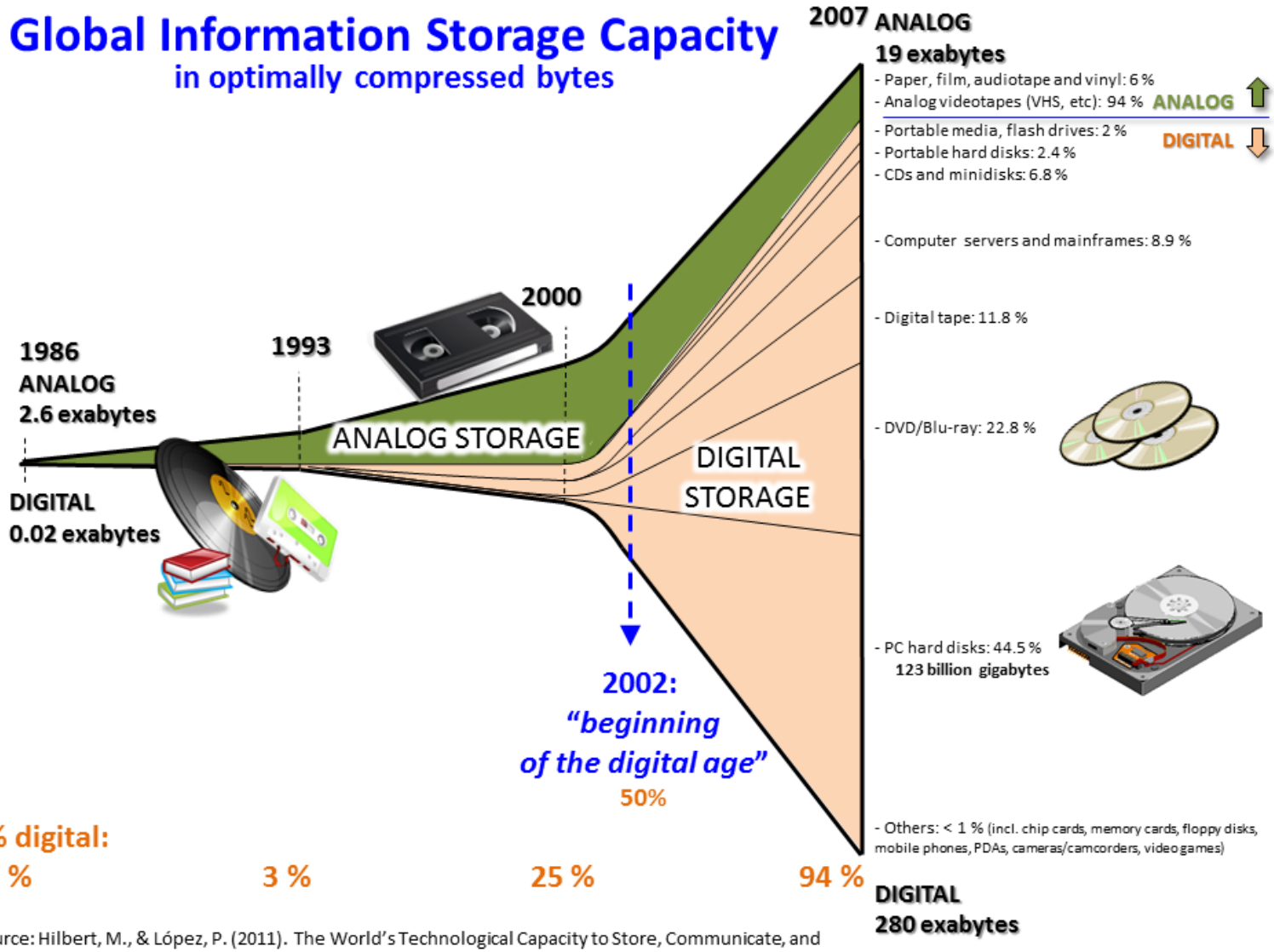
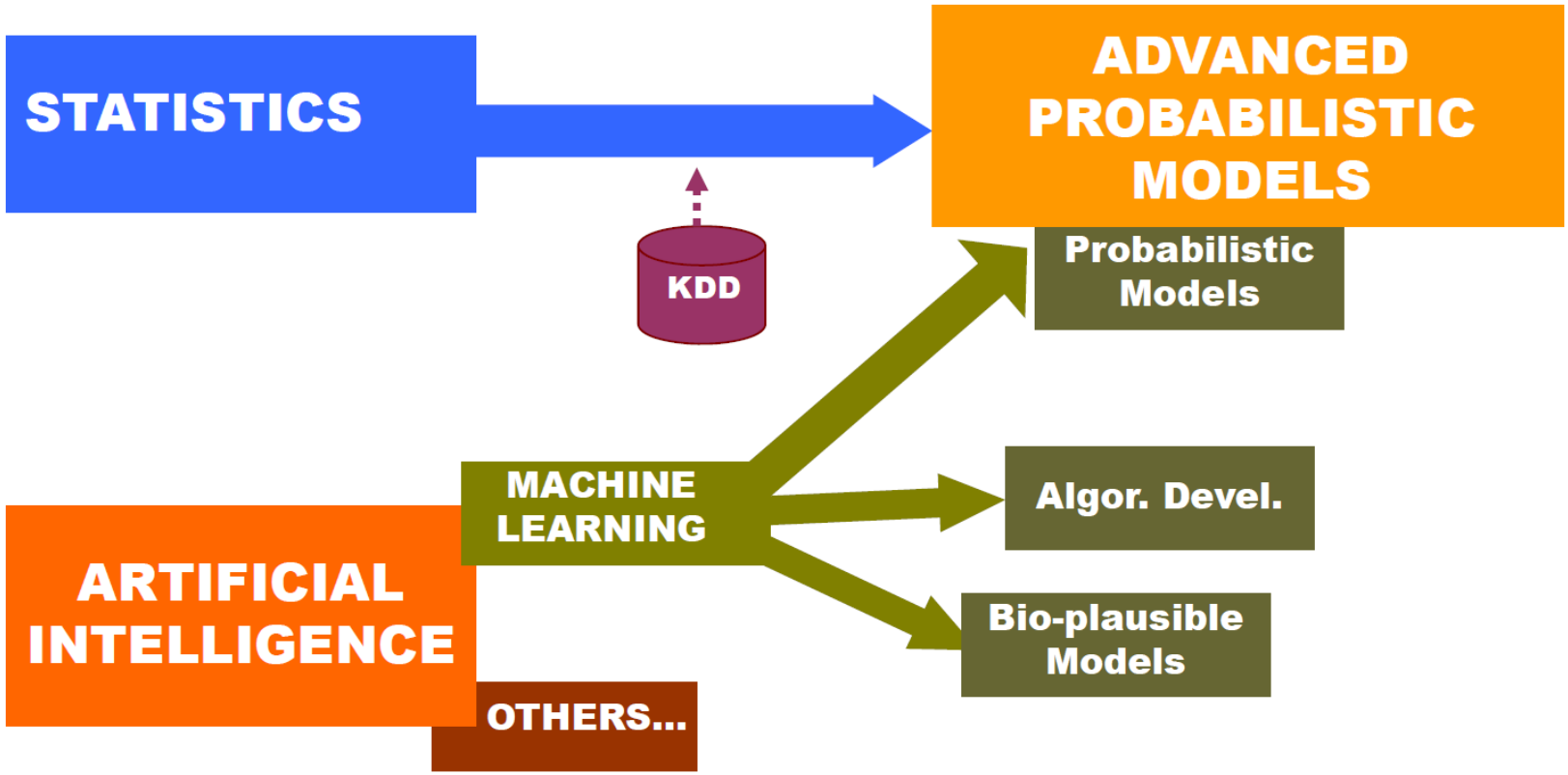
Data growth rate



Source: Hilbert, M., & López, P. (2011). The World's Technological Capacity to Store, Communicate, and Compute Information. *Science*, 332(6025), 60 –65. http://www.martinhilbert.net/WorldInfoCapacity.html

What's DATA MINING?: A historicist view point



Source: Lluis Belanche – SOCO -UPC

Big Data vs Survey based data

Big Data characteristics:

Volume

The quantity of generated and stored data. The size of the data determines the value and potential insight- and whether it can actually be considered big data or not.

Variety

The type and nature of the data. This helps people who analyze it to effectively use the resulting insight.

Velocity

In this context, the speed at which the data is generated and processed to meet the demands and challenges that lie in the path of growth and development.

Variability

Inconsistency of the data set can hamper processes to handle and manage it.

Veracity

The quality of captured data can vary greatly, affecting accurate analysis.

Purpose collected data (Surveys) is a fundamental issue

Surveys Overview

- Today the word "survey“ is used most often to describe a method of gathering information from a sample of individuals. This "sample" is usually just a fraction of the population being studied.
- Not only do surveys have a wide variety of purposes, they also can be conducted in many ways
  - including over the telephone, by mail, or in person.
  - Nonetheless, all surveys do have certain characteristics in common.
- Unlike a census, where all members of the population are studied, surveys gather information from only a portion of a population of interest
  - the size of the sample depending on the purpose of the study.

What is a Survey

- In a good survey, the sample is not selected haphazardly or only from persons who volunteer to participate.
- It is scientifically chosen so that each person in the population will have a measurable chance of selection.
  - This way, the results can be reliably projected from the sample to the larger population.
- Information is collected by means of standardized procedures so that every individual is asked the same questions in more or less the same way.
  - The use of questionnaires is strongly recommended.
  - All of the survey's results should be presented in completely anonymous summaries, such as statistical tables and charts.

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TOPIC 3. KNOWLEGDE DISCOVERY

3-1. Component And Factor Analysis

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Data Collection in Traffic and Transport

- Data from network sensors collecting traffic data from a rich variety of detection stations and sensor types, based on traditional or advanced ICT sources, as for example:
  - Traffic Detection Stations: inductive loop detectors, radars, magnetometers…
  - Antennas to capture Bluetooth or Wi-Fi equipped devices
  - CCTV image processing (e.g. License Plate Recognition, emulation of Traffic Detection Stations)
  - Capture of digital footprints, e.g. TAGs
  - GPS tracking of fleets
  - *Call Detail Records from mobile phones*
- Socioeconomic data from authorities (CAD support currently)
- Data collected from surveys

Common Data in Computer Science

- Facial Recognition
- Facial Expression Recognition
- Data Comprension
- Dimension Reduction

Challenge: Facial Recognition

- Want to identify specific person, based on facial image
- Robust to glasses, lighting,…

  ⇒ Can't just use the given 256 x 256 pixels

Why Factor or Component Analysis?

- We study phenomena that can not be directly observed
  - ego, personality, intelligence in psychology
  - Underlying factors that govern the observed data

- We want to identify and operate with underlying latent factors rather than the observed data
  - E.g. topics in news articles
  - Transcription factors in genomics

- We want to discover and exploit hidden relationships
  - “beautiful car” and “gorgeous automobile” are closely related
  - So are “driver” and “automobile”
  - But does your search engine know this?
  - Reduces noise and error in results

Why Factor or Component Analysis?

- Discover a new set of factors/dimensions/axes against which to represent, describe or evaluate the data
  - For more effective reasoning, insights, or better visualization
  - Reduce noise in the data
  - Typically a smaller set of factors: dimension reduction
  - Better representation of data without losing much information
  - Can build more effective data analyses on the reduced-dimensional space: classification, clustering, pattern recognition
- Factors are combinations of observed variables
  - May be more effective bases for insights, even if physical meaning is obscure
  - Observed data are described in terms of these factors rather than in terms of original variables/dimensions

Basic Concept

- Areas of variance in data are where items can be best discriminated and key underlying phenomena observed
  - Areas of greatest “signal” in the data
- If two items or dimensions are highly correlated or dependent
  - They are likely to represent highly related phenomena
  - If they tell us about the same underlying variance in the data, combining them to form a single measure is reasonable
    - Parsimony
    - Reduction in Error
- So the goal is to combine related variables, and focus on uncorrelated or independent ones, especially those along which the observations have high variance
- Obtaining a smaller set of variables that explain most of the variance in the original data, in more compact and insightful form
  - Dimension reduction technique

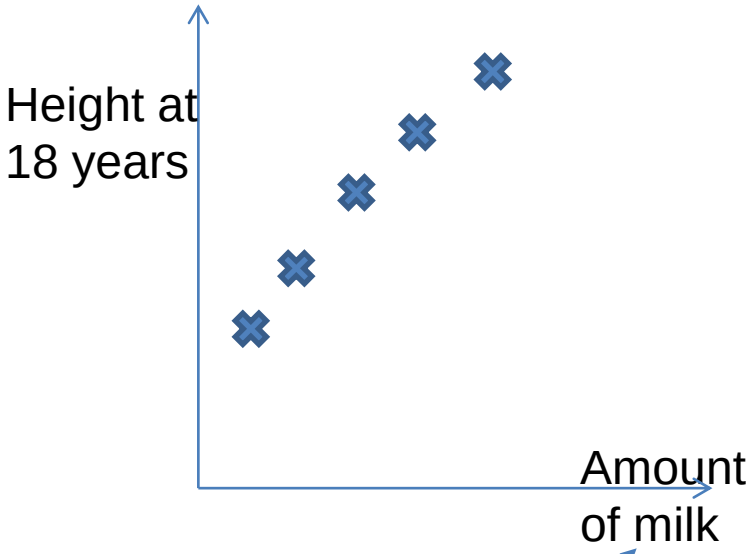
Basic Concept

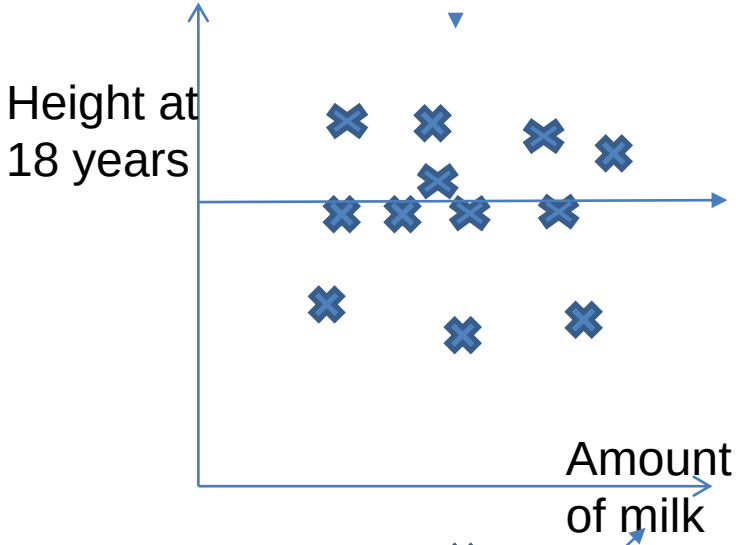
- What if the dependences and correlations are not so strong or direct?
- And suppose you have 3 variables, or 4, or 5, or 10000?
- Look for the phenomena underlying the observed covariance/co-dependence in a set of variables
  - Once again, phenomena that are uncorrelated or independent, and especially those along which the data show high variance
- These phenomena are called “factors” or “principal components” or “independent components,” depending on the methods used
  - Factor analysis: based on variance/covariance/correlation
  - Independent Component Analysis: based on independence

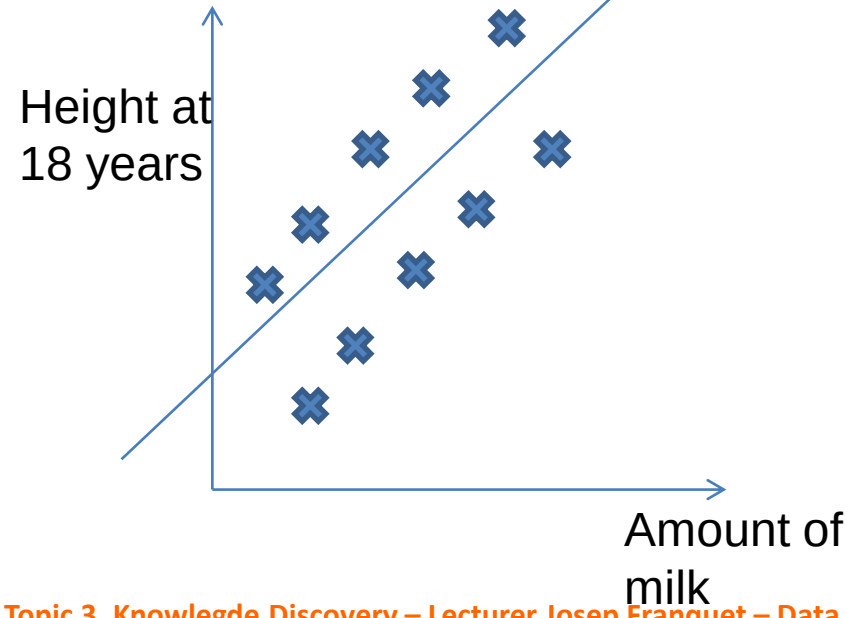
PCA Applications

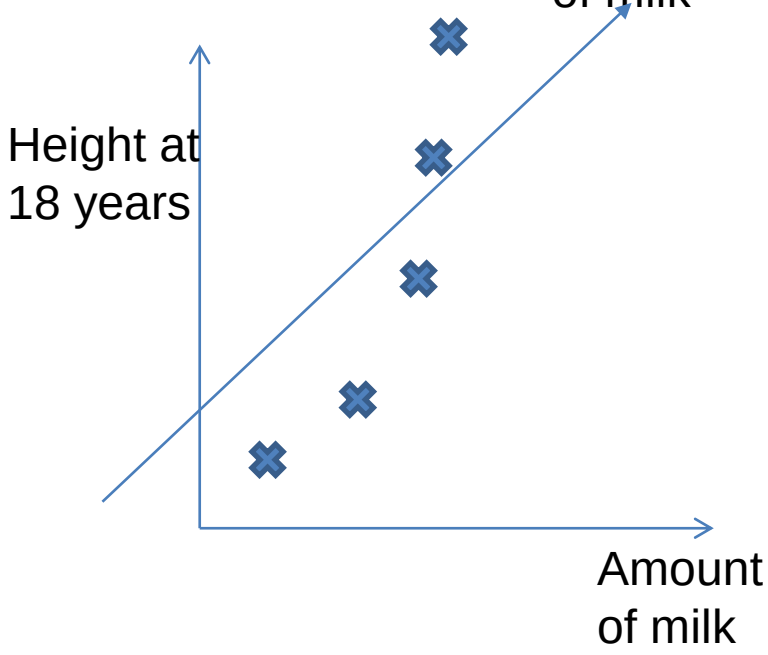
- Data Visualization
- Data Compression
- Noise Reduction
- Data Classification
- Trend Analysis
- Factor Analysis

What does structure mean? Example in two variables









Data Visualization

Example:

- Given 53 blood and urine samples (features) from 65 people.

- How can we visualize the measurements?

Data Visualization

- Matrix format (65x53)

Instances

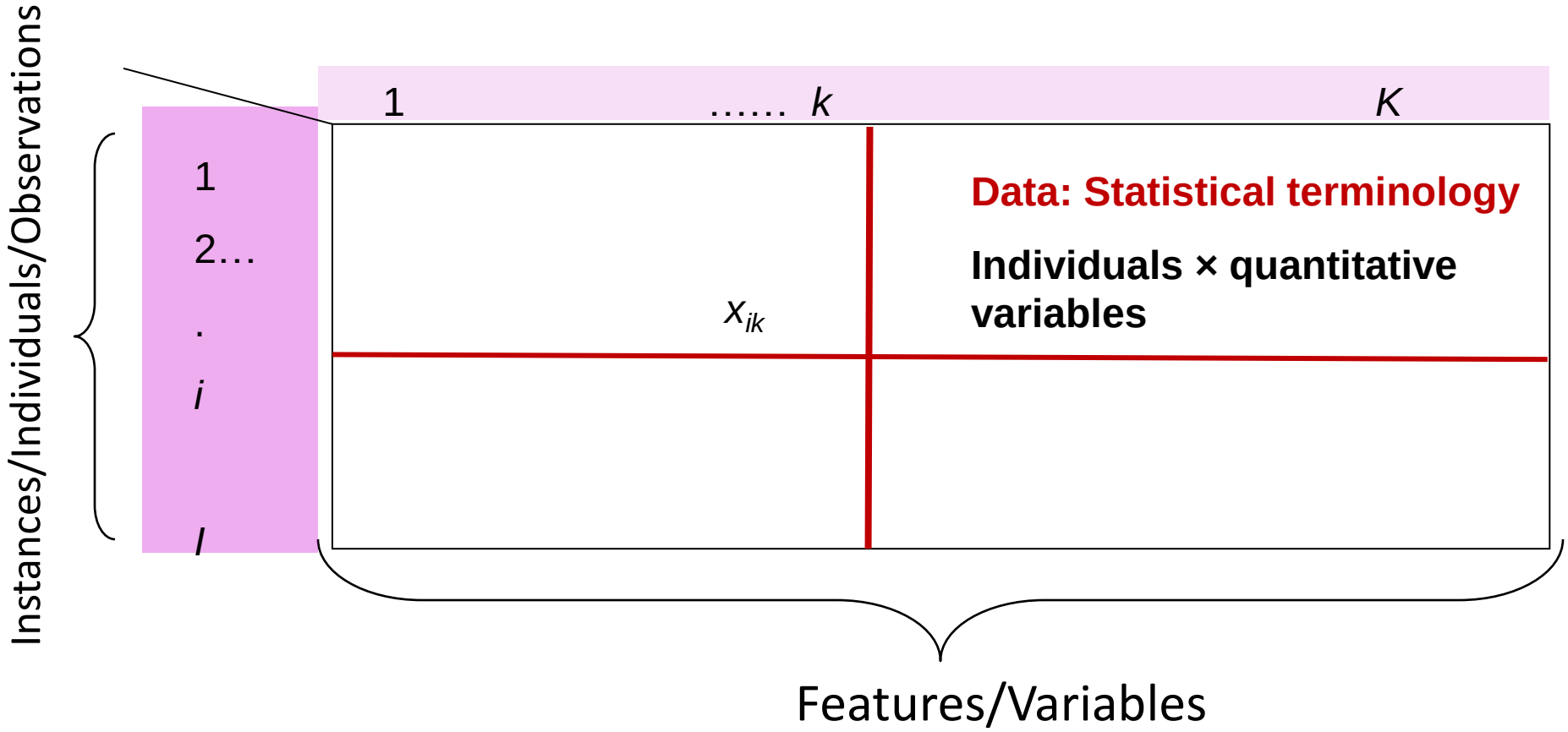
	H-WBC	H-RBC	H-Hgb	H-Hct	H-MCV	H-MCH	H-MCHC
A1	8.0000	4.8200	14.1000	41.0000	85.0000	29.0000	34.0000
A2	7.3000	5.0200	14.7000	43.0000	86.0000	29.0000	34.0000
A3	4.3000	4.4800	14.1000	41.0000	91.0000	32.0000	35.0000
A4	7.5000	4.4700	14.9000	45.0000	101.0000	33.0000	33.0000
A5	7.3000	5.5200	15.4000	46.0000	84.0000	28.0000	33.0000
A6	6.9000	4.8600	16.0000	47.0000	97.0000	33.0000	34.0000
A7	7.8000	4.6800	14.7000	43.0000	92.0000	31.0000	34.0000
A8	8.6000	4.8200	15.8000	42.0000	88.0000	33.0000	37.0000
A9	5.1000	4.7100	14.0000	43.0000	92.0000	30.0000	32.0000

Features

Difficult to see the correlations between the features...

Data Visualization

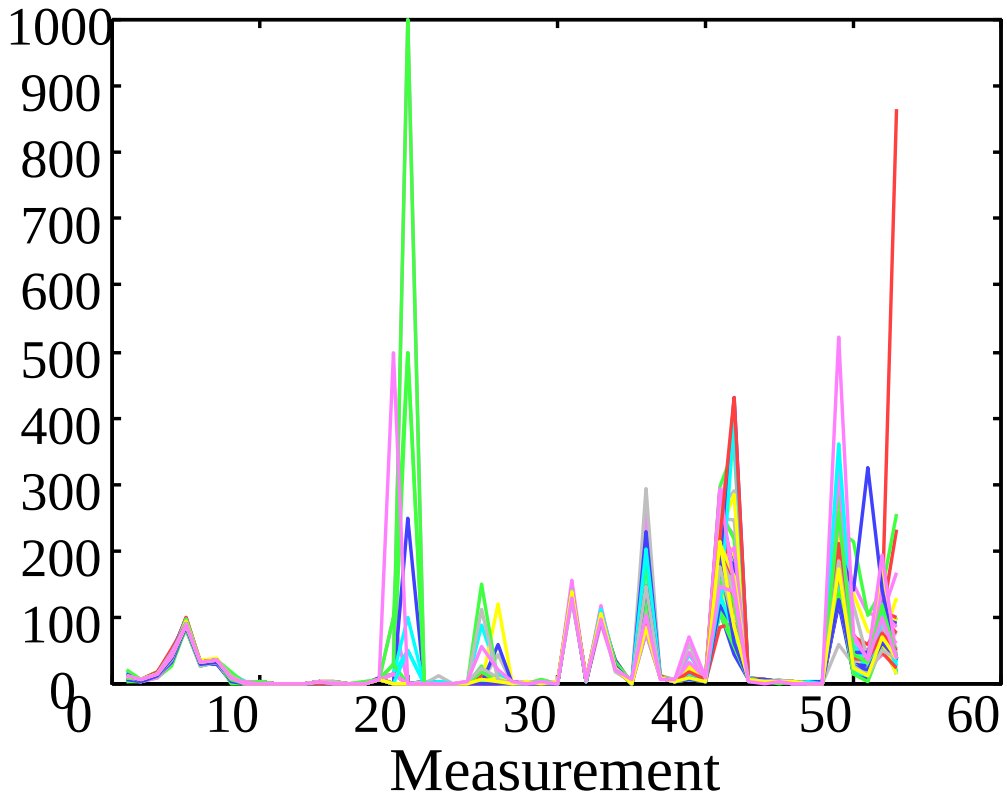
- Matrix format (65x53) :Duality of the table



Difficult to see the correlations between the features...

Data Visualization

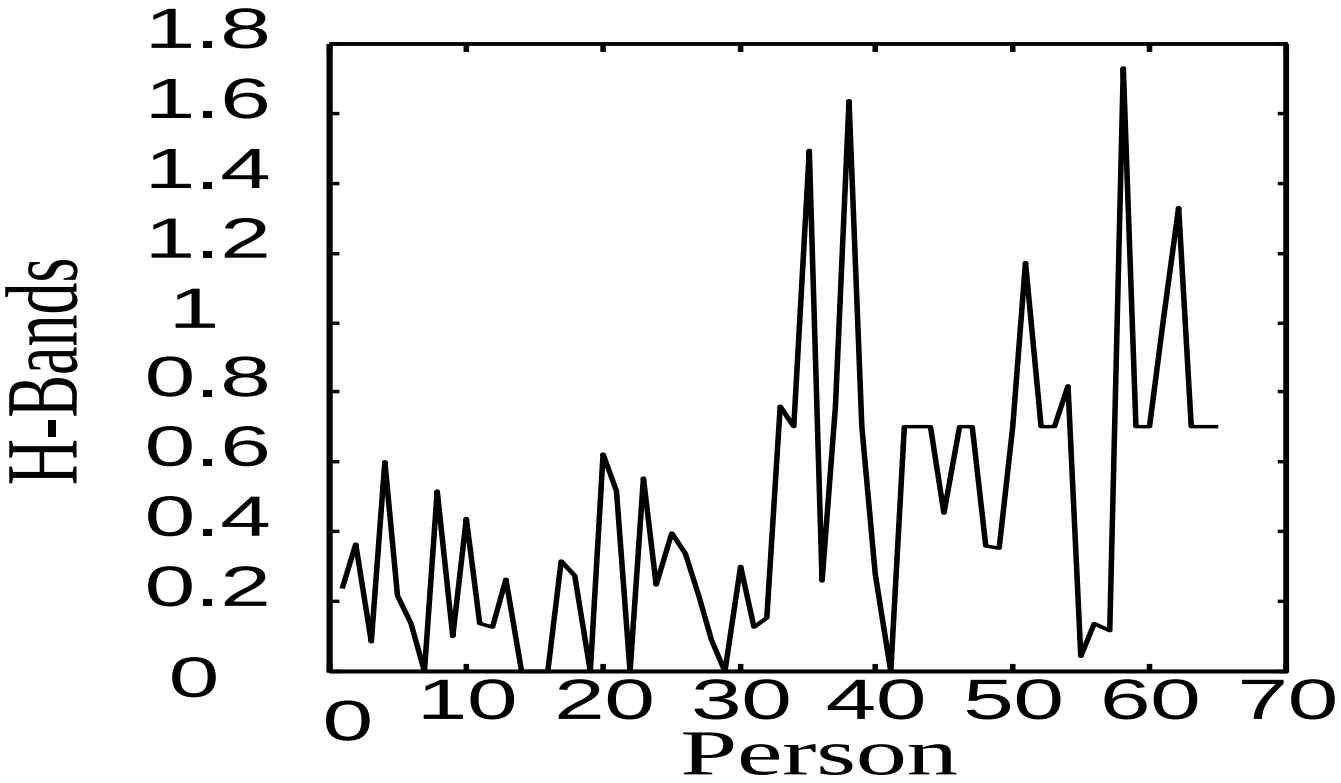
- Spectral format (65 pictures, one for each person)



Difficult to compare the different patients...

Data Visualization

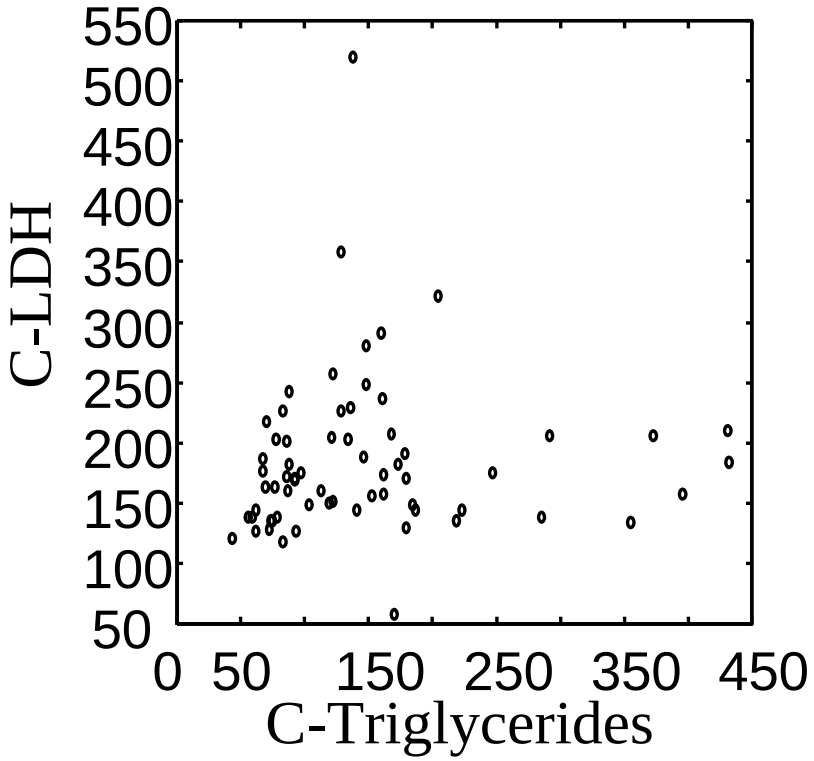
- Spectral format (53 pictures, one for each feature)



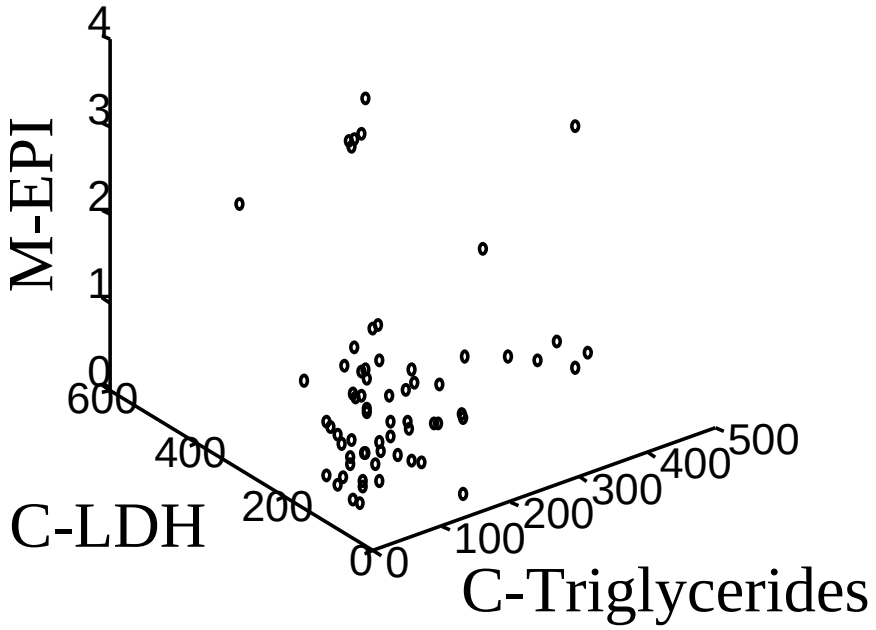
Difficult to see the correlations between the features...

Data Visualization

Bi-variate



Tri-variate



- **How can we visualize the other variables???**

… difficult to see in 4 or higher dimensional spaces...

Data Visualization

- Is there a representation better than the coordinate axes?
- Is it really necessary to show all the 53 dimensions?
  - … what if there are strong correlations between the features?
- How could we find
  the *smallest* subspace of the 53-D space that
  keeps the *most information* about the original data?

- Solution: **Principal Component Analysis**

Principle Component Analysis

1. **Compresses the information**
   - Finds the directions with most variability
   - Projects the information down on these dimensions
   - The goal of PCA is to reduce the dimensionality of the data while **retaining as much as possible of the variation present in the dataset.**
2. **Presents the information in simple plots**
   - **Scores plot**
     - Projection of data onto subspace
   - **Loadings plot**
     - Plot of relation between original variables and subspace dimensions

Principle Component Analysis

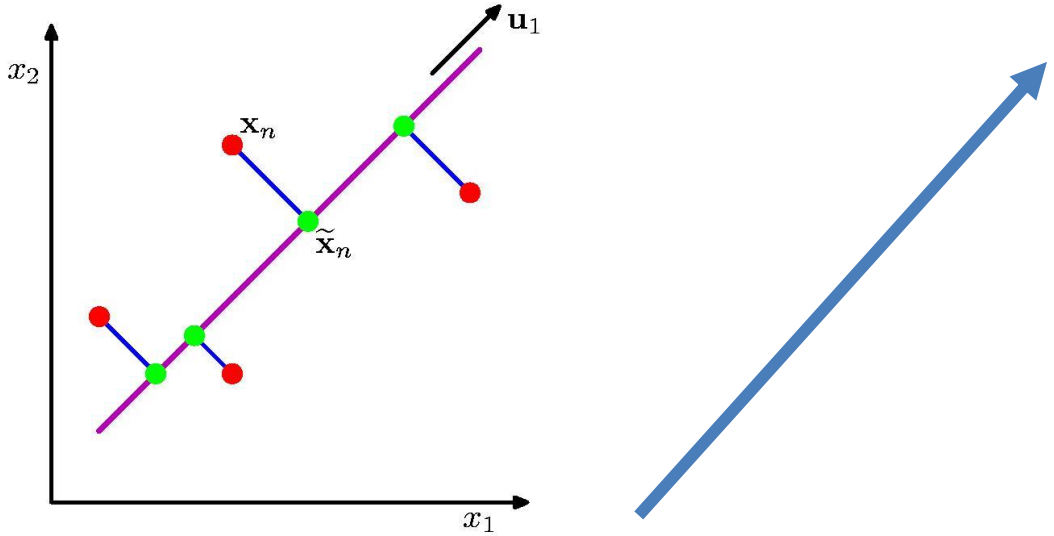
Goals of PCA: Highlight ...

- The structure of the row-individuals through an Euclidean representation to **detect the individuals that are similar from the point of view of the active variables**
- The structure of the column-variables a representation that **evidences the variables highly correlated**

This method aims at discovering the data structure, the underlying system, the patterns, the general rules but also the clues towards hidden information and explain:

- The variability of the individuals from the variables point of view
- The dispersion of the variables from the individuals point of view

Principle Component Analysis



Orthogonal projection of data onto lower-dimension linear space that...

- maximizes variance of projected data (purple line)
- minimizes mean squared distance between
  - data point and
  - projections (sum of blue lines)

Principle Components Analysis

Idea:

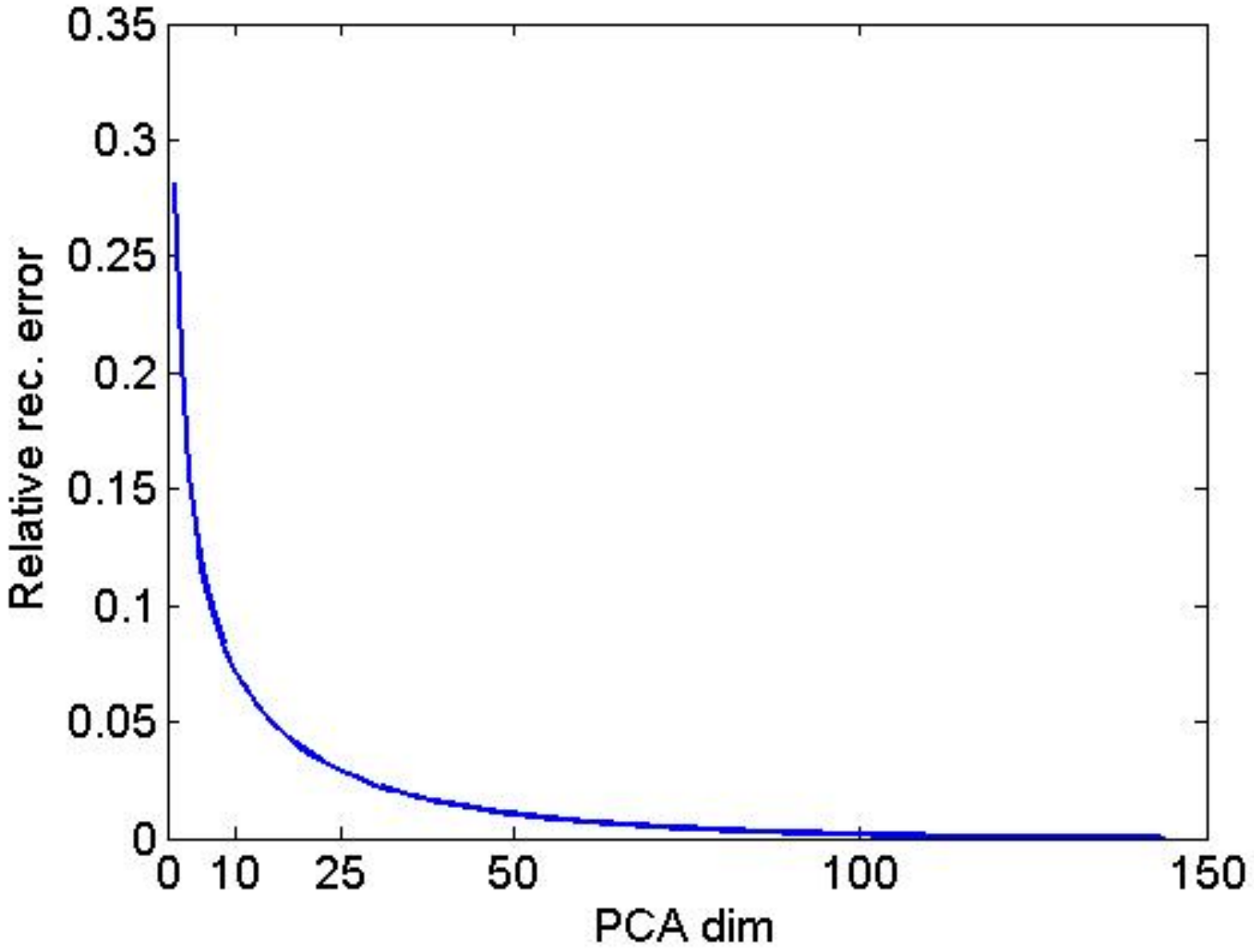
- Given data points in a d-dimensional space, project into lower dimensional space while preserving as much information as possible
  - Eg, find best planar approximation to 3D data
  - Eg, find best 12-D approximation to 10^4-D data

- In particular, choose projection that minimizes *squared error* in reconstructing original data

Image Compresion Example

- Divide the original 372x492 image into patches
- Each patch is an instance that contains 12x12 pixels on a grid
- View each as a 144-D vector

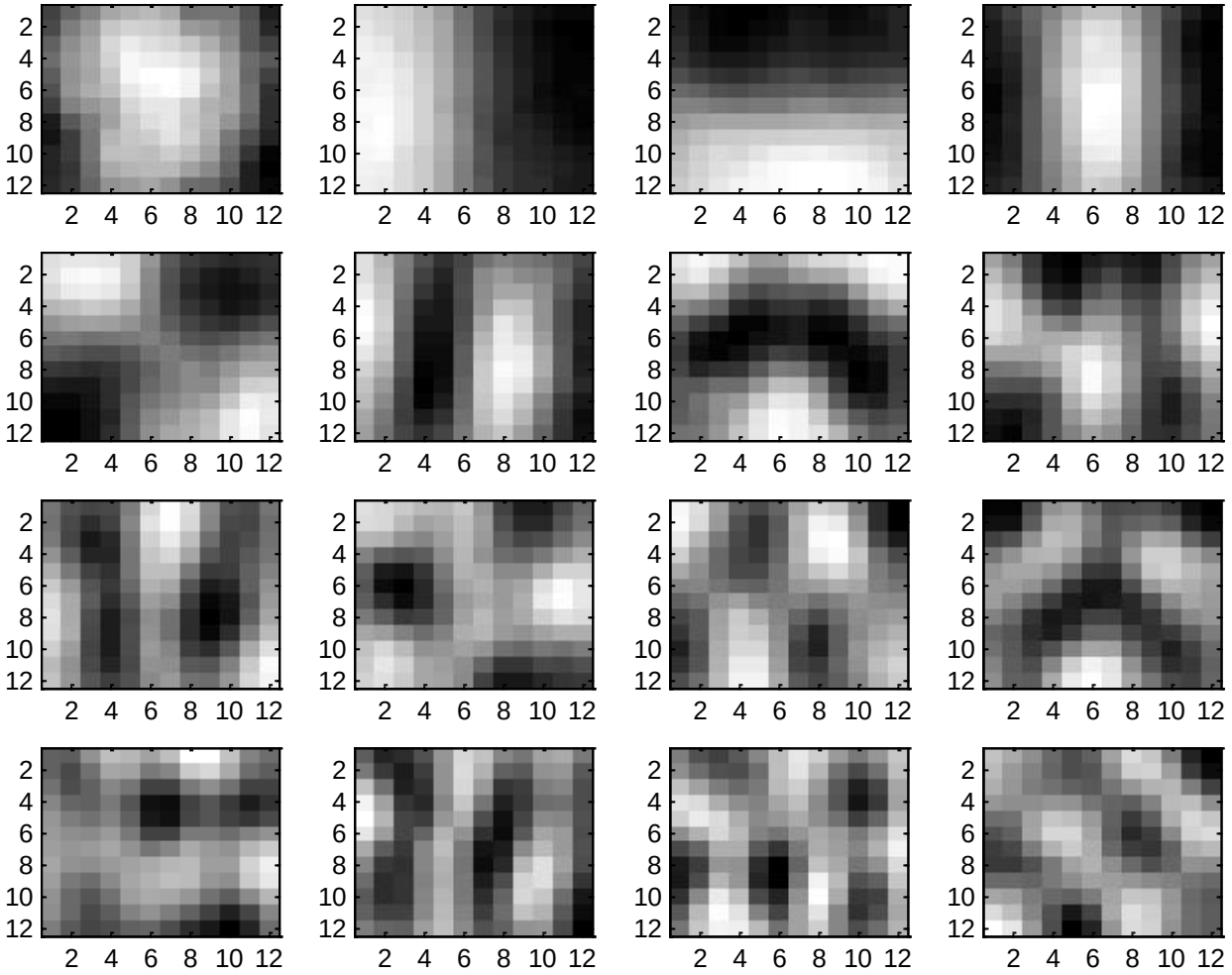
L_2 error and PCA dim



PCA compression: 144D) 60D

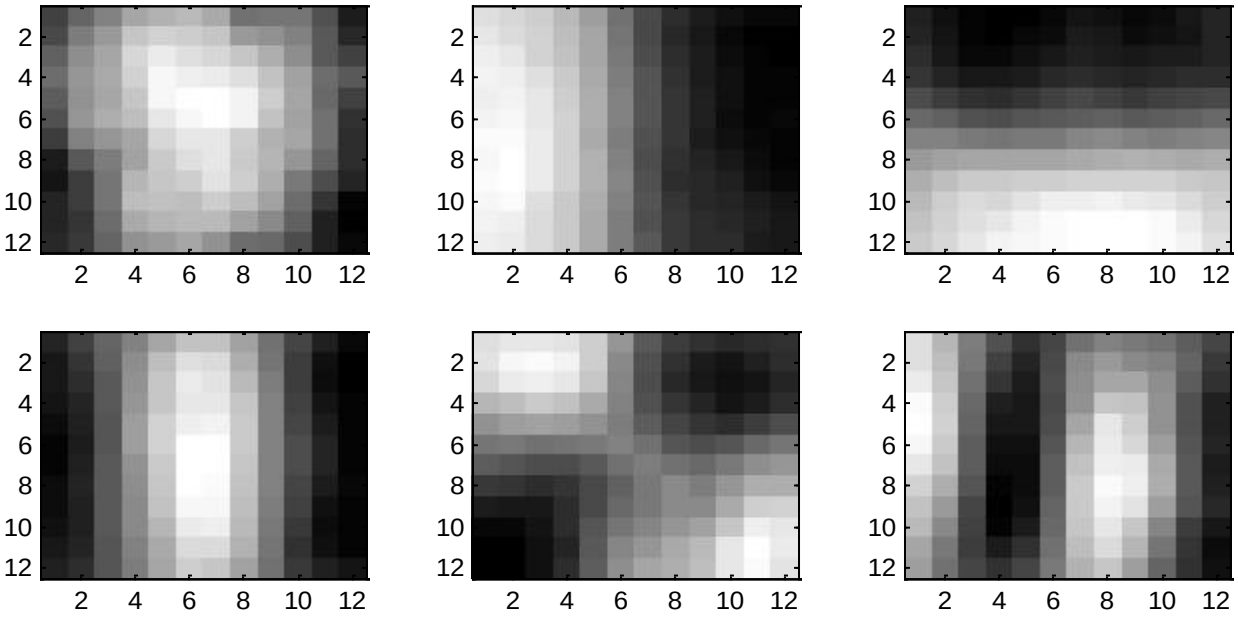
PCA compression: 144D) 16D

16 most important eigenvectors



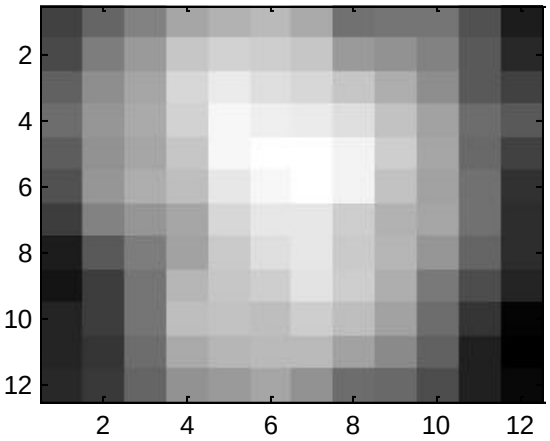
PCA compression: 144D) 6D

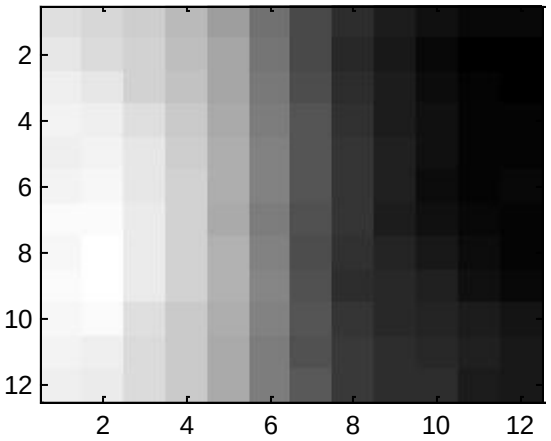
6 most important eigenvectors

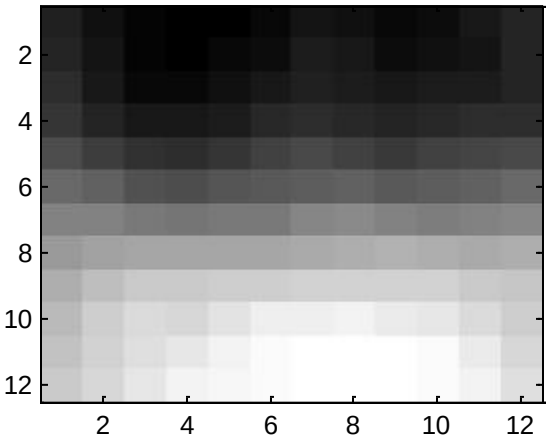


PCA compression: 144D) 3D

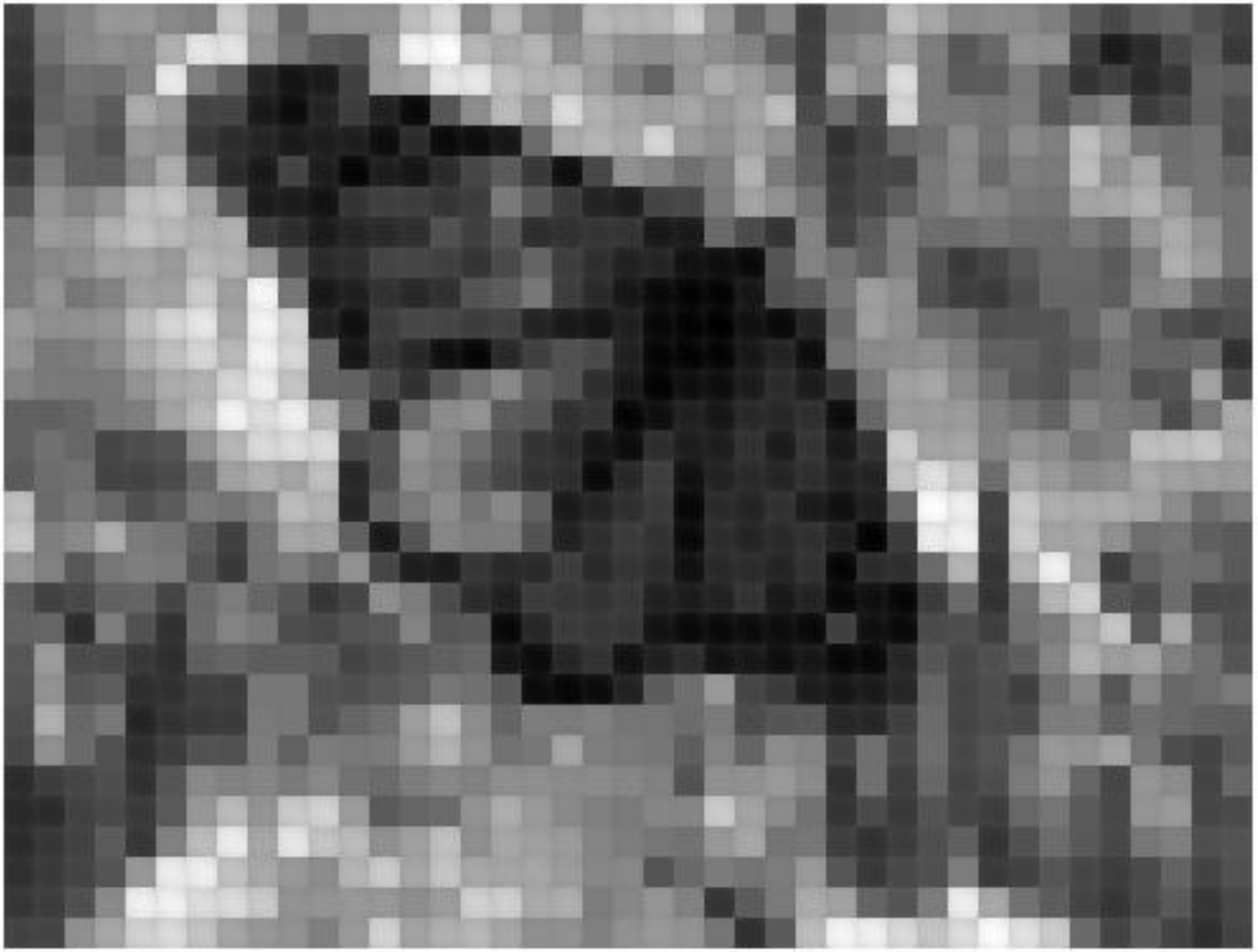
3 most important eigenvectors



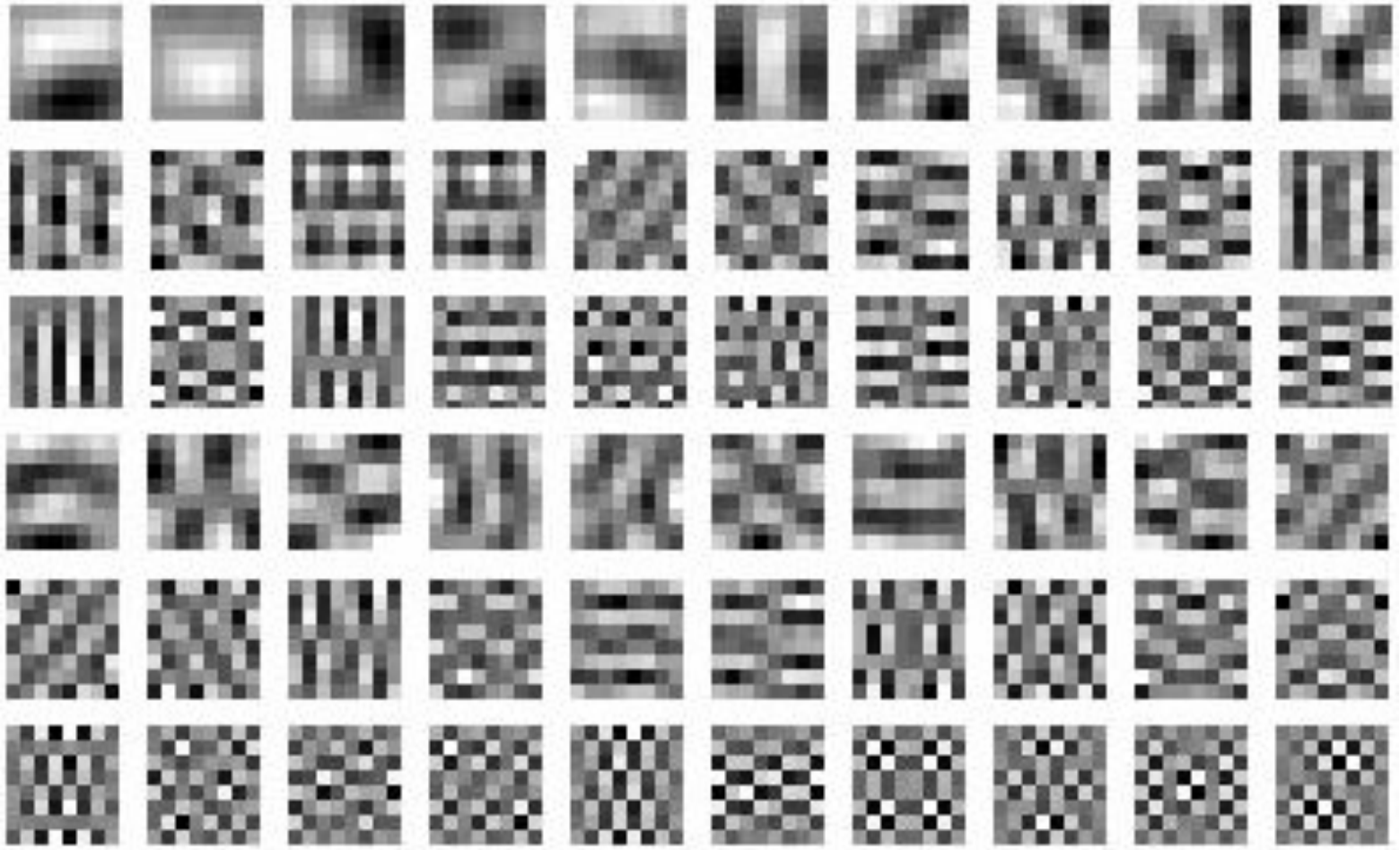




PCA compression: 144D) 1D

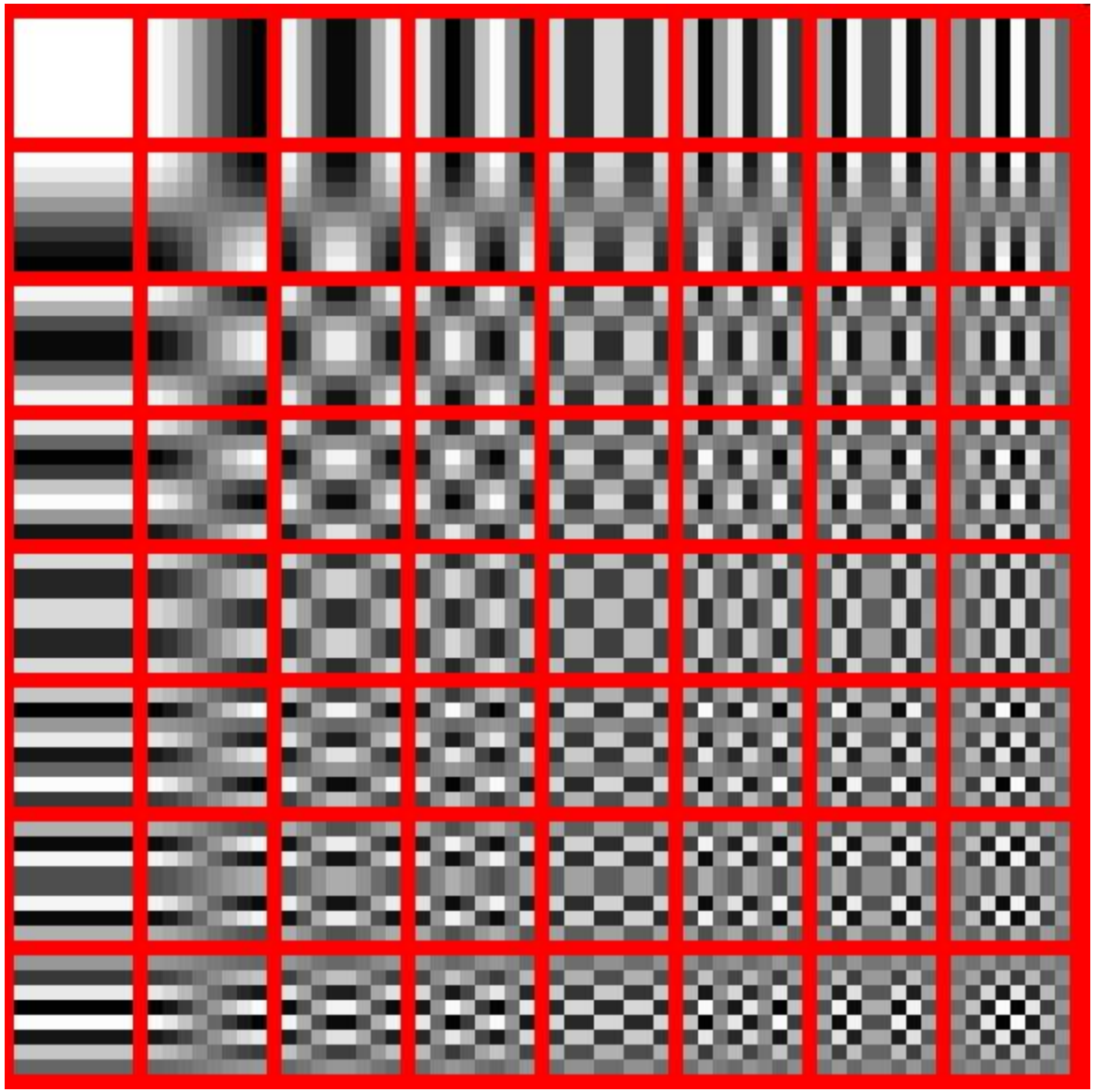


60 most important eigenvectors



Looks like the discrete cosine bases of JPG!...

2D Discrete Cosine Basis



http://en.wikipedia.org/wiki/Discrete_cosine_transform

Noisy filtering applications

- Noisy picture

Noisy filtering applications

- Denoised image using 15 PCA components

The Principal Components

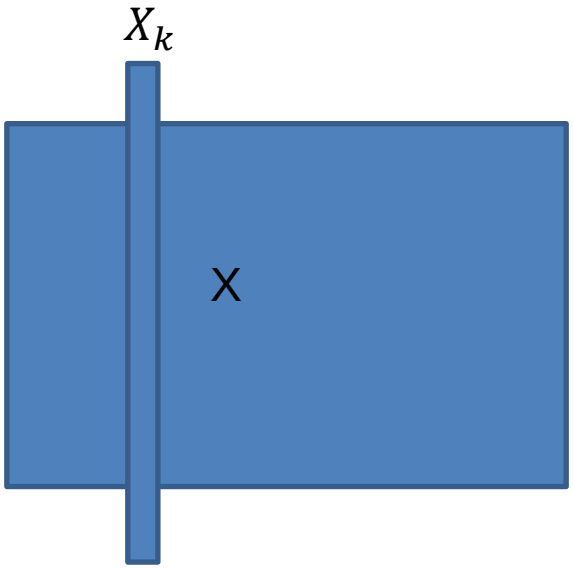
- **Vectors** originating from the center of mass, in PCA, either matrix *Y* or matriz Z are used with general terms:

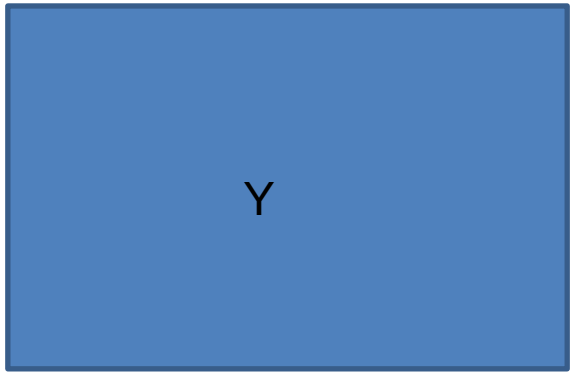
$$y_{ik} = \left(x_{ik} - \bar{x}_k\right)$$

$$z_{ik} = \frac{\left(x_{ik} - \bar{x}_k\right)}{s_k}$$

Normalized

- Principal component #1 points in the direction of the **largest variance (inertia)**.
- Each subsequent principal component…
  - is **orthogonal** to the previous ones, and
  - points in the directions of the **largest variance of the residual subspace**

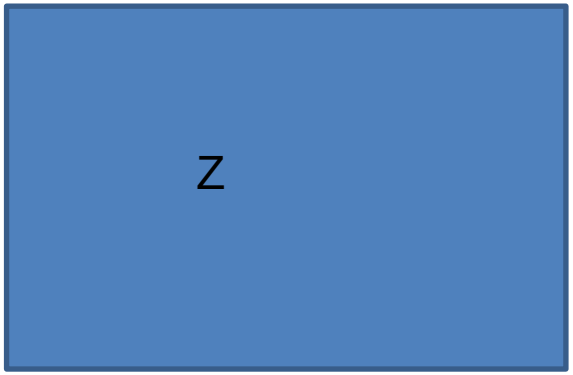




$\overline{x_k}$ s_k

$$y_{ik} = \left(x_{ik} - \overline{x}_k\right)$$

$$z_{ik} = \frac{\left(x_{ik} - \overline{x}_k\right)}{s_k}$$



Geometric Rationale of PCA

- Degree to which the variables are linearly correlated is represented by their covariances.

$$y_{ik} = \left(x_{ik} - \bar{x}_k\right)$$

$$C_{ij} = \frac{1}{I-1}\sum_{m=1}^{I}\left(X_{mi} - \bar{X}_i\right)\left(X_{mj} - \bar{X}_j\right)$$

Covariance of variables *i* and *j*

Sum over all *I* objects

Value of variable *i*

Mean of variable *i*

Value of variable *j* in object *m*

Mean of variable *j*

Geometric Rationale of PCA

- Normalized PCA: Degree to which the variables are linearly correlated is represented by their correlations.

$$z_{ik} = \frac{\left(x_{ik} - \bar{x}_k\right)}{s_k}$$

$$C_{ij} = \frac{1}{I-1}\sum_{m=1}^{I}\frac{\left(X_{mi} - \bar{X}_i\right)}{S_i}\frac{\left(X_{mj} - \bar{X}_j\right)}{S_j}$$

Correlation of variables *i* and *j*

Sum over all *I* objects

Value of variable *i*

St deviation of variable *i*

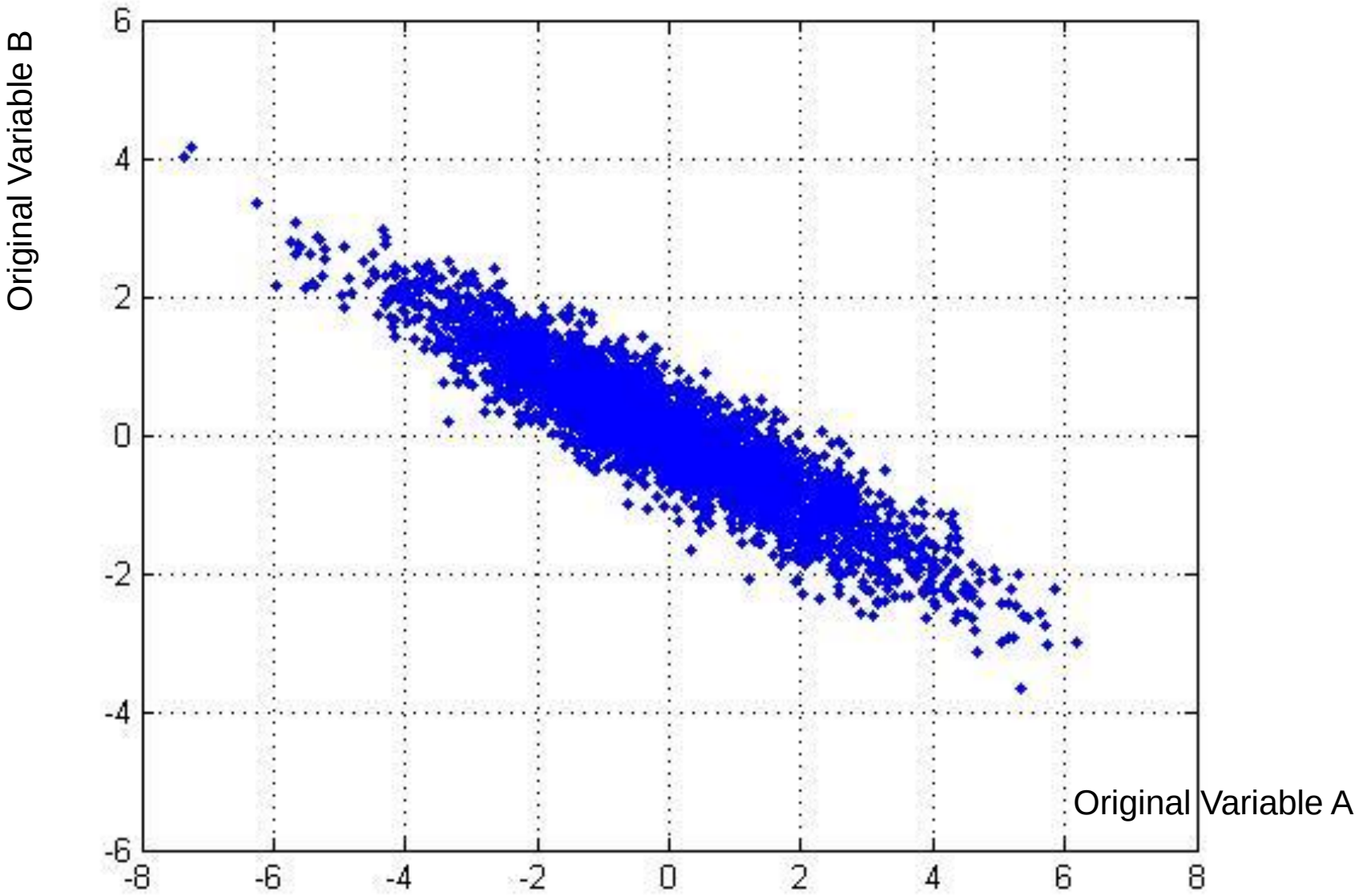
Mean of variable *i*

Value of variable *j* in object *m*

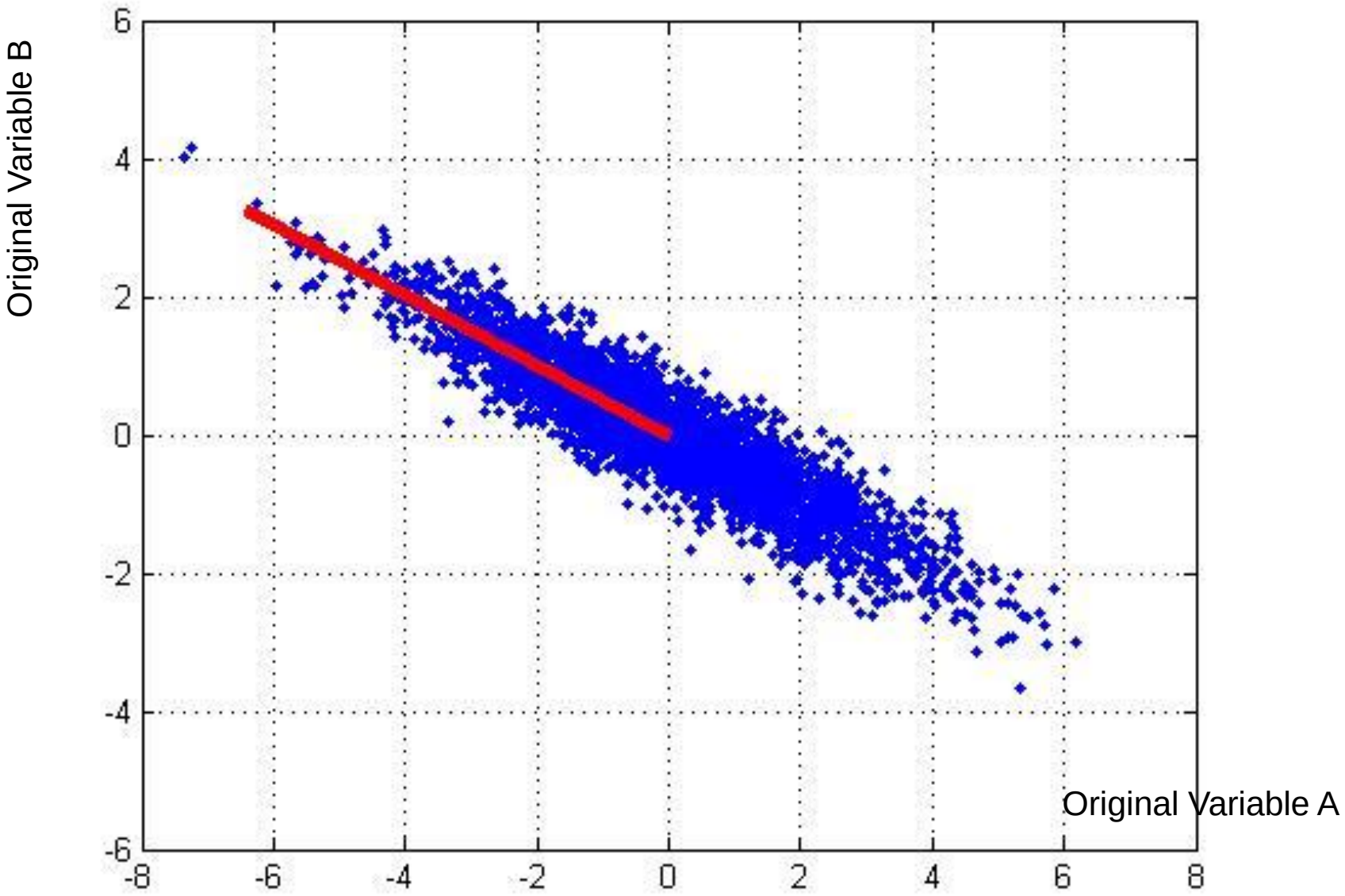
St deviation of variable *j*

Mean of variable *j*

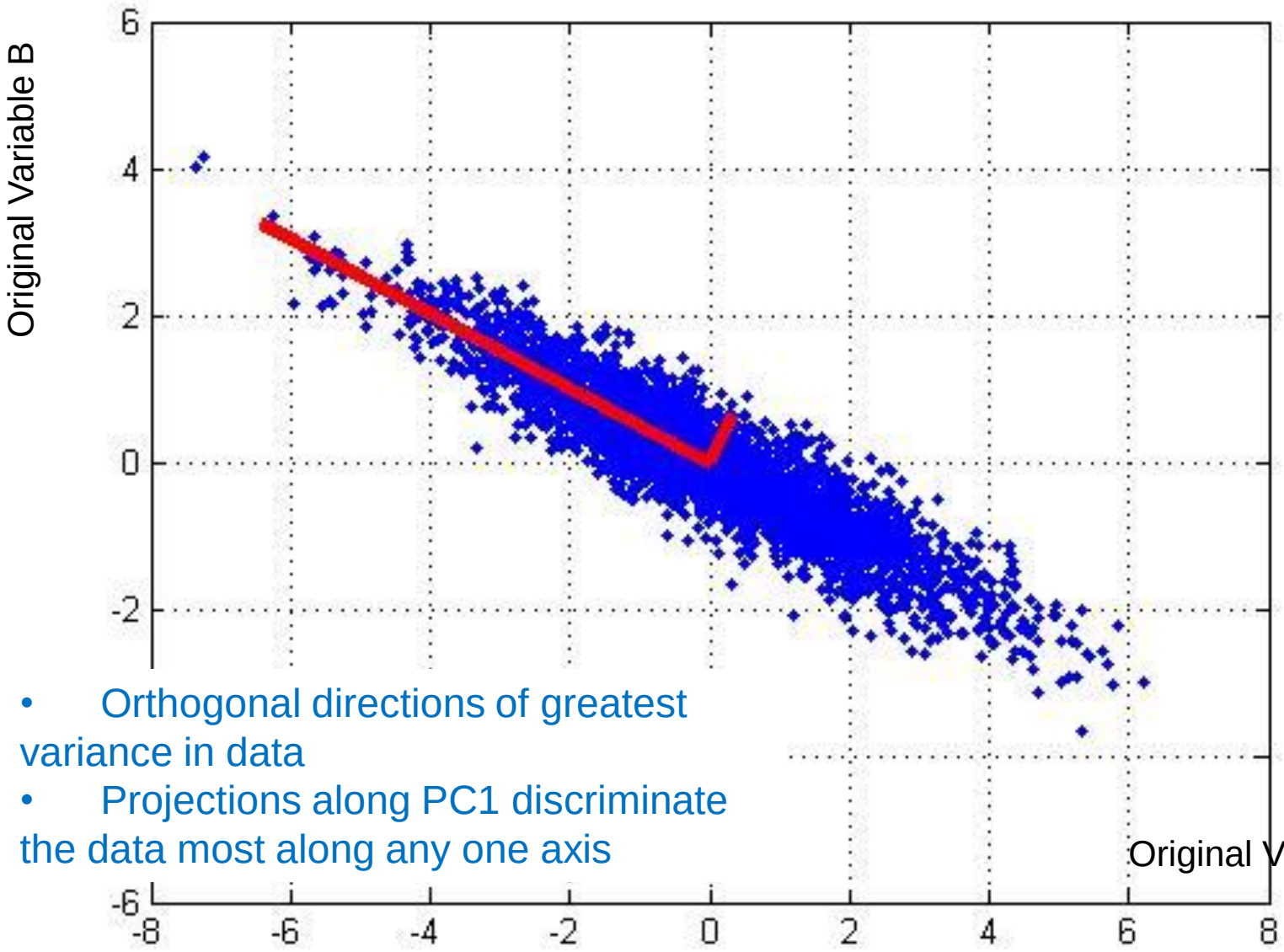
2D Gaussian dataset



1st PCA axis


Original Variable B
Original Variable A
6
4
2
0
-2
-4
-6
-8
-6
-4
-2
0
2
4
6
8

2nd PCA axis



- Orthogonal directions of greatest variance in data
- Projections along PC1 discriminate the data most along any one axis

Principal Components

- First principal component is the direction of greatest variability (covariance) in the data
- Second is the next orthogonal (uncorrelated) direction of greatest variability
  - So first remove all the variability along the first component, and then find the next direction of greatest variability
- And so on …

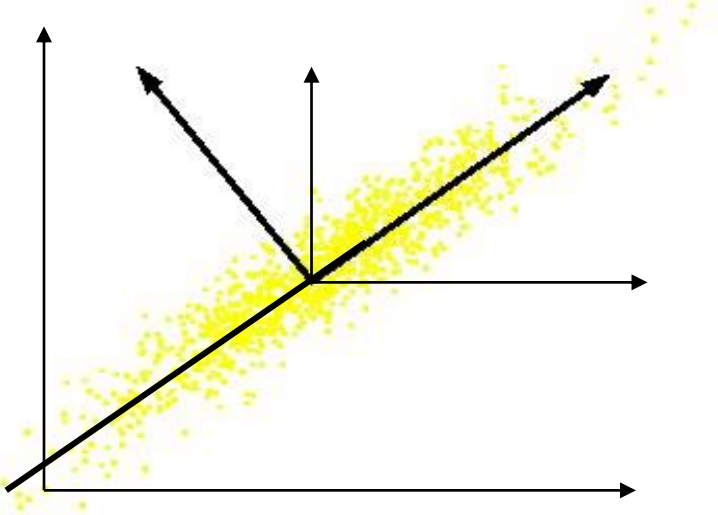
Principal Components Analysis (PCA)

- Principle
  - Linear projection method to reduce the number of parameters
  - Transfer a set of correlated variables into a new set of uncorrelated variables
  - Map the data into a space of lower dimensionality
  - Form of unsupervised learning

- Properties
  - It can be viewed as a rotation of the existing axes to new positions in the space defined by original variables
  - New axes are orthogonal and represent the directions with maximum variability

Computing the Components

- Data points are vectors in a multidimensional space
- Projection of vector **x** onto an axis (dimension) **u** is **x.u**
- Direction of greatest variability is that in which the average square of the projection is greatest
  - I.e. **u** such that $E((\mathbf{x}.\mathbf{u})^2)$ over all **x** is maximized
  - Usually, just subtract the mean along each dimension, thus center the original axis system at the centroid of all data points, for simplicity.
  - This direction of **u** is the direction of the first Principal Component



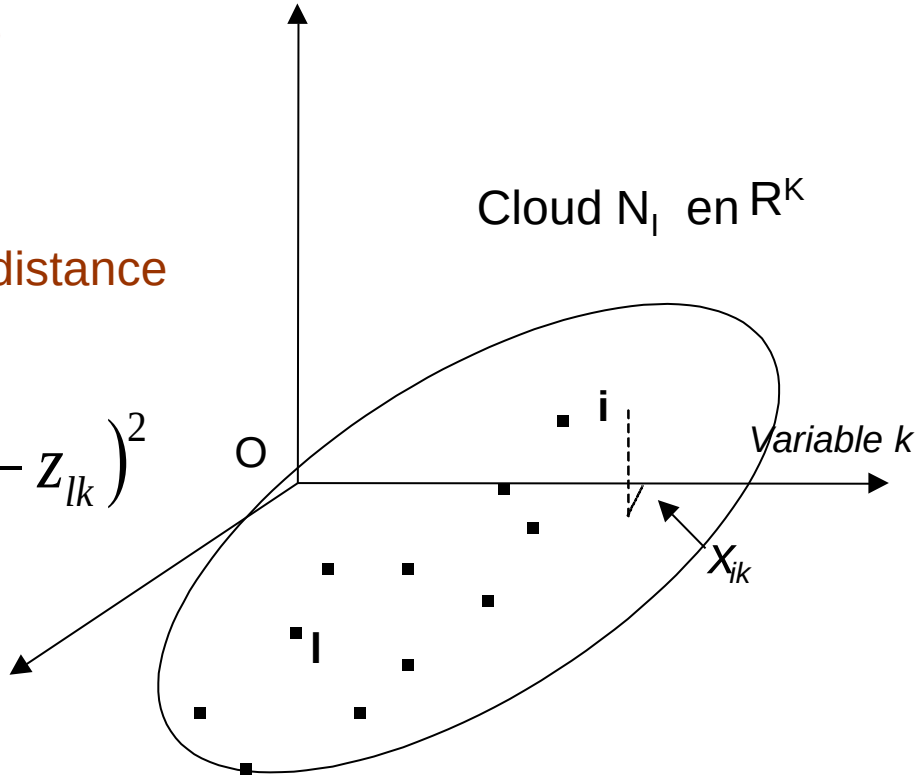
Computing the Components

Principal component analysis

Cloud of individuals

Classical Euclidean distance

$$d^2(i,l) = \sum_{k \in K} \left(z_{ik} - z_{lk}\right)^2$$



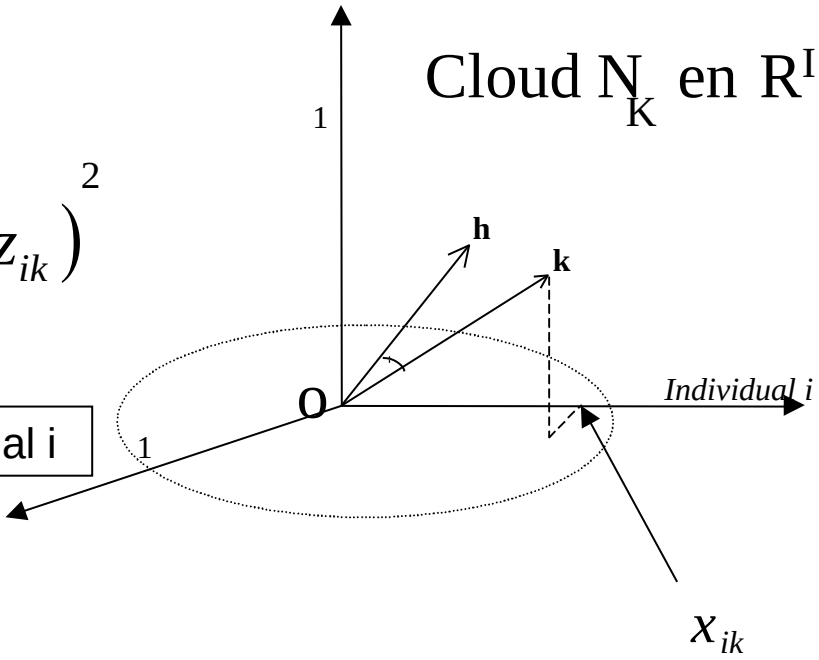
Computing the Components

Principal component analysis

Cloud of variables

$$d^2(h,k) = \sum_{i \in I} \frac{1}{I} \left(z_{ih} - z_{ik} \right)^2$$

weight of individual i



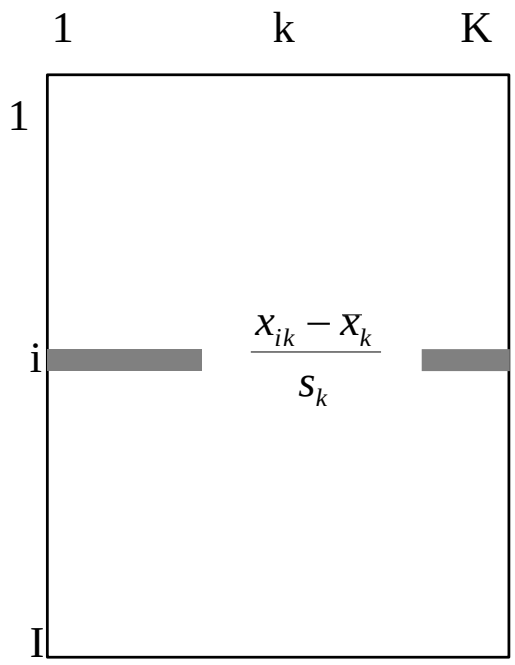
However, it is usual to analyze the relationships between variables through the linear correlation coefficient

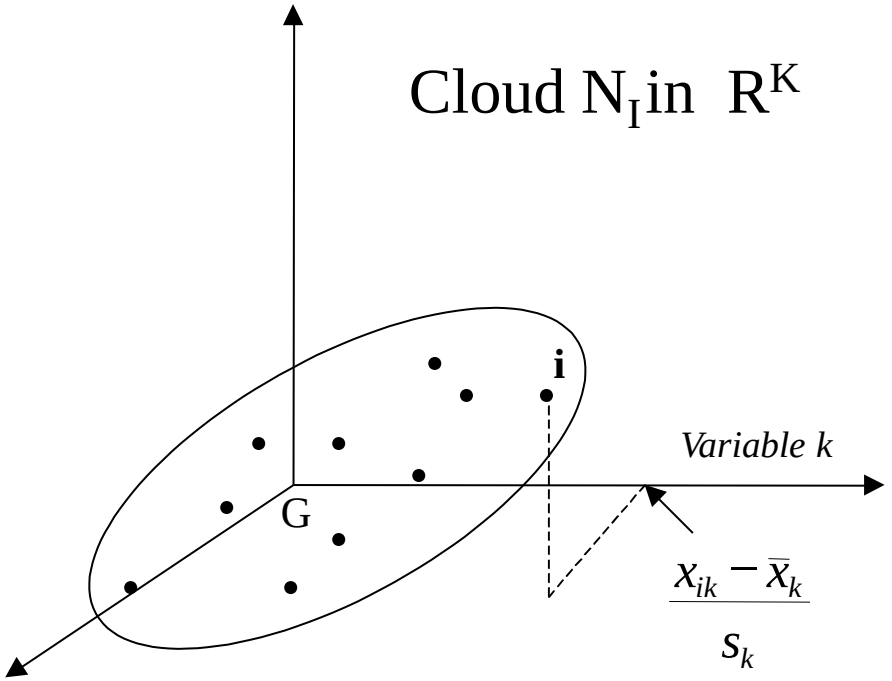
$$r(k,h) = \frac{1}{I} \sum_{i \in I} \left(\frac{x_{ik} - \bar{x}_k}{s_k} \right) \cdot \left(\frac{x_{ih} - \bar{x}_h}{s_h} \right) = \frac{s_{k,h}}{s_k s_h}$$

Computing the Components

In the individual space

$$d^2(i,l) = \sum_k \left(\frac{x_{ik} - x_{lk}}{s_k} \right)^2 = \sum_k (z_{ik} - z_{lk})^2$$





Computing the Components

- $E((\mathbf{z}.\mathbf{u})^2) = E((\mathbf{z}.\mathbf{u})^T(\mathbf{z}.\mathbf{u})) = E(\mathbf{u}^T.\mathbf{z}^T.\mathbf{z}.\mathbf{u})$
- The matrix $\mathbf{C} = \mathbf{Z}^T.\mathbf{Z}$ contains the correlations (similarities) of the original axes based on how the data values project onto them
- So we are looking for w that maximizes $\mathbf{u}^T\mathbf{C}\mathbf{u}$, subject to **u** being unit-length
- It is maximized when w is the principal eigenvector of the matrix **C**, in which case
  - $\mathbf{u}^T\mathbf{C}\mathbf{u} = \mathbf{u}^T\lambda\mathbf{u} = \lambda$ if **u** is unit-length, where λ is the principal eigenvalue of the correlation matrix C
  - The eigenvalue denotes the amount of variability captured along that dimension

Why the Eigenvectors?

- Maximize $\mathbf{u}^T\mathbf{Z}^T\mathbf{Z}\mathbf{u}$

$$\text{s.t } \mathbf{u}^T\mathbf{u} = 1$$

- Construct Langrangian $\mathbf{u}^T\mathbf{Z}^T\mathbf{Z}\mathbf{u} - \lambda\mathbf{u}^T\mathbf{u}$
- Vector of partial derivatives set to zero

$$\mathbf{Z}^T\mathbf{Z}\mathbf{u} - \lambda\mathbf{u} = (\mathbf{Z}^T\mathbf{Z} - \lambda\mathbf{I})\,\mathbf{u} = 0$$

- As $\mathbf{u} \neq \mathbf{0}$ then $\mathbf{u}$ must be an eigenvector of $\mathbf{Z}^T\mathbf{Z}$ with eigenvalue λ
- Diagonalization $\mathbf{Z}^T\mathbf{Z}=\mathbf{U}\,\mathbf{\Sigma}\,\mathbf{U}^T$, where $\mathbf{\Sigma}$ diag matrix with eigenvalues

Singular Value Decomposition

- The first root is called the principal eigenvalue which has an associated orthonormal ($\mathbf{u}^T\mathbf{u} = 1$) *eigenvector* $\mathbf{u}$
- Subsequent roots are ordered such that $\lambda_1 > \lambda_2 > \ldots > \lambda_S$ with rank($\mathbf{C}$) ($S \leq \text{Min}(I,K)$) non-zero values.
- Eigenvectors form an orthonormal basis i.e. $\mathbf{u}_i^T\mathbf{u}_j = \delta_{ij}$
- The eigenvalue decomposition of $\mathbf{Z}^T\mathbf{Z} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{U}^T$

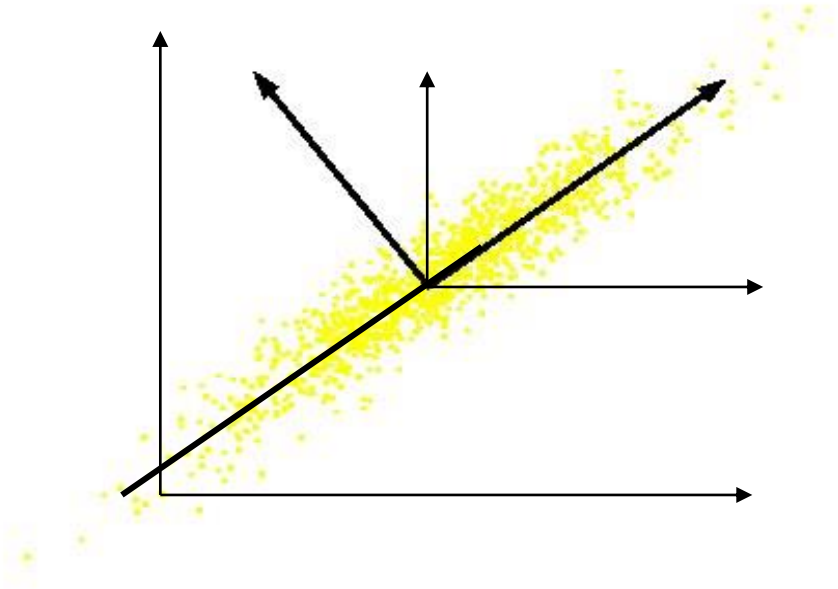
  where $\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_S]$ s-by-s matrix whose columns are the eigenvectors of $\mathbf{Z}^T\mathbf{Z}$ and $\boldsymbol{\Sigma} = \text{diag}[\lambda_1, \lambda_2, \ldots, \lambda_S]$

- Similarly the eigenvalue decomposition of $\mathbf{Z}\mathbf{Z}^T = \mathbf{V}\boldsymbol{\Sigma}\mathbf{V}^T$
- The SVD is closely related to the above $\mathbf{Z}^T = \mathbf{U}\,\boldsymbol{\Sigma}^{1/2}\,\mathbf{V}^T$
- The left eigenvectors **U,** right eigenvectors **V,**

  singular values = square root of eigenvalues**.**

Computing the Components

- So, the new axes are the eigenvectors of the matrix of correlations of the original variables, which captures the similarities of the original variables based on how data samples project to them



- Geometrically: centering followed by rotation
  - Linear transformation

PCs, Variance and Least-Squares

- The first PC retains the greatest amount of variation in the sample
- The k^{th} PC retains the k^{th} greatest fraction of the variation in the sample
- The k^{th} largest eigenvalue of the correlation matrix C is the variance in the sample along the k^{th} PC

- The least-squares view: PCs are a series of linear least squares fits to a sample, each orthogonal to all previous ones

Principal component definition

Coordinates of the individuals on u_s: $\mathbf{F_s = Zu_s}$

$\boldsymbol{F}_s$ is:

• The vector of the coordinates of the individuals on axis *s (=one new variable)*

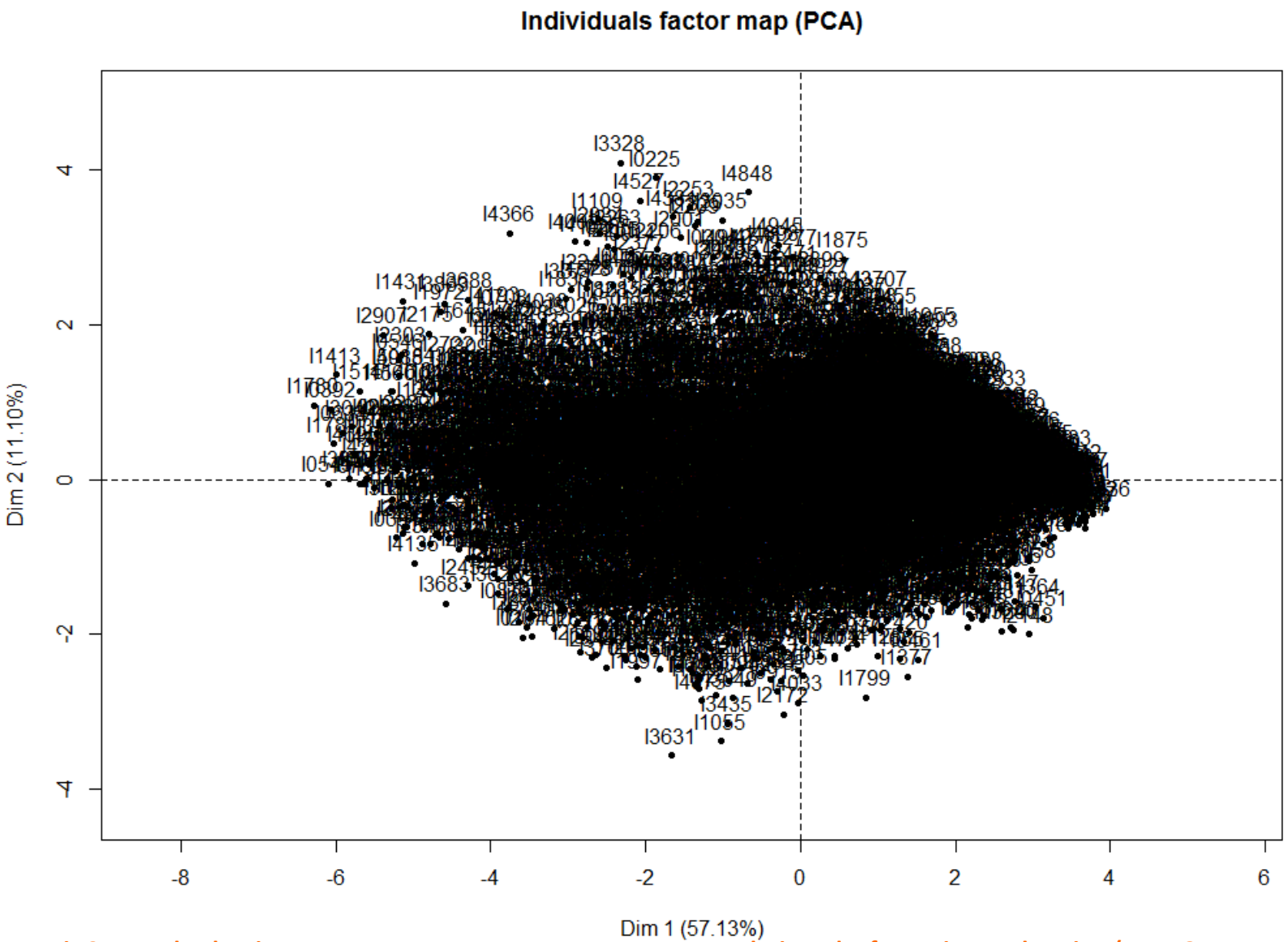
• a lineal combination of the original variables (coefficients = elements of u_s)

• centered with variance λ_s

$\boldsymbol{F}_s$ *is called the* s_{th} *principal component (Ix1)*

The principal axes $\boldsymbol{u}_s$ are orthogonal.
Thus a series of synthetic variables is defined, called principal components.
They are uncorrelated and constitute the best summary of the initial variables.

Principal component definition: scores plot



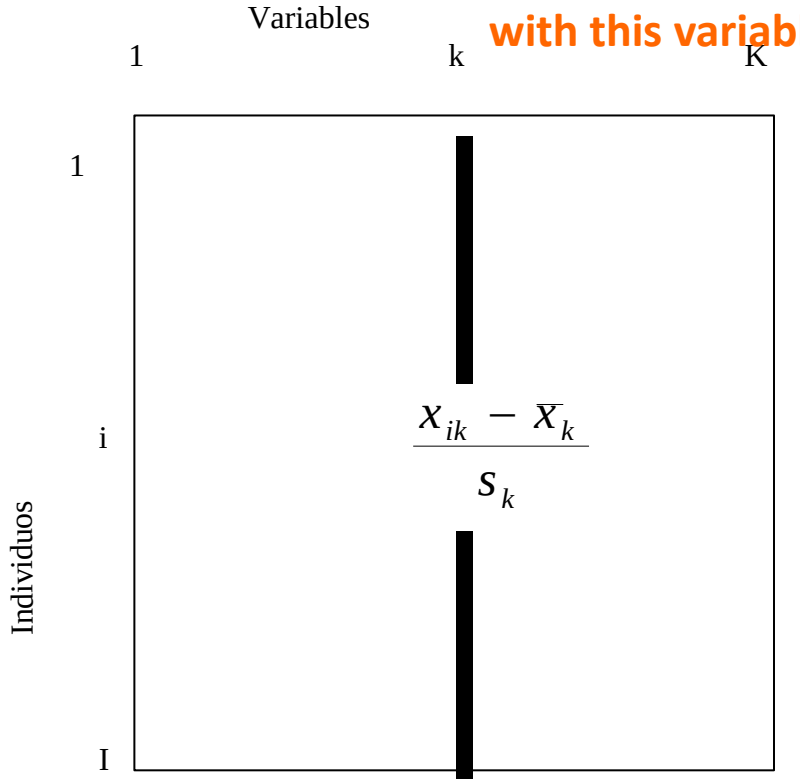
Some more algebrea: In the variables space …

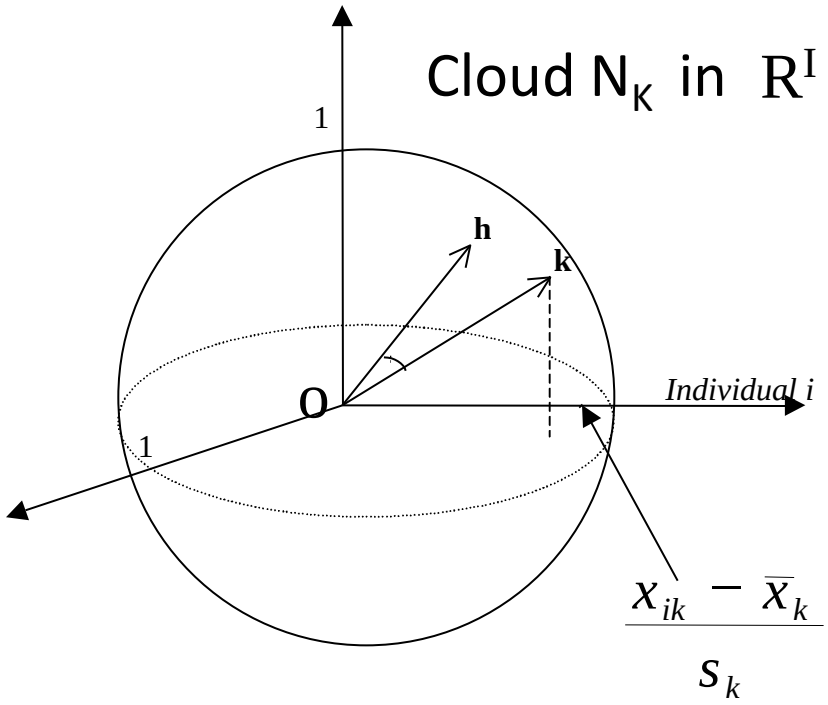
In R^I, because of the variables normalization, all the variables lie on the hypersphere with radius 1 . To center the variable means:

In R^I, the cosine of the angle between two vectors is equal to the correlation between the two variables.

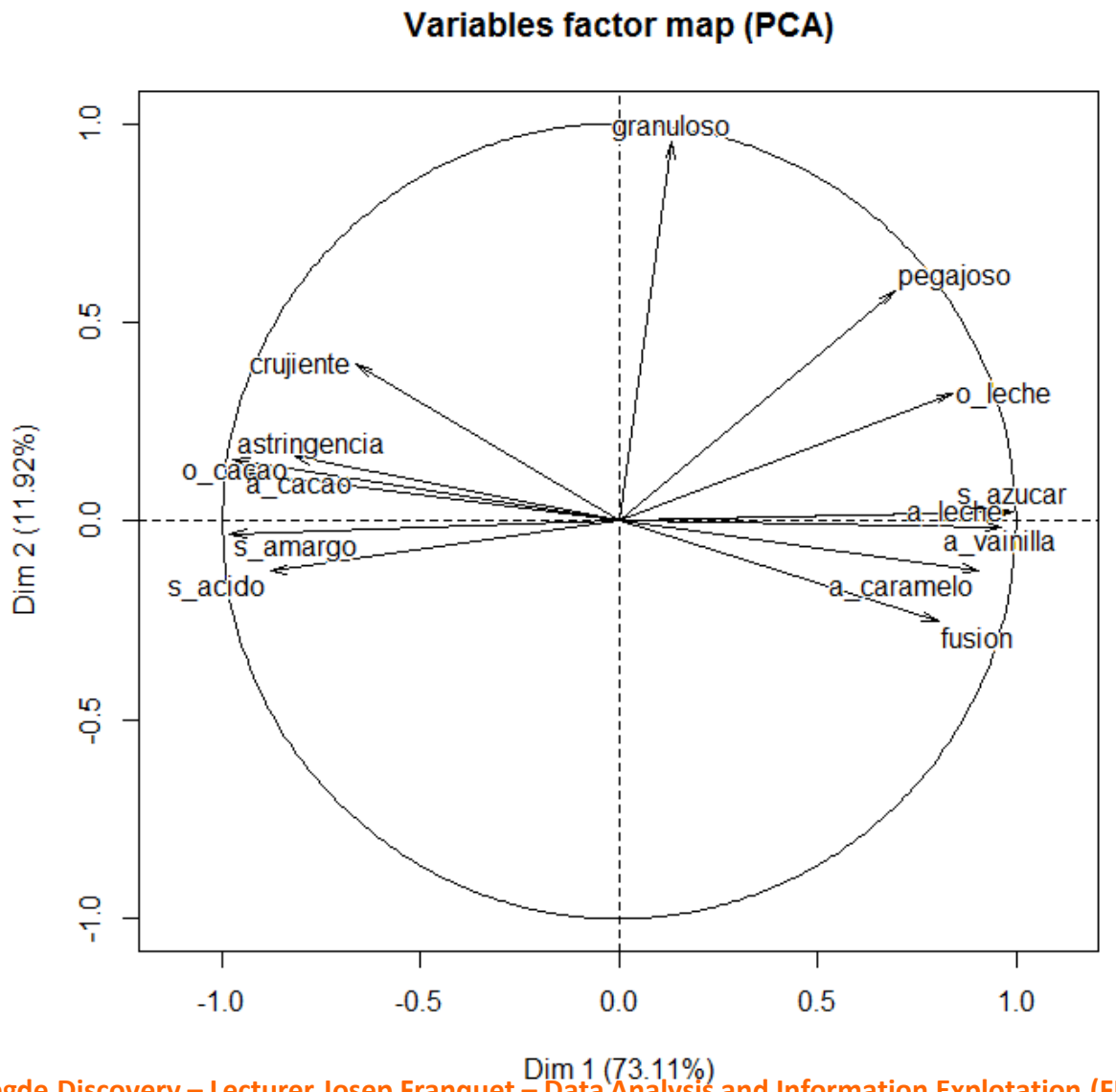
Cloud of variables

As the variables are centered and standardized, **the projection on v_1 of any variable is equal to the coefficient of correlation with this variable**.



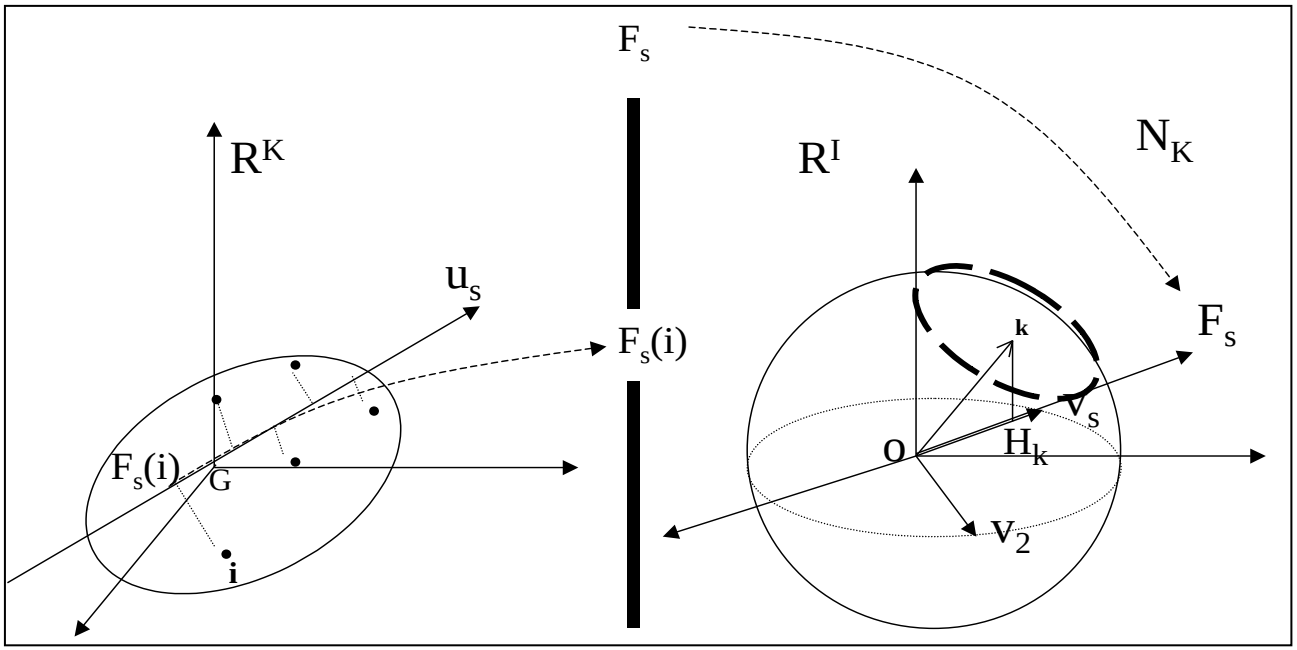


Variable factor map: Loadings Plot



Principal components

Factor *s* or principal component *s* on individuals: projection of all points of the cloud of individuals on the axis *s* noted F_s



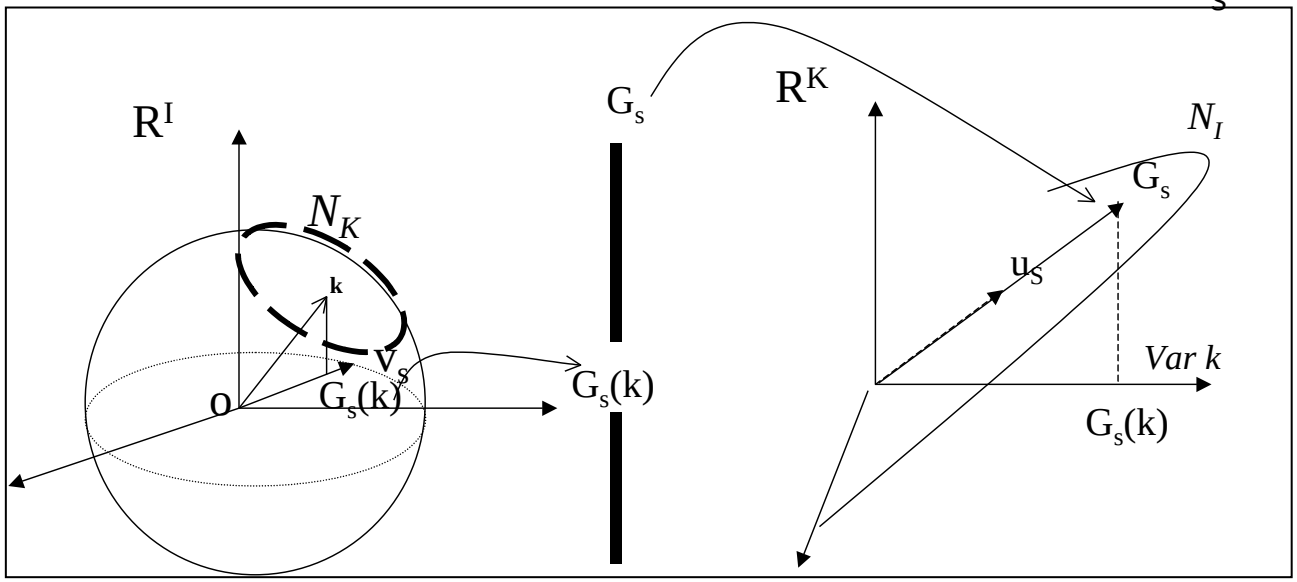
$$v_s = \frac{1}{\sqrt{\lambda_s}} F_s$$

Relationship between the factor F_s and factorial axis v_s

Principal component analysis

Factor *s* on the variables G_s: projection of the *K* variables on the factorial axis v_s.

The set of values is the factor *s* on the variables noted G_s



Relationship between axes u_s and factor G_s $\quad u_s = \frac{1}{\sqrt{\lambda_s}} G_s$

Principal component analysis

Transition relationships

They are deduced from the relationships between axes and factors:

$$F_s(i) = \frac{1}{\sqrt{\lambda_s}} \sum_k \frac{x_{ik} - \bar{x}_k}{s_k} G_s(k)$$

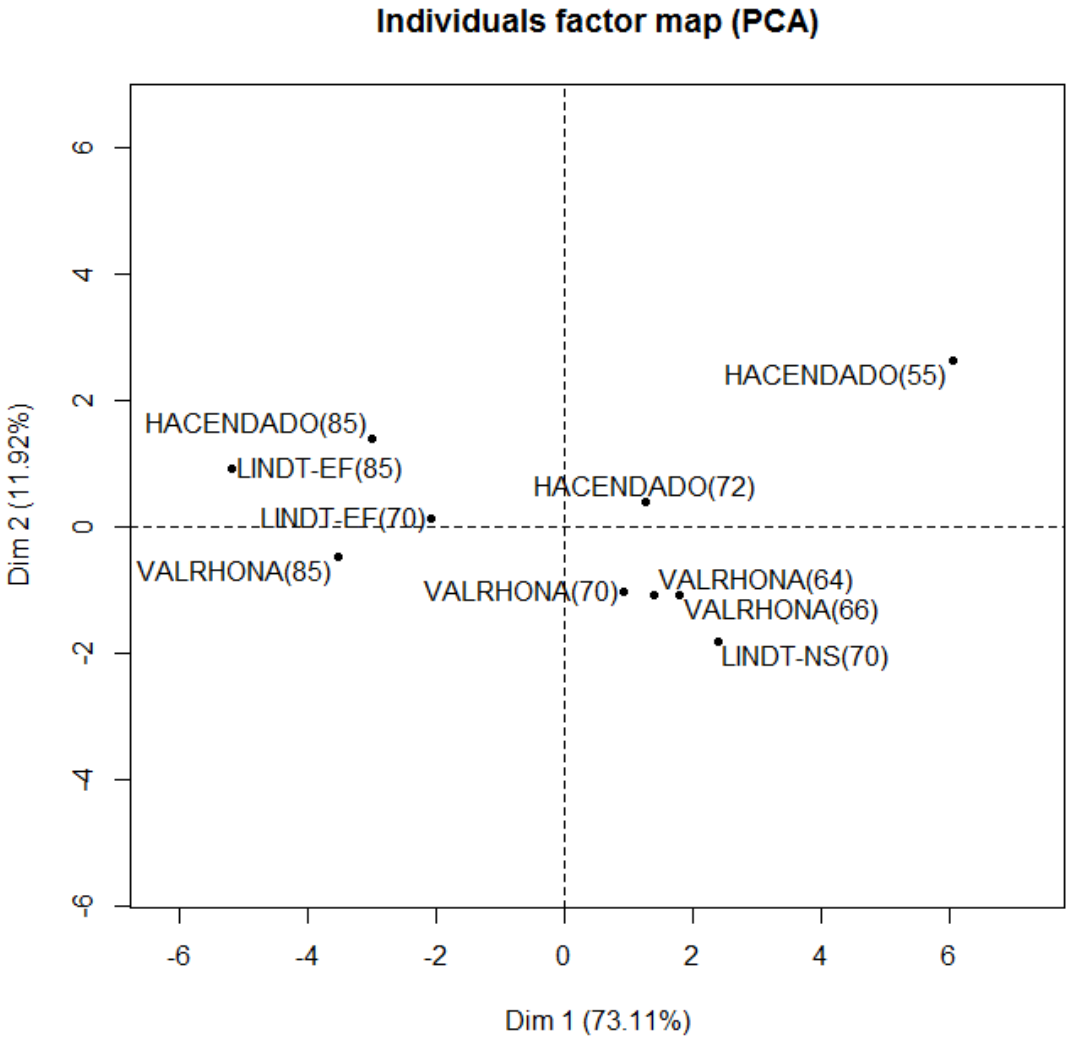
$$G_s(k) = \frac{1}{I} \frac{1}{\sqrt{\lambda_s}} \sum_i \frac{x_{ik} - \bar{x}_k}{s_k} F_s(i)$$

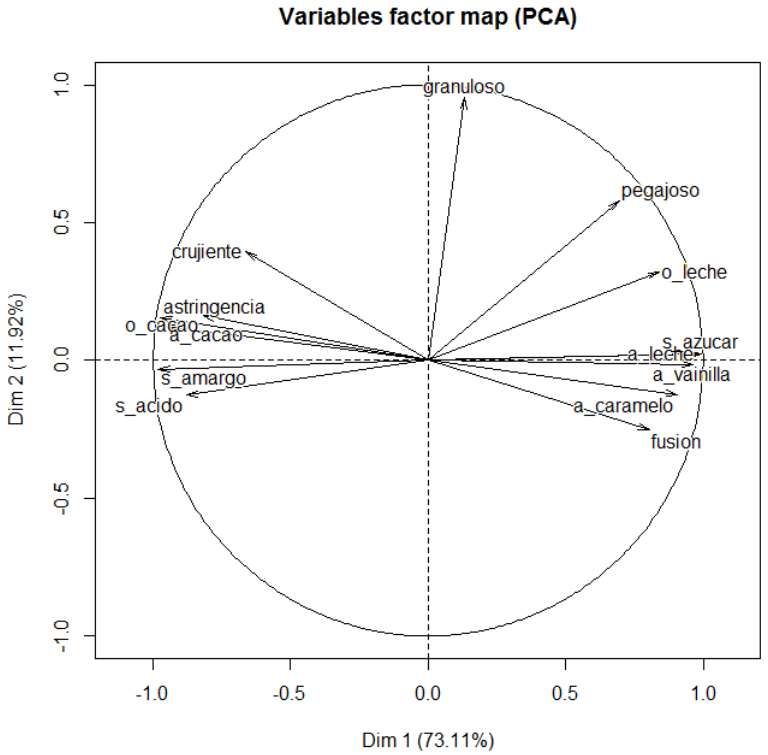
In practice, they are computed :

$$G_s(k) = \sqrt{\lambda_s}\, u_{sk}$$

$$G_s(k) = corr(k, F_s)$$

Simultaneous reading of both graphics





Principal component analysis

Helps to interpretation

Quality representation of the projection of the cloud on an axis, a plane, etc.

$$\frac{\sum_{1}^{q} \lambda_s}{\sum_{1}^{K} \lambda_s}$$

	eigenvalue	percentage of variance	cumulative percentage of variance
comp 1	4.57	57.13	57.13
comp 2	0.89	11.10	68.23

Principal component analysis

Quality of representation of an element on an axis:

$$QLT_s(i) = \frac{\left(OH_i^s\right)^2}{(Oi)^2} = \cos^2\theta$$

Contribution of a row-element to the inertia of an axis $\frac{1}{I} \cdot \frac{F_s^2(i)}{\lambda_s}$

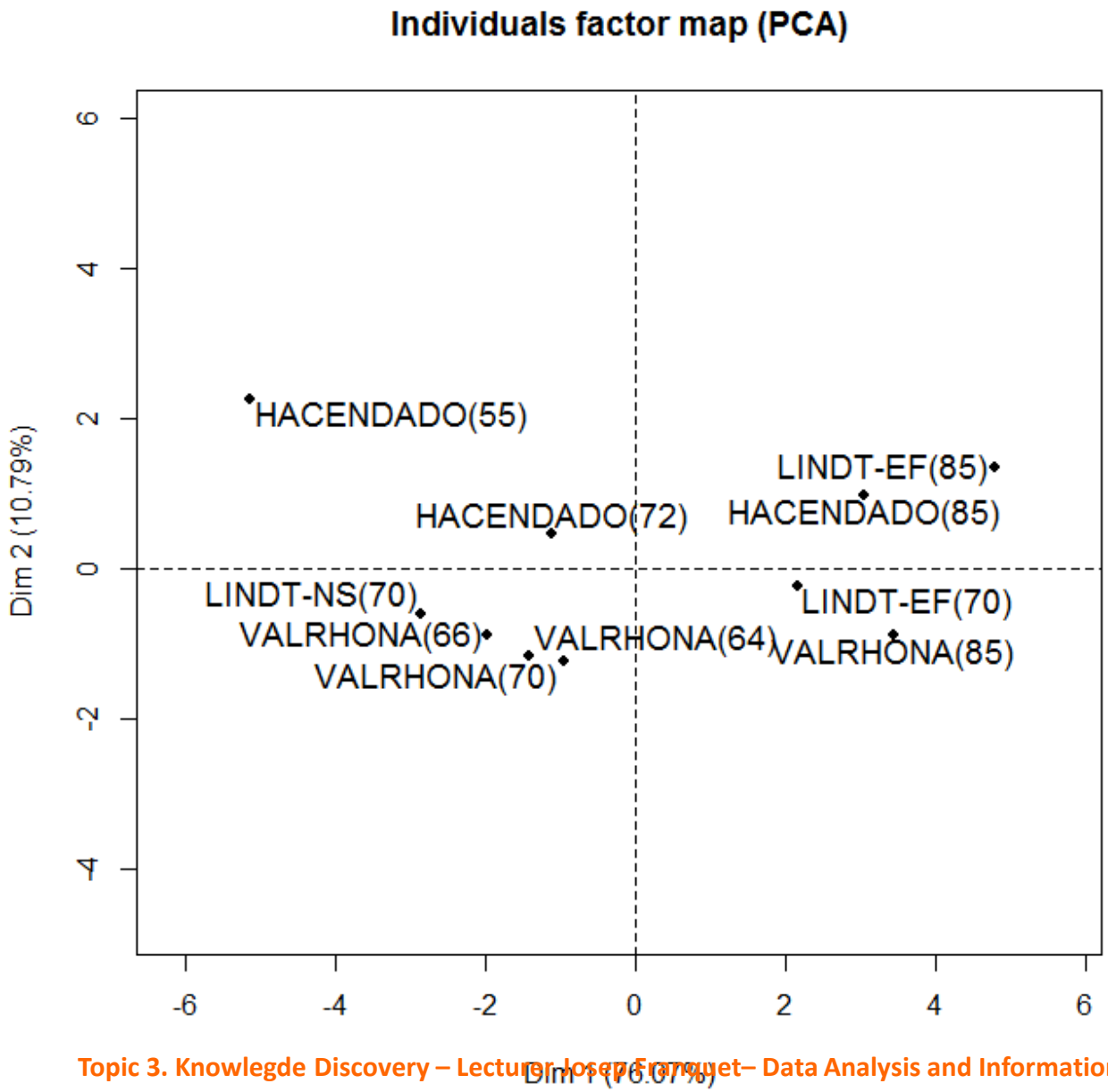
Contribution of a column-element to the inertia of an axis $\frac{G_s^2(k)}{\lambda_s}$

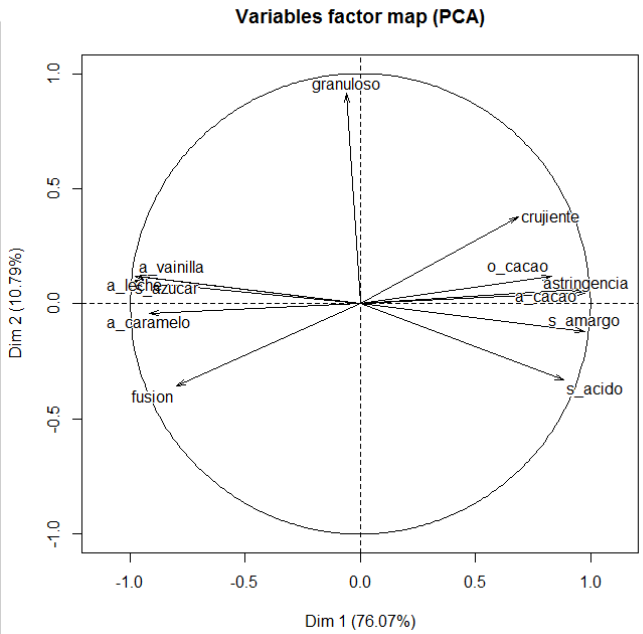
Individuals

	Dist	Dim.1	ctr	cos2	Dim.2	ctr	cos2
VALRHONA(85)	3.974	-3.536	12.212	0.792	-0.461	1.276	0.013
VALRHONA(70)	2.028	0.919	0.824	0.205	-1.030	6.354	0.258
VALRHONA(66)	2.530	1.792	3.137	0.502	-1.087	7.082	0.185
VALRHONA(64)	2.161	1.401	1.918	0.420	-1.086	7.064	0.252
LINDT-NS(70)	3.548	2.390	5.581	0.454	-1.803	19.478	0.258
LINDT-EF(85)	5.477	-5.176	26.178	0.893	0.923	5.104	0.028
LINDT-EF(70)	2.878	-2.083	4.239	0.524	0.141	0.119	0.002
HACENDADO(85)	3.472	-2.998	8.783	0.746	1.383	11.458	0.159
HACENDADO(72)	1.603	1.256	1.542	0.614	0.401	0.965	0.063
HACENDADO(55)	6.598	6.035	35.586	0.837	2.619	41.100	0.158

Variables (the 10 first)

	Dim.1	ctr	cos2	Dim.2	ctr	cos2
o_cacao	-0.818	6.536	0.669	0.162	1.568	0.026
o_leche	0.841	6.904	0.707	0.323	6.236	0.104
s_azucar	0.993	9.624	0.985	0.022	0.029	0.000
s_acido	-0.878	7.534	0.771	-0.127	0.966	0.016
s_amargo	-0.980	9.378	0.960	-0.033	0.065	0.001
a_cacao	-0.949	8.807	0.901	0.126	0.949	0.016
a_leche	0.983	9.431	0.965	0.025	0.037	0.001
a_caramelo	0.907	8.041	0.823	-0.124	0.926	0.015
a_vainilla	0.962	9.036	0.925	-0.014	0.011	0.000
astringencia	-0.971	9.221	0.944	0.155	1.440	0.024


Individuals factor map (PCA)
HACENDADO(55)
HACENDADO(72)
LINDT-EF(85)
HACENDADO(85)
LINDT-NS(70)
VALRHONA(66)
VALRHONA(64)
VALRHONA(70)
LINDT-EF(70)
VALRHONA(85)
Dim 2 (10.79%)
Dim 1 (76.07%)


Variables factor map (PCA)
granuloso
crujiente
a_vainilla
o_cacao
a_leche
a_azucar
astringencia
a_cacao
a_caramelo
s_amargo
fusion
s_acido
Dim 2 (10.79%)
Dim 1 (76.07%)

Principal component analysis

Supplementary individuals and variables

• In order to project a supplementary or illustrative individual: its values for each of the variables, but centered (centered or standardized) are computed. Then the transition relationships are used to place it on every axis.

$$F_s(i^+) = \frac{1}{\sqrt{\lambda_s}} \sum_k \frac{x_{i^+k} - \bar{x}_k}{s_k} G_s(k)$$

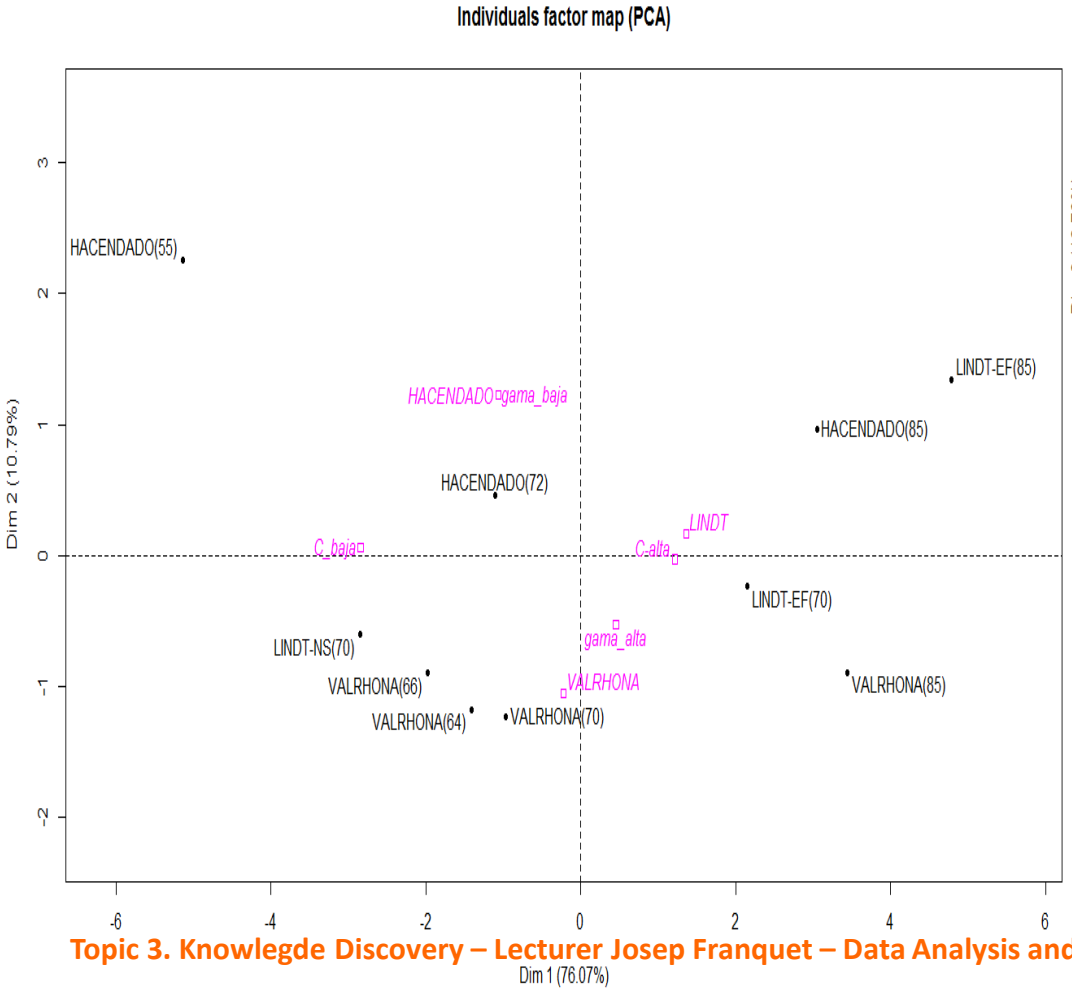
•A supplementary quantitative variable is placed on the axes through its correlations with the principal components.

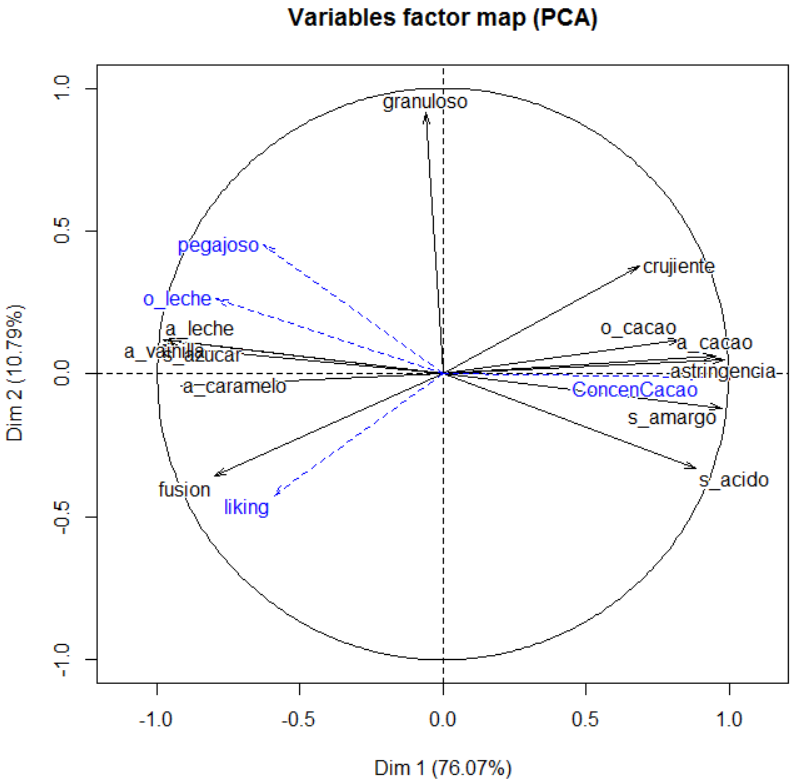
$$G_s(k^+) = corr(k^+, F_s)$$

• A category of a **supplementary categorical variable** (with *m* categories) is placed at the centroid of the individuals that belong to this category.

Individuals vs Variables Spaces

- Separate representation of both clouds
- The two clouds are not in the same space; They do not have the same referential
- Similarities between individuals are interpreted as corresponding to similar behavior as far as the active variables are concerned
- Proximities between variables are interpreted as correlations


Individuals factor map (PCA)
HACENDADO(55)
HACENDADO-gama_baja
HACENDADO(85)
LINDT-EF(85)
HACENDADO(72)
LINDT
C_baja
C-alta
LINDT-EF(70)
gama_alta
LINDT-NS(70)
VALRHONA(66)
VALRHONA
VALRHONA(85)
VALRHONA(64)
VALRHONA(70)
Dim 2 (10.79%)
Dim 1 (76.07%)


Variables factor map (PCA)
granuloso
pegajoso
crujiente
o_leche
a_leche
a_vainilla
s_azucar
o_cacao
a_cacao
astringencia
a_caramelo
ConcenCacao
s_amargo
s_acido
fusion
liking
Dim 2 (10.79%)
Dim 1 (76.07%)

Some more algebrea: Transition relationships between spaces

The total inertia of both clouds is the same

$$Inertia = \frac{1}{I}\sum_k \sum_i \left(\frac{x_{ik} - \bar{x}}{s_k} \right)^2 = \text{sum of variances}$$

Inertia total= nr of variables when the variables are standardized

In general, the inertia is equal to
- the sum of variances of the variables
- the sum of the trace of the variance-covariance matrix

Thus, this analysis performs a decomposition of the total inertia equivalent in both spaces. The inertia projected onto the same rank axis are equal.

How Many PCs?

- For K original dimensions, correlation matrix is K x K, and has up to K eigenvectors. So K PCs.
- Where does dimensionality reduction come from?
  - Retain a given percentage of data variability: 0.80 or 0.90 or 0.95.
  - Kaiser criteria: retain PCs with eigenvalue > mean(eigenvalues)
    - PCA Normalized: mean(eigenvalues) = 1

Principal Component Analysis (PCA)

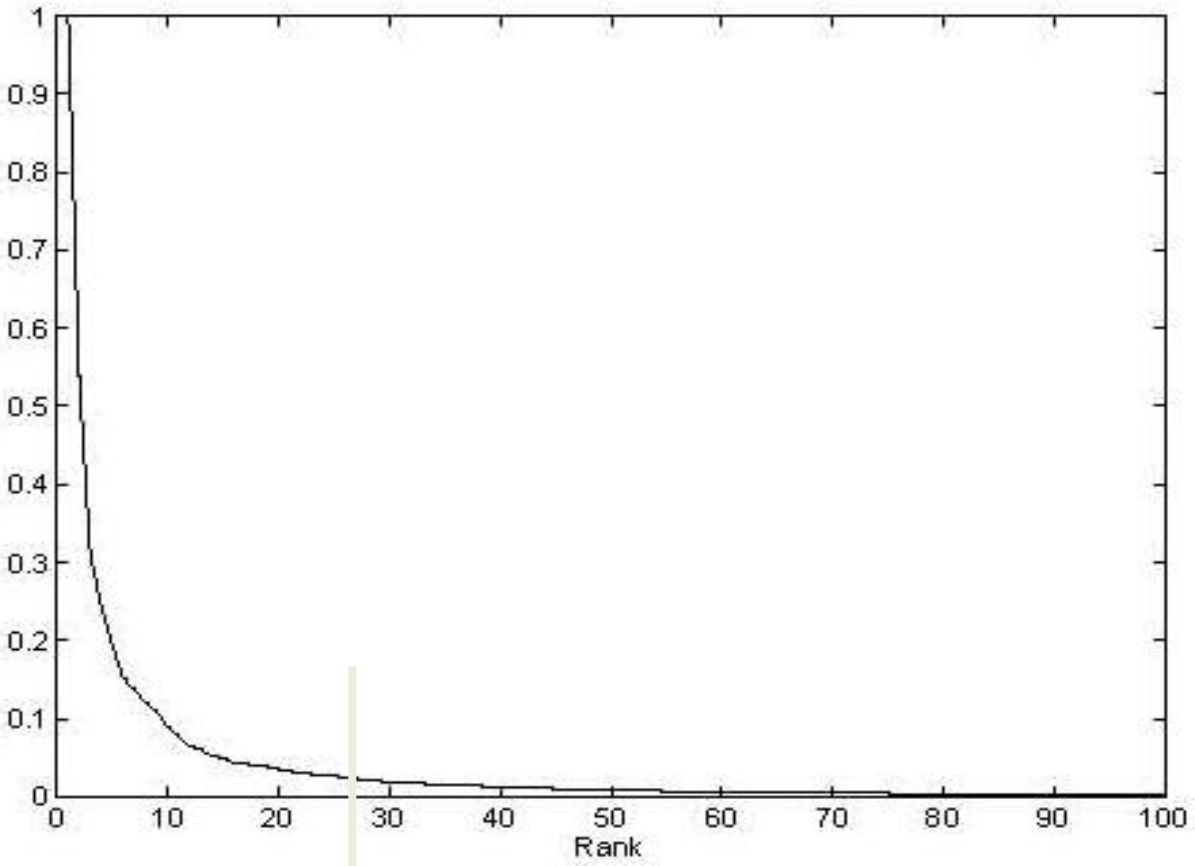
- How many principal components to keep?
  - To choose *K*, the following criterion can be used:

$$\frac{\sum_{i=1}^{K} \lambda_i}{\sum_{i=1}^{N} \lambda_i} > Threshold \quad \text{(e.g., 0.9 or 0.95)}$$

- Unfortunately for some data sets to meet this requirement we need K almost equal to I. That is, no effective data reduction is possible.

Principal Component Analysis (PCA)

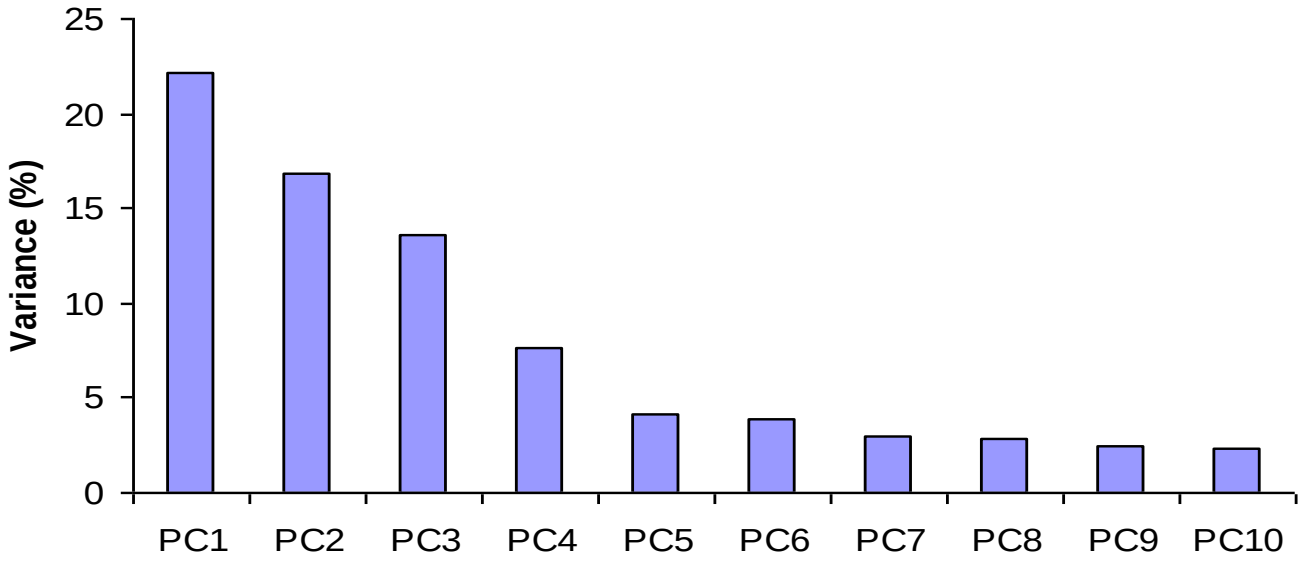
- Eigenvalue spectrum



Scree plot

Dimensionality Reduction

Can *ignore* the components of lesser significance.



You do loose some information, but if the eigenvalues are small, you don't lose much

- K dimensions in original data
- calculate K eigenvectors and eigenvalues
- choose only the first p eigenvectors, based on their eigenvalues
- final data set has only p dimensions

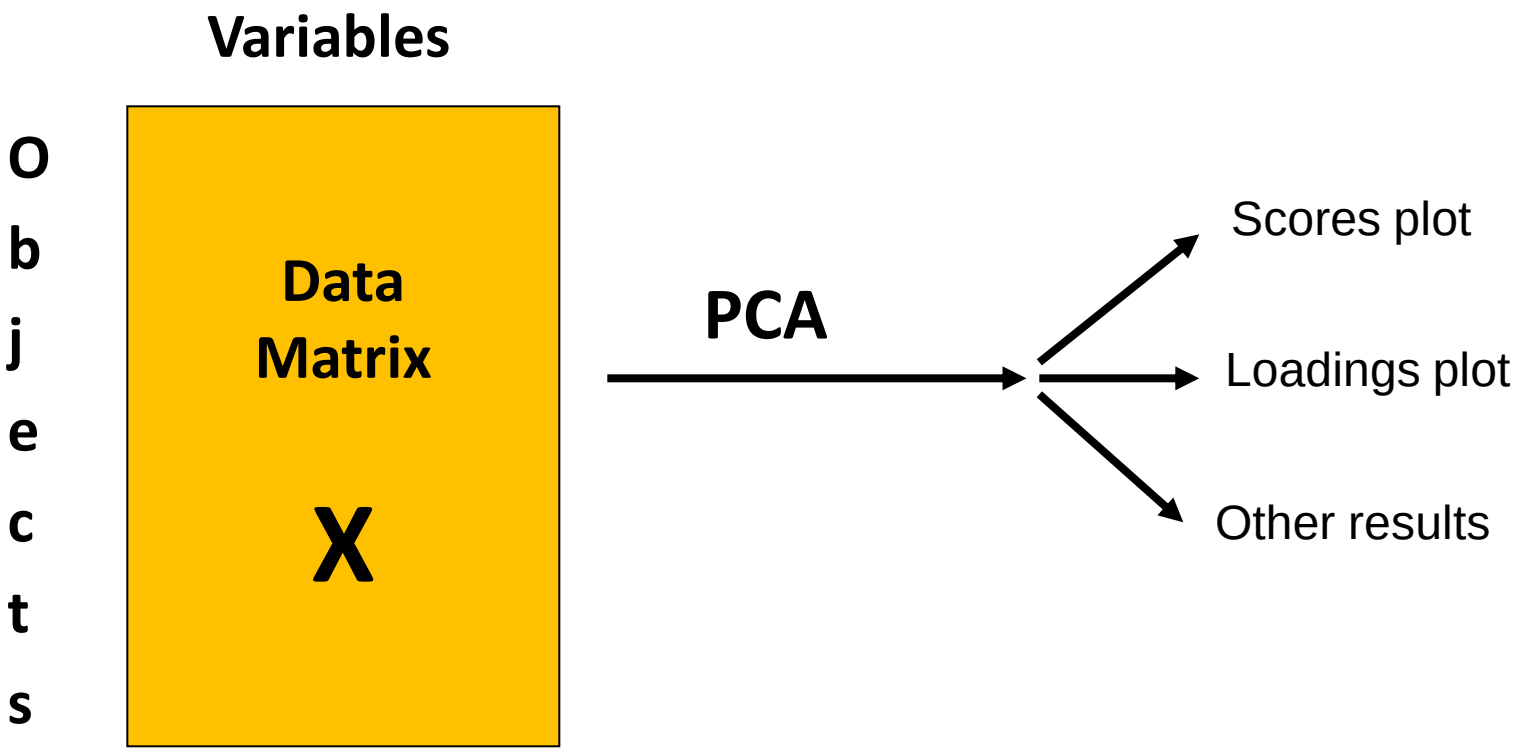
Principal Component Analysis (PCA)

- Probably the most widely-used and well-known of the "standard" multivariate methods
- Invented by Pearson (1901) and Hotelling (1933)
- First applied in ecology by Goodall (1954) under the name "factor analysis" ("principal factor analysis" is a synonym of PCA).

Principal Component Analysis (PCA)

- PCA takes a data matrix of *I* objects by *K* variables, which may be correlated, and summarizes it by uncorrelated axes (principal components or principal axes) that are linear combinations of the original *K* variables
- The first *k* components display as much as possible of the variation among objects.

Principal component analysis



The main plots

- **PCA Model : $X=TP^T + E$**

  The matrix X is modelled as components (systematic effects) plus residuals, E (noise)

- **Scores plot**
  - For interpreting relations among samples
- **Loadings plot**
  - For interpreting relations among variables
- **Explained variance plot**
- **Addition of supplementary variables is very useful for interpretation**

Loadings plots

- Usually 2-dimensions are shown, firstly PC1 and PC2.
- Higher dimension PCs, (PCk,PCk') relationships have to be checked.
- For spectroscopy and other continuous measurements, 1-dimensional plots are used.

Guidelines for how to interpret the plots

- Variables which are close have high correlation
- Samples which are close are similar
- Variables on opposite side of origin have negative correlation
- Objects on the right are dominated by variables to the right and so on….

PCA Conclusions

- PCA
  - finds orthonormal basis for data
  - Sorts dimensions in order of “importance”
  - Discard low significance dimensions

- Uses:
  - Get compact description
  - Ignore noise
  - Improve classification (hopefully)

- Not magic:
  - Doesn’t know class labels
  - Can only capture linear variations

- One of many tricks to reduce dimensionality!