Certificate Data Science for Managment

Introduction to Dimensionality Reduction

X – HEC, Spring 2020

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https://github.com/jchiquet/CourseUnsupervisedLearningX

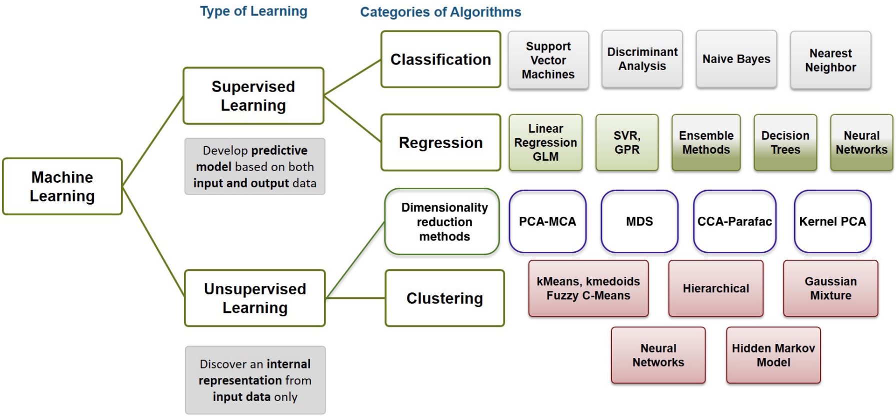
Part I

Introduction

Packages required for reproducing the slides

```
library(tidyverse)  # opinionated collection of packages for data manipulation
library(GGally)     # extension to ggplot vizualization system
library(FactoMineR) # PCA and oter linear method for dimension reduction
library(factoextra) # fancy plotting for FactoMineR output
# color and plots themes
library(RColorBrewer)
pal <- brewer.pal(10, "Set3")
theme_set(theme_bw())
```

Machine Learning



Supervised vs Unsupervised Learning

Supervised Learning

- Training data $\mathcal{D}_n = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}, X_i \sim^{\text{i.i.d}} \mathbb{P}$
- Construct a predictor $\hat{f} : \mathcal{X} \to \mathcal{Y}$ using $\mathcal{D}_n$
- Loss $\ell(y, f(x))$ measures how well $f(x)$ predicts y
- Aim: minimize the generalization error
- Task: Regression, Classification

$\rightsquigarrow$ The goal is clear: predict y based on x (regression, classification)

Unsupervised Learning

- Training data $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$
- Loss? , Aim?
- Task: **Dimension reduction**, Clustering

$\rightsquigarrow$ The goal is less well defined, and *validation* is questionable

Dimension Reduction?

Figure: source: F. Belardi

- How to view a high-dimensional dataset ?
- High-dimension: dimension larger than 2!
- *Projection* in a 2D space.

Dimension Reduction?

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Dimension Reduction?

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- *Projection* in a 2D space.

Companion data set: 'crabs'

Morphological Measurements on Leptograpsus Crabs

Description: *small data, low-dimensional*

The crabs data frame has 200 rows and 8 columns, describing 5 morphological measurements on 50 crabs each of two colour forms and both sexes, of the species *Leptograpsus variegatus* collected at Fremantle, W. Australia.

Figure: A leptograpsus Crab

Companion data set: 'crabs' I

Table header

```
crabs <- MASS::crabs %>% select(-index) %>%
  rename(sex = sex,
         species          = sp,
         frontal_lob      = FL,
         rear_width       = RW,
         carapace_length = CL,
         carapace_width  = CW,
         body_depth       = BD)
crabs %>% select(sex, species) %>% summary() %>% knitr::kable("latex")
```

	sex	species
	F:100	B:100
	M:100	O:100

```
dim(crabs)

## [1] 200   7
```

Companion data set: 'crabs' II

Table header

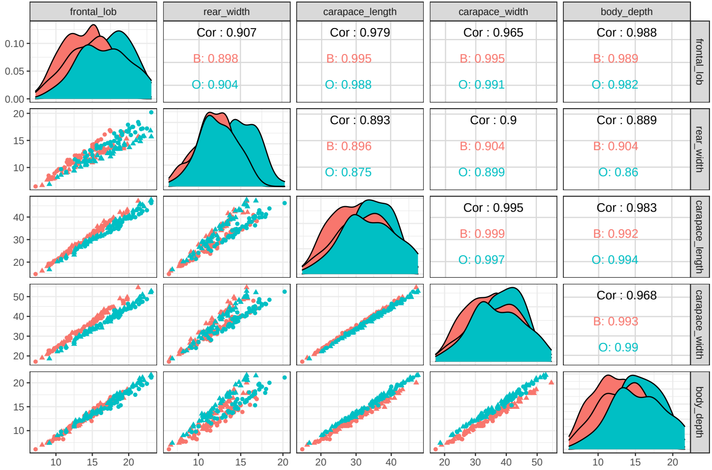
```r
crabs %>% head(15) %>% knitr::kable("latex")
```

species	sex	frontal_lob	rear_width	carapace_length	carapace_width	body_depth
B	M	8.1	6.7	16.1	19.0	7.0
B	M	8.8	7.7	18.1	20.8	7.4
B	M	9.2	7.8	19.0	22.4	7.7
B	M	9.6	7.9	20.1	23.1	8.2
B	M	9.8	8.0	20.3	23.0	8.2
B	M	10.8	9.0	23.0	26.5	9.8
B	M	11.1	9.9	23.8	27.1	9.8
B	M	11.6	9.1	24.5	28.4	10.4
B	M	11.8	9.6	24.2	27.8	9.7
B	M	11.8	10.5	25.2	29.3	10.3
B	M	12.2	10.8	27.3	31.6	10.9
B	M	12.3	11.0	26.8	31.5	11.4
B	M	12.6	10.0	27.7	31.7	11.4
B	M	12.8	10.2	27.2	31.8	10.9
B	M	12.8	10.9	27.4	31.5	11.0

Companion data set: 'crabs'

Pairs plot of attributes

```r
ggpairs(crabs, columns = 3:7, aes(colour = species, shape = sex))
```



⇝ Pairs plot don't help...

Companion data set: 'crabs'

Correlation matrix

```
crabs %>%  select(-species, -sex) %>% cor( ) %>% kable('latex', digits = 3)
```

	frontal_lob	rear_width	carapace_length	carapace_width	body_depth
frontal_lob	1.000	0.907	0.979	0.965	0.988
rear_width	0.907	1.000	0.893	0.900	0.889
carapace_length	0.979	0.893	1.000	0.995	0.983
carapace_width	0.965	0.900	0.995	1.000	0.968
body_depth	0.988	0.889	0.983	0.968	1.000

Very high correlation!

- much redundancy?
- hidden factor?

$\leadsto$ dimension reduction might hem

Another example: 'snp'

Genetics variant in European population

Description: *medium/large data, high-dimensional*

500, 000 Genetics variants (SNP – Single Nucleotide Polymorphism) for 3000 individuals (1 meter × 166 meter (height × width)

- SNP : 90 % of human genetic variations

- coded as 0, 1 or 2 (10, 1 or 2 allel different against the population reference)

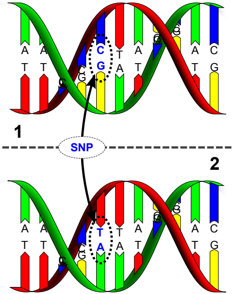


Figure: SNP (wikipedia)

Summarize 500,000 variables in 2

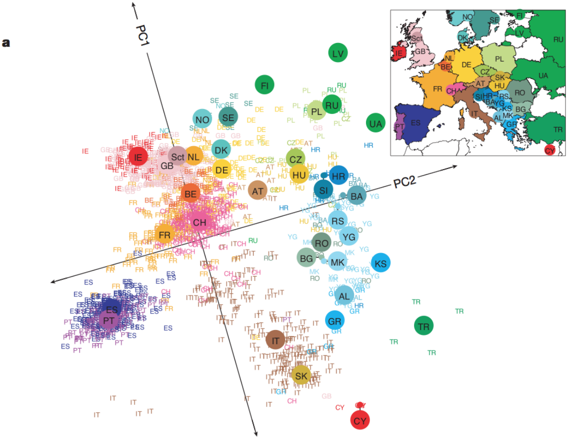


Figure: PCA output source: Nature "Gene Mirror Geography Within Europe", 2008

⇝ How much information is lost?

Theoretical argument: dimensionality Curse

High Dimension Geometry Curse

- Folks theorem: In high dimension, everyone is alone.
- Theorem: If $\mathbf{x}_1, \dots, \mathbf{x}_n$ in the hypercube of dimension d such that their coordinates are i.i.d then

$$d^{-1/p}\left(\max \|\mathbf{x}_i - \mathbf{x}_{i'}\|_p - \min \|\mathbf{x}_i - \mathbf{x}_{i'}\|_p\right) = 0 + O\left(\sqrt{\frac{\log n}{d}}\right)$$

$$\frac{\max \|\mathbf{x}_i - \mathbf{x}_{i'}\|_p}{\min \|\mathbf{x}_i - \mathbf{x}_{i'}\|_p} = 1 + O\left(\sqrt{\frac{\log n}{d}}\right).$$

$\rightsquigarrow$ When d is large, all the points are almost equidistant
Hopefully, the data **are not really leaving in d** dimension (think of the SNP example)

Dimension reduction: goals summary

Main objective: find a **low-dimensional representation** that captures the "essence" of (high-dimensional) data

Application in Machine Learning

Preprocessing, Regularization

- compression, denoising, anomaly detection
- Reduce overfitting in supervised learning (improve performances)

Application in statistics and data analysis

Better understand the data

- descriptive/exploratory methods
- visualization: difficult to plot and interpret $> 3d$!

Dimension reduction: problem setup

Settings

- Training data : $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \in \mathbb{R}^d$, (i.i.d.)
- Space $\mathbb{R}^d$ of possibly high dimension $(n \ll d)$

Dimension Reduction Map

Construct a map Φ from the space $\mathbb{R}^d$ into a space $\mathbb{R}^{d'}$ of smaller dimension:

$$\begin{aligned} \Phi : \quad & \mathbb{R}^d \to \mathbb{R}^{d'}, d' \ll d \\ & \mathbf{X} \mapsto \Phi(\mathbf{X}) \end{aligned}$$

How should we design/construct Φ?

Criterion

- **Geometrical approach**
- Reconstruction error
- Relationship preservation

Form of the map Φ

- **Linear** or non-linear ?
- tradeoff between **interpretability** and versatility ?
- tradeoff between high or **low** computational resource

Part II

Principal Component Analysis

Some references. . .

. . . biased choices!

- Analyse en composantes principales, Course AgroParisTech
  Carine Ruby, Stéphane Robin
  http://www.agroparistech.fr/IMG/pdf/AnalyseComposantesPrincipales-AgroParisTech.pdf
- Exploratory Multivariate Analysis by Example using R,
  Husson, Le, Pages, 2017.
  Chapman & Hall
- Multiple Factor Analysis by Example using R,
  J. Pagès 2015.
  CRC Press
- An Introduction to Statistical Learning
  G. James, D. Witten, T. Hastie and R. Tibshirani
  http://faculty.marshall.usc.edu/gareth-james/ISL/

PCA and classical Linear methods

Principal component Analysis (PCA) is for continuous data

Non continuous data

- Correspondence analysis (CA): contingency table
- Multiple correspondence analysis (MCA): categorical data
- Multiple factor analysis (MFA): multi-table, array data

$\rightsquigarrow$ Basic adaptation that build on PCA to deal with non-continuous data
$\rightsquigarrow$ smart encoding of non-continuous data to continuous ones

We will focus on PCA, as the mother or most linear (and non-linear) methods.

The data matrix

The data set is a $n \times d$ matrix $\mathbf{X} = (x_{ij})$ with values in $\mathbb{R}$:

- each row $\mathbf{x}_i$ represents an individual/observation
- each col $\mathbf{x}^j$ represents a variable/attribute

```
crabs %>% head(6) %>% knitr::kable("latex")
```

species	sex	frontal_lob	rear_width	carapace_length	carapace_width	body_depth
B	M	8.1	6.7	16.1	19.0	7.0
B	M	8.8	7.7	18.1	20.8	7.4
B	M	9.2	7.8	19.0	22.4	7.7
B	M	9.6	7.9	20.1	23.1	8.2
B	M	9.8	8.0	20.3	23.0	8.2
B	M	10.8	9.0	23.0	26.5	9.8

Objectives

Individual/Observations

- similarity between observations with respect to all the variables
- Find pattern ($\sim$ partition) between individuals

Variables

- linear relationships between variables
- visualization of the correlation matrix
- find synthetic variables

Link between the two

- characterization of the groups of individuals with variables
- specific observations to understand links between variables

Outline

Principal Component Analysis

1. Background: high-school algebra
2. Geometric approach to PCA
3. Principal axes and variance maximization
4. Representation and interpretation
5. Additional tools and Complements
6. Beyond linear methods

Vectors in $\mathbb{R}^n$

Definition and Basics

A vector $\mathbf{x} \in \mathbb{R}^d$ is defined by a d-uplet $(x_1, x_2, \ldots, x_d)$, *its coordinates*.

Elementary operations

- Addition of two vectors (define a parallelogram)
- Multiplication by a scalar (streching)

$$\mathbf{x} + \mathbf{y} = \begin{pmatrix} x_1 + y_1 \\ x_2 + y_2 \\ \vdots \\ x_d + y_d \end{pmatrix}$$

$$\lambda \mathbf{x} = \begin{pmatrix} \lambda x_1 \\ \lambda x_2 + c \\ \vdots \\ \lambda x_d \end{pmatrix}, \quad \lambda, c \in \mathbb{R}.$$

Properties

- associativity: $(\mathbf{x} + \mathbf{y}) + \mathbf{z} = \mathbf{x} + (\mathbf{y} + \mathbf{z})$
- commutativity: $\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}$
- linearity: $\lambda(\mathbf{x} + \mathbf{y}) = \lambda \mathbf{x} + \lambda \mathbf{y}$
- $(\lambda_1 + \lambda_2)\mathbf{x} = \lambda_1 \mathbf{x} + \lambda_2 \mathbf{x}$

Vectors in $\mathbb{R}^n$

Dot/Inner product and norm

Dot product of 2 vectors: sum of the products between each coordinate:

$$\langle \mathbf{x}, \mathbf{y} \rangle \equiv \mathbf{x} \cdot \mathbf{y} \equiv \mathbf{x}^\top \mathbf{y} \triangleq \sum_{i=1}^{d} x_i \, y_j .$$

- $\mathbf{x}^\top \mathbf{y} = \mathbf{y}^\top \mathbf{x}$
- $\mathbf{x}^\top (\mathbf{y} + \mathbf{z}) = \mathbf{x}^\top \mathbf{y} + \mathbf{x}^\top \mathbf{z}$
- $\lambda(\mathbf{x}^\top \mathbf{y}) = (\lambda(\mathbf{x})^\top \mathbf{y} = \mathbf{x}^\top (\lambda \mathbf{y})$
- if $\mathbf{x} = \mathbf{0}$, then $\mathbf{x}^\top \mathbf{x} = 0$.

(Euclidean) norm (a.k.a length, magnitude)

$$\|\mathbf{x}\| = \sqrt{\mathbf{x}^\top \mathbf{x}}. \quad \text{we have } \|\lambda \mathbf{x}\| = |\lambda| \|\mathbf{x}\|.$$

Vectors in $\mathbb{R}^n$

Distances and orthogonality

(Euclidean) distance between 2 vectors

$$\mathsf{dist}(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|.$$

Remark that when $\mathbf{x}$ and $\mathbf{y}$ are orthogonal and non zero, distances between $\mathbf{x}$ and $\mathbf{y}$ and $\mathbf{x}$ and $(-\mathbf{y})$ are the same. Then,

$$(\mathbf{x} - \mathbf{y})^\top (\mathbf{x} - \mathbf{y}) = (\mathbf{x} + \mathbf{y})^\top (\mathbf{x} + \mathbf{y}) \Leftrightarrow \mathbf{x}^\top \mathbf{y} = 0,$$

which motivates the following definition of orthornality:

Orthogonality

Two vectors $\mathbf{x}, \mathbf{y} \neq \mathbf{0}$ are orthogonal iff $\mathbf{x}^\top \mathbf{y} = 0$.

(Euclidean) distance between 2 vectors

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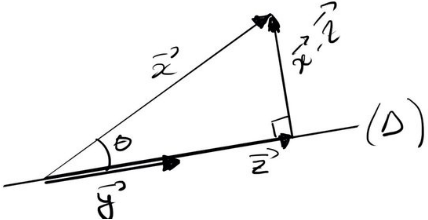
Orthogonal projection of $\mathbf{x}$ onto $\mathbf{y}$



It is the vector $\mathbf{z}$ such that

1. $\mathbf{z} = \lambda \mathbf{y}$
2. $\mathbf{y}$ is orthogonal to $\mathbf{x} - \mathbf{z}$

We find $\lambda = \mathbf{x}^\top \mathbf{y} / \|\mathbf{y}\|^2$

Thanks to Pythagoras theorem,

$$\cos(\theta) = \frac{\|\mathbf{z}\|}{\|\mathbf{x}\|} = \lambda \frac{\|\mathbf{y}\|}{\|\mathbf{x}\|}$$

and then we end with the following geometric definition of the dot product

Dot product: geometric definition

$$\mathbf{x}^\top \mathbf{y} = \cos(\theta) \|\mathbf{x}\| \, \|\mathbf{y}\|$$

Orthogonal projection of $\mathbf{x}$ onto $\mathbf{y}$

It is the vector $\mathbf{z}$ such that

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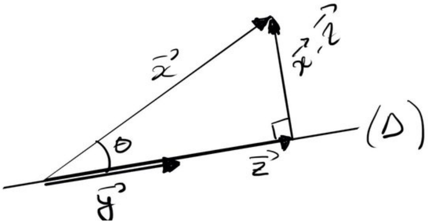

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Dot product: geometric definition

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Outline
Principal Component Analysis

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The data set is a $n \times d$ matrix $\mathbf{X} = (x_{ij})$ with values in $\mathbb{R}$:

- each row $\mathbf{x}_i$ represents an individual/observation
- each col $\mathbf{x}^j$ represents a variable/attribute

$$
\mathbf{X} = \begin{array}{cc}
 & \begin{array}{cccccc} \mathbf{x}^1 & \mathbf{x}^2 & \dots & \mathbf{x}^j & \dots & \mathbf{x}^d \end{array} \\
\begin{array}{c} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_i \\ \vdots \\ \mathbf{x}_n \end{array} &
\begin{pmatrix}
x_{11} & x_{12} & \dots & x_{1j} & \dots & x_{1d} \\
x_{21} & x_{22} & \dots & x_{2j} & \dots & x_{2d} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
x_{i1} & x_{i2} & \dots x_{ij} & \dots & x_{id} & \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
x_{n1} & x_{n2} & \dots x_{nj} & \dots & x_{nd} &
\end{pmatrix}
\end{array}
$$

```r
crabs %>% head(3) %>% knitr::kable("latex")
```

species	sex	frontal_lob	rear_width	carapace_length	carapace_width	body_depth
B	M	8.1	6.7	16.1	19.0	7.0
B	M	8.8	7.7	18.1	20.8	7.4
B	M	9.2	7.8	19.0	22.4	7.7

Cloud of observation in $\mathbb{R}^d$

Individuals can be represented in the variable space $\mathbb{R}^d$ as a point cloud

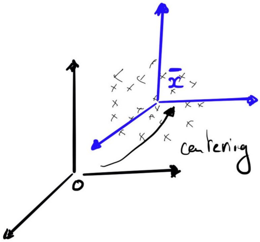


Figure: Example in $\mathbb{R}^3$

Center of Intertia

(or barycentrum, or empirical mean)

$$\bar{\mathbf{x}} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i = \begin{pmatrix} \sum_{i=1}^{n} x_{i1}/n \\ \sum_{i=1}^{n} x_{i2}/n \\ \vdots \\ \sum_{i=1}^{n} x_{id}/n \end{pmatrix}$$

We center the cloud $\mathbf{X}$ around $\mathbf{x}$ denote this by $\mathbf{X}^c$

$$\mathbf{X}^c = \begin{pmatrix} x_{11} - \bar{x}_1 & \dots & x_{1j} - \bar{x}_j & \dots & x_{1d} - \bar{x}_d \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{i1} - \bar{x}_1 & \dots & x_{ij} - \bar{x}_j & \dots & x_{id} - \bar{x}_d \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{n1} - \bar{x}_1 & \dots & x_{nj} - \bar{x}_j & \dots & x_{nd} - \bar{x}_d \end{pmatrix}$$

Inertia and Variance

Total Inertia: distance of the individuals to the center of the cloud

$$I_T = \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{d}(x_{ij}-\bar{x}_j)^2 = \frac{1}{n}\sum_{i=1}^{n}\|\mathbf{x}_i-\bar{\mathbf{x}}\|^2 = \frac{1}{n}\sum_{i=1}^{n}\mathsf{dist}^2(\mathbf{x}_i,\bar{\mathbf{x}})$$

I_T is proportional to the total variance

Let $\hat{\mathbf{\Sigma}}$ be the empirical variance-covariance matrix

$$I_T = \frac{1}{n}\sum_{j=1}^{p}\sum_{i=1}^{n}(x_{ij}-\bar{x}_j)^2 = \sum_{j=1}^{n}\frac{1}{n}\|\mathbf{x}^j-\bar{x}_j\|^2 = \sum_{j=1}^{n}\mathbb{V}(\mathbf{x}^j) = \mathrm{trace}\Big(\hat{\mathbf{\Sigma}}\Big)$$

- $\rightsquigarrow$ Good representation has large inertia (much variability)
- $\rightsquigarrow$ Large dispertion $\sim$ Large distances between points

Inertia with respect to an axix

The Inertia of the cloud wrt axe Δ is the sum of the distances between all points and their orthogonal projection on Δ.

$$I_\Delta = \frac{1}{n}\sum_{i=1}^{n} \mathsf{dist}^2(\mathbf{x}_i, \mathsf{proj}_\Delta(\mathbf{x}_i))$$

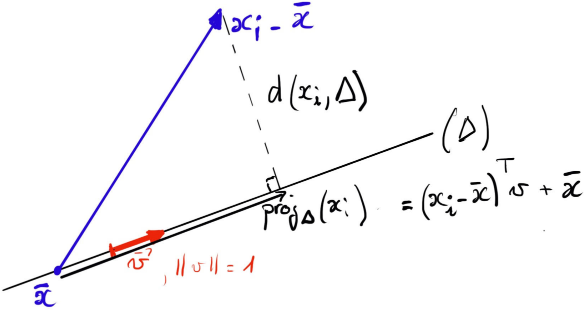
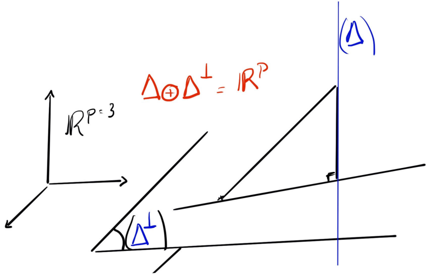


Figure: Projection of $\mathbf{x}_i$ onto a line Δ passing through $\bar{\mathbf{x}}$

Decomposition of total Inertia (1)

Let $\Delta^\perp$ the orthogonal subspace Δ is $\mathbb{R}^n$



Theorem (Huygens)

A consequence of the above (Pythagoras Theorem) is the decomposition of the following total inertia:

$$I_T = I_\Delta + I_{\Delta^\perp}$$

By projecting the cloud $\mathbf{X}$ onto Δ, with loss the inertia measured by $\Delta^\perp$

Decomposition of total Inertia (2)

Consider only subspaces with dimension 1 (that is, lines or axes). We can decompose $\mathbb{R}^p$ the sum of p othogonal axis.

$$\mathbb{R}^p = \Delta_1 \oplus \Delta_2 \oplus \cdots \oplus \Delta_p$$

$\rightsquigarrow$ These axes form a new basis for representing the point cloud.

Theorem (Huygens)

$$I_T = I_{\Delta_1} + I_{\Delta_2} + \cdots + I_{\Delta_p}$$

Outline

Principal Component Analysis

Finding the best axis (1)

Definition of the problem

- The best axis Δ_1 is the "closest" to the point cloud
- Inertia of Δ_1 measures the distance between the data and Δ_1
- Δ_1 is defined by the director vector $\mathbf{u}_1$, such as $\|\mathbf{u}_1\| = 1$
- $\Delta_1^\perp$ is defined by the normal vector $\mathbf{u}_1$, such as $\|\mathbf{u}_1\| = 1$

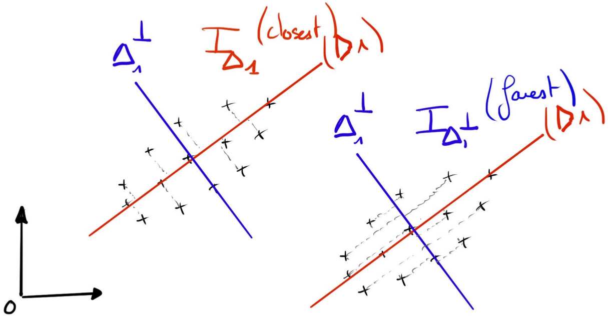
$\rightsquigarrow$ The best axis Δ_1 is the one with the minimal Inertia.

Finding the best axis (2)

Stating the optimization problem

Since $\Delta_1 \oplus \Delta_1^\perp = \mathbb{R}^p$ and $I_T = I_{\Delta_1} + I_{\Delta_1^\perp}$, then

$$\underset{\mathbf{u}\in\mathbb{R}^p:\|\mathbf{u}\|=1}{\text{minimize}}\ I_{\Delta_1} \Leftrightarrow \underset{\mathbf{u}\in\mathbb{R}^p:\|\mathbf{u}\|=1}{\text{maximize}}\ I_{\Delta_1^\perp}$$



Finding the best axis (3)

Stating the problem (algebraically)

Find $\mathbf{u}_1; \|\mathbf{u}_1\| = 1$ that minimizes

$$
\begin{aligned}
I_{\Delta_1^\perp} &= \frac{1}{n}\sum_{i=1}^{n} \text{dist}(x_i, \Delta_1^\perp)^2 \\
&= \frac{1}{n}\sum_{i=1}^{n} \mathbf{u}_1^\top(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^\top \mathbf{u}_1 \\
&= \mathbf{u}_1^\top \left(\sum_{i=1}^{n} \frac{1}{n}(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^\top \right) \\
&= \mathbf{u}_1^\top \hat{\mathbf{\Sigma}} \mathbf{u}_1
\end{aligned}
$$

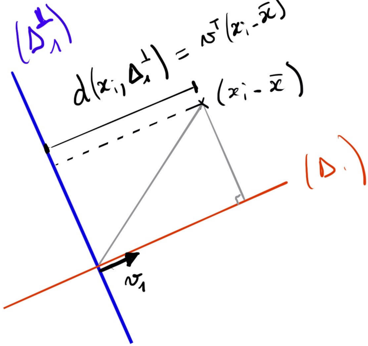


Figure: Geometrical insight

Finding the best axis (4)

We solve a simple constraint maximization problem with the method of Lagrange multipliers:

$$\underset{\mathbf{u}_1 : \|\mathbf{u}_1\|=1}{\text{maximize}}\, \mathbf{u}_1^\top \hat{\boldsymbol{\Sigma}} \mathbf{u}_1 \Leftrightarrow \underset{\mathbf{u}_1 \in \mathbb{R}^p, \lambda_1 > 0}{\text{maximize}}\, \mathbf{u}_1^\top \hat{\boldsymbol{\Sigma}} \mathbf{u}_1 - \lambda_1(\|\mathbf{u}_1\| - 1)$$

By straightforward (vector) differentiation, an using that $\mathbf{u}_1^\top \mathbf{u}_1 = 1$

$$\begin{cases} 2\hat{\boldsymbol{\Sigma}}\mathbf{u}_1 - 2\lambda_1 \mathbf{u}_1 = 0 \\ \mathbf{u}_1^\top \mathbf{u}_1 - 1 = 0 \end{cases} \Leftrightarrow \begin{cases} \hat{\boldsymbol{\Sigma}}\mathbf{u}_1 = \lambda_1 \mathbf{u}_1 \\ \mathbf{u}_1^\top \hat{\boldsymbol{\Sigma}} \mathbf{u}_1 = \lambda_1 \mathbf{u}_1^\top \mathbf{u}_1 = \lambda_1 = I_{\Delta_1}^\perp \end{cases}$$

- $\mathbf{u}_1$ is the first eigen vector of $\hat{\boldsymbol{\Sigma}}$
- λ_1 is the first eigen value of $\hat{\boldsymbol{\Sigma}}$

$\rightsquigarrow$ **Δ_1 is defined by the first eigen vector of $\hat{\boldsymbol{\Sigma}}$**
$\rightsquigarrow$ **Variance "carried" by Δ_1 is equal to the largest eigen value of $\hat{\boldsymbol{\Sigma}}$**

Finding the following axes

Second best axis

Find Δ_2 with dimension 1, director vector $\mathbf{u}_2$ orthogonal to Δ_1 solving

$$\underset{\mathbf{u}_2 \in \mathbb{R}^p}{\text{maximize}}\, I_{\Delta_2^\perp} = \mathbf{u}_2^\top \hat{\boldsymbol{\Sigma}} \mathbf{u}_2, \quad \text{with } \|\mathbf{u}_2\| = 1, \mathbf{u}_1^\top \mathbf{u}_2 = 0.$$

$\rightsquigarrow$ $\mathbf{u}_2$ is the second eigen vector of $\hat{\boldsymbol{\Sigma}}$ with eigen value λ_2

And so on!

PCA is roughly a matrix factorisation problem

$$\hat{\boldsymbol{\Sigma}} = \mathbf{U} \boldsymbol{\Lambda} \mathbf{U}^\top, \quad \mathbf{U} = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2, & \dots & \mathbf{u}_p \end{pmatrix}, \quad \boldsymbol{\Lambda} = \mathrm{diag}(\lambda_1, \dots, \lambda_p)$$

- $\mathbf{U}$ is an orthogonal matrix of normalized eigen vectors.
- $\boldsymbol{\Lambda}$ is diagonal matrix of ordered eigen values.

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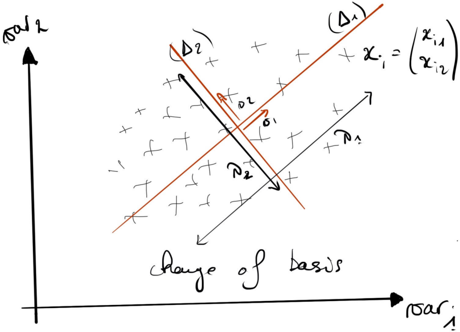
- $\mathbf{\Lambda}$ is diagonal matrix of ordered eigen values.

Interpretation in $\mathbb{R}^p$

$\mathbf{V}$ describes a new orthogonal basis and a rotation of data in this basis
$\rightsquigarrow$ PCA is an appropriate rotation on axes that maximizes the variance

$$\begin{cases} \Delta_1 & \oplus & \dots & \oplus & \Delta_p \\ \mathbf{u}_1 & \perp & \dots & \perp & \mathbf{u}_2 \\ \lambda_1 & > & \dots & > & \lambda_p \\ I_{\Delta_1^\perp} & > & \dots & > & I_{\Delta_p^\perp} \end{cases}$$



Outline

Principal Component Analysis

Contribution of each axis and quality of the representation

Δ_k is carrying inertia/variance defined by its orthogonal, thus

$$I_T = I_{\Delta_1^\perp} + \cdots + I_{\Delta_p^\perp} = \lambda_1 + \cdots + \lambda_p$$

Relative contribution of axis k

$$\mathrm{contrib}(\Delta_k) = \frac{\lambda_k}{\sum_{k=1}^{p} \lambda_j} = \frac{\lambda_k}{\mathrm{trace}\left(\hat{\Sigma}\right)} \times 100$$

$\rightsquigarrow$ Percentage of explained inertia/variance explained

Global quality of the representation on the first k axes

$$\mathrm{contrib}(\Delta_1, \dots, \Delta_k) = \frac{\lambda_1 + \cdots + \lambda_k}{\mathrm{trace}\left(\hat{\Sigma}\right)} \times 100$$

A few axes may explain a large proportion of the total variance.
$\rightsquigarrow$ This paves the way for dimension reduction

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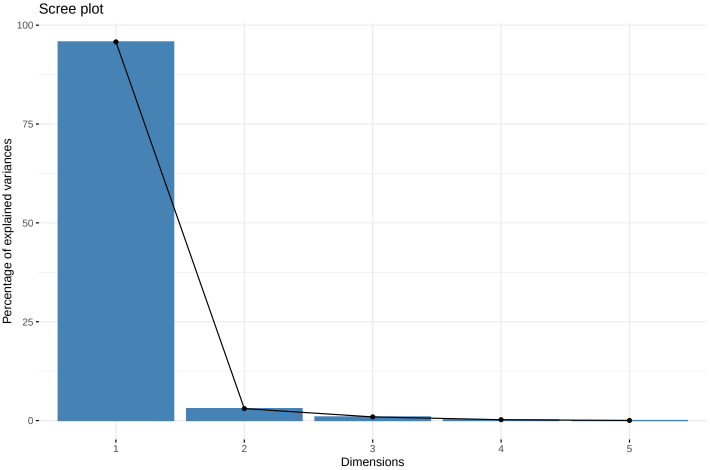
A few axes may explain a large proportion of the total variance.
$\rightsquigarrow$ This paves the way for dimension reduction

Scree plot: 'crabs'

```
crabs_pca <- select(crabs, -species, -sex) %>% FactoMineR::PCA(graph = FALSE)
fviz_eig(crabs_pca)
```



$\rightsquigarrow$ We will see during labs why everything is carried by the first axis

Outline

Principal Component Analysis

Individuals: representation in the new basis

Projection of point $\mathbf{x}_i$ axis k

The projection of $\mathbf{x}_i$ onto axis Δ_k is $c_{ik}\mathbf{u}_k$, with

$$c_{ik} = \mathbf{u}_k^\top (\mathbf{x}_i - \bar{\mathbf{x}}),$$

the coordinate of i in the basis $\mathbf{u}_k$ (along axis Δ_k).

Coordinates of i in the new basis

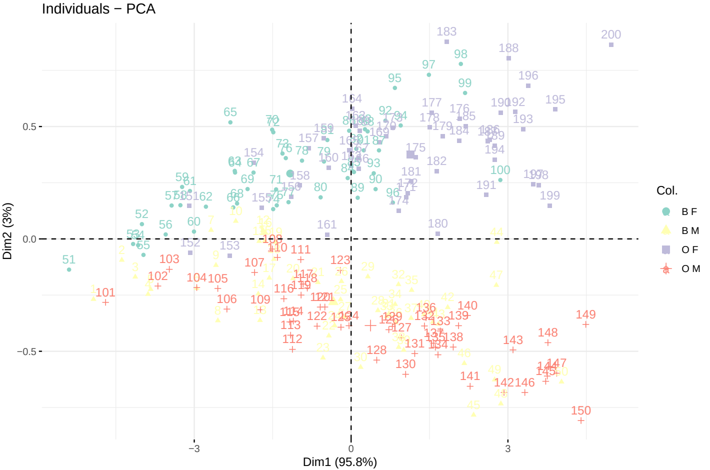
Coordinates of i in the new basis $\{\mathbf{u}1, \dots, \mathbf{u}_d\}$ is thus

$$\mathbf{c}_i = (\mathbf{U}^\top(\mathbf{x}_i - \bar{\mathbf{x}}))^\top = (\mathbf{x}_i - \bar{\mathbf{x}})^\top \mathbf{U} = \mathbf{X}_i^c \mathbf{U}, \quad \tilde{\mathbf{x}}_i \in \mathbb{R}^p.$$

- $\mathbf{U}$ are often the called the **loadings**, or **weights**
- $\tilde{\mathbf{c}}_i$ are the **scores** or **coordinates** in the new space for the individuals

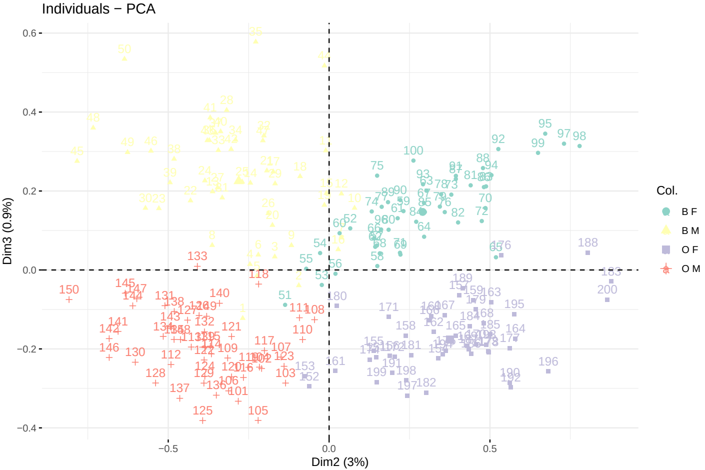
Individual visualization: projection in the new basis (1)

```r
fviz_pca_ind(crabs_pca, col.ind = paste(crabs$species, crabs$sex), palette = pal)
```



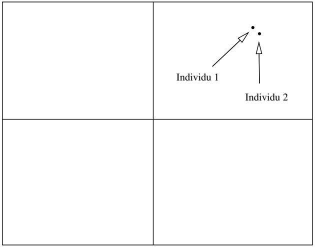
Individual visualization: projection in the new basis (2)

```
fviz_pca_ind(crabs_pca, axes = c(2,3), col.ind = paste(crabs$species, crabs$sex), p
```



Warning: about distances after projection

Close projection doesn't mean close individuals!



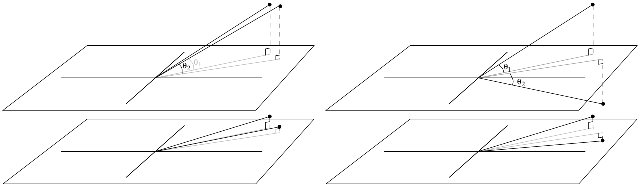


Figure: Same projections but different situations (source: E. Matzner)

⇝ Only work when individuals are well represented in the lower space

Individual: quality of the representation

Property

- An individual i is well represented by Δ_k if it is close to this axis.
- In other word, vector $\mathbf{x}_i - \bar{\mathbf{x}}$ and $\mathbf{u}_k$ are close to collinear

We use the cosine of the angle θ_{ik} between $\mathbf{x}_i - \bar{\mathbf{x}}$ and $\mathbf{u}_k$ to measure the degree of co-linearity:

$$\cos 2(\theta_{ik}) = \frac{\left(\mathbf{u}_k^\top (\mathbf{x}_i - \bar{\mathbf{x}})\right)^2}{\|\mathbf{x}_i - \bar{\mathbf{x}}\|^2 \cancel{\|\mathbf{u}_k\|^2}}$$

```r
factoextra::get_pca_ind(crabs_pca)$cos2 %>% head(3) %>% kable("latex")
```

Dim.1	Dim.2	Dim.3	Dim.4	Dim.5
0.9961694	0.0029565	0.0006132	6.29e-05	1.98e-04
0.9994582	0.0004598	0.0000800	1.60e-06	5.00e-07
0.9980940	0.0016699	0.0000663	8.50e-05	8.48e-05

Individual: contribution to an axis

Property

- Inertia "explained" by Δ_k is inertia of $\Delta_k^\perp$
- $I_{\Delta_k^\perp} = n^{-1} \sum_{i=1}^n \text{dist}^2(\Delta_k^\perp, \mathbf{x}_i)$

Contribution of $\mathbf{x}_i$ to axis Δ_k is the proportion of variance/inertia carried by individual i:

$$\text{contr}(\mathbf{x}_i) = \frac{n^{-1}\text{dist}^2(\Delta_k^\perp, \mathbf{x}_i)}{I_{\Delta_k^\perp}} = \frac{\left(\mathbf{u}_k^\top(\mathbf{x}_i - \bar{\mathbf{x}})\right)^2}{n\lambda_k}$$

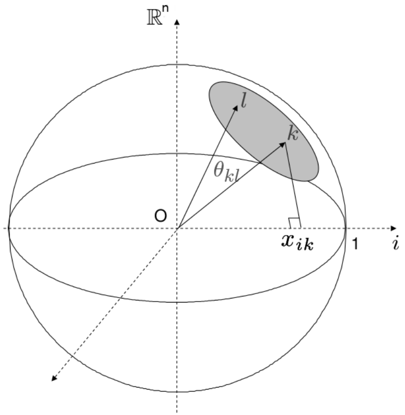
```
factoextra::get_pca_ind(crabs_pca)$contr %>% head(3) %>% kable("latex")
```

Dim.1	Dim.2	Dim.3	Dim.4	Dim.5
2.535166	0.2375409	0.1602617	0.0688010	1.4097141
2.008687	0.0291717	0.0165027	0.0013421	0.0027214
1.779751	0.0940074	0.0121362	0.0651696	0.4231593

Outline

Principal Component Analysis

Cloud of variables in $\mathbb{R}^n$



Direct equivalence between geometry and statistics (collinearity $\equiv$ correlation)

$$\cos(\theta_{kl}) = \frac{\langle \mathbf{x}^k, \mathbf{x}^\ell \rangle}{\|\mathbf{x}^k\| \|\mathbf{x}^\ell\|} = \rho(\mathbf{x}^k, \mathbf{x}^\ell)$$

Principal Components

Dual representation

A symmetric reasoning can be made in $\mathbb{R}^n$ for the variables, like with the individuals in $\mathbb{R}^p$.
$\rightsquigarrow$ New axes are linear combinason of the original variables, which can be seen as **new variables** in the new latent space

Principal component

It is the linear combinason formed by the orginal variables with weights given by the loadings $\mathbf{u}_k$

$$\mathbf{f}_k = \sum_{j=1}^{p} \mathbf{u}_k(\mathbf{x}^j - \bar{x}_j) = \mathbf{X}^c \mathbf{u}_k, \quad \mathbf{f}_k \in \mathbb{R}^n$$

Sometimes called "factors" in factor analysis, as latent (hidden) variables.

Variable representation in the new space

Connection with original variables

- essential for interpretation
- answer to the question: how reading the axis of the individual map
- use correlation to measure connection to original variable

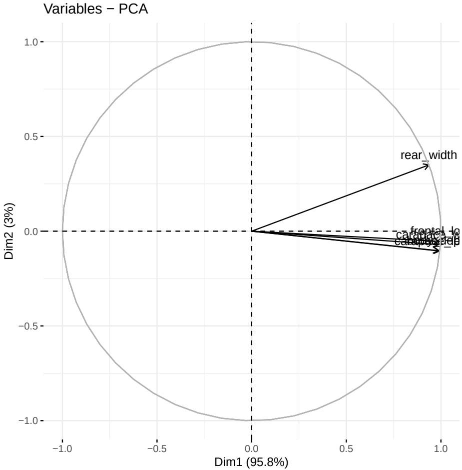
$$\mathbb{V}(\mathbf{f}_k) = \mathbb{V}(\mathbf{X}^c\mathbf{u}_k) = \mathbf{u}_k^\top(\mathbf{X}^c)^\top\mathbf{X}^c\mathbf{u}_k = \lambda_k\mathbf{u}_k^\top\mathbf{u}_k = \lambda_k$$

$$\mathrm{cov}(\mathbf{f}_k, (\mathbf{x}^j - \bar{x}_j)) = \mathbf{u}_k\top\mathbf{X}^{c\top}\mathbf{X}^c e_j = \mathbf{u}_k\lambda_k e_j = \lambda_k\mathbf{u}_{kj}$$

$$\mathrm{cor}(\mathbf{f}_k, (\mathbf{x}^j - \bar{x}_j)) = \sqrt{\frac{\lambda_k}{\mathbb{V}(\mathbf{x}^j)}}\mathbf{u}_{kj}$$

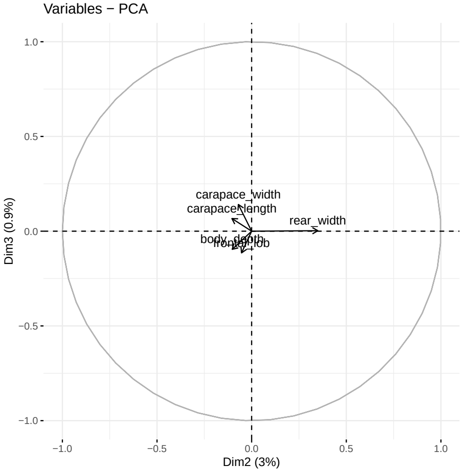
Variable vizualisation: correlation circle (1)

```r
fviz_pca_var(crabs_pca)
```



Variable vizualisation: correlation circle (2)

```
fviz_pca_var(crabs_pca, axes = c(2,3))
```



Warning: about angle after projection

Close projection doesn't mean close variable!

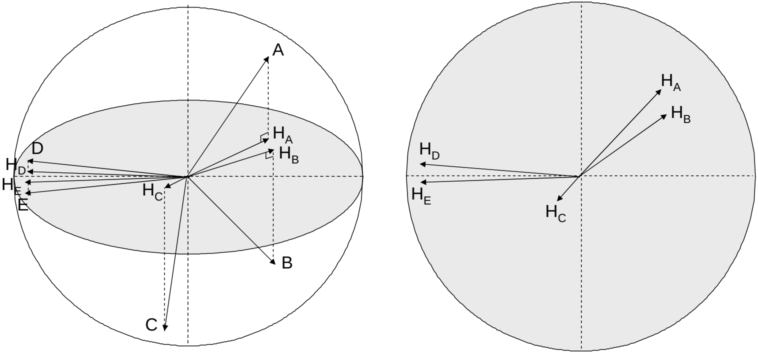


Figure: Same angle but different situations (source: J. Josse)

⇝ Only work when variables are well represented in the latent space

Variable: quality of the representation

Same story as for individuals

Property

- An variable j is well represented by Δ_k if its projection is close to $\mathbf{f}_k$.
- High collinearity means high absolute correlation and high cosine.
- use cosine to the square of the angle between the original and new variables.

$\rightsquigarrow$ The projection of j must be close to the boundardy of the correlation circle

```
factoextra::get_pca_var(crabs_pca)$cos2 %>% head(3) %>% kable("latex")
```

	Dim.1	Dim.2	Dim.3	Dim.4	Dim.5
frontal_lob	0.9785672	0.0028712	0.0131372	0.0054085	0.0000159
rear_width	0.8775551	0.1223552	0.0000067	0.0000780	0.0000051
carapace_length	0.9835409	0.0109140	0.0044722	0.0000000	0.0010728

Variable: contribution to an axis

Similarly to individuals, we can measure the contribution of the original variables to the construction of the new ones.

```
factoextra::get_pca_var(crabs_pca)$contr %>% kable("latex")
```

	Dim.1	Dim.2	Dim.3	Dim.4	Dim.5
frontal_lob	20.43435	1.892860	28.171511	48.5702186	0.9310620
rear_width	18.32502	80.663877	0.014350	0.7006226	0.2961274
carapace_length	20.53821	7.195170	9.590266	0.0002087	62.6761450
carapace_width	20.35027	3.261487	42.584703	0.7954467	33.0080946
body_depth	20.35215	6.986605	19.639170	49.9335034	3.0885710

$\rightsquigarrow$ What do you think of the first axe ?

Outline

Principal Component Analysis

Unifying view of variables and individuals

Principal components

The full matrix of principal component connects individual coordinates to latent factors:

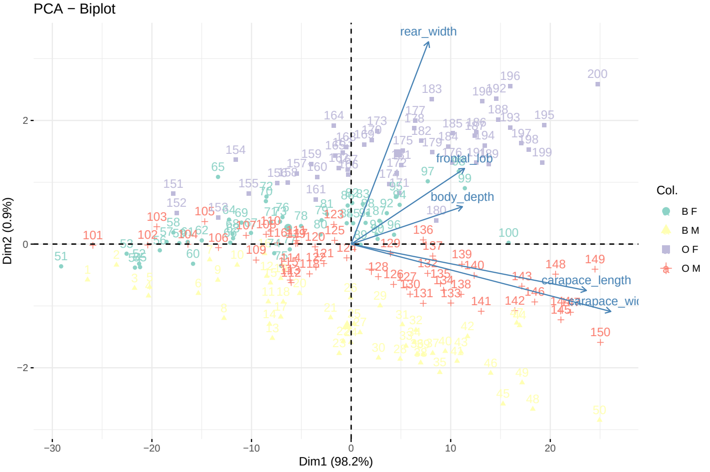
$$\mathrm{PC} = \mathbf{X}^c\mathbf{U} = \begin{pmatrix} \mathbf{f}_1 & \mathbf{f}_2 & \dots & \mathbf{f}_d \end{pmatrix} = \begin{pmatrix} \mathbf{c}_1^\top \\ \mathbf{c}_2^\top \\ \dots \\ \mathbf{c}_d^\top \end{pmatrix}$$

- new variables (latent factor) are seen column-wise
- new coordinates are seen row-wise

$\rightsquigarrow$ Everything can be interpreted on a single plot, called the biplot

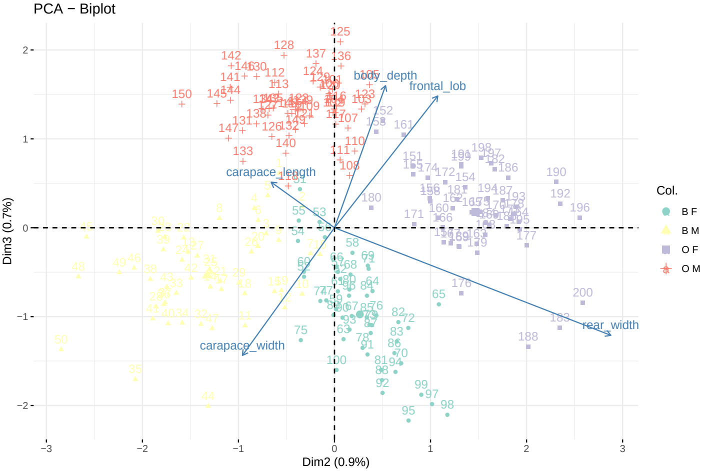
Biplot (1)

```
FactoMineR::PCA(select(crabs, -species, -sex), scale.unit = FALSE, graph = FALSE) %
  factoextra::fviz_pca_biplot(
    axes = c(1,2), col.ind = paste(crabs$species, crabs$sex), palette = pal
  )
```



Biplot (2)

```
FactoMineR::PCA(select(crabs, -species, -sex), scale.unit = FALSE, graph = FALSE) %
  factoextra::fviz_pca_biplot(
    axes = c(2,3), col.ind = paste(crabs$species, crabs$sex), palette = pal
  )
```



Reconstruction formula

Recall that $\mathbf{F} = (\mathbf{f}_1, \ldots, \mathbf{f}_d)$ is the matrix of Principal components. Then,

- $\mathbf{f}_k = \mathbf{X}^c \mathbf{u}_k$ for projection on axis k
- $\mathbf{F} = \mathbf{X}^c \mathbf{U}$ for all axis.

Using orthogonality of $\mathbf{U}$, we get pack the original data as follows, without loss ($\mathbf{U}^T$ performs the inverse rotation of $\mathbf{U}$):

$$\mathbf{X}^c = \mathbf{F}\mathbf{U}^\top$$

We obtain an approximation $\tilde{\mathbf{X}}^c$ (compression) of the data $\mathbf{X}^c$ by considering a subset $\mathcal{S}$ of PC, typically $\mathcal{S} = 1, \ldots, K$ with $K \ll d$.

$$\tilde{\mathbf{X}}^c = \mathbf{F}_{\mathcal{S}}\mathbf{U}_{\mathcal{S}}^\top = \mathbf{X}^c \mathbf{U}_{\mathcal{S}}\mathbf{U}_{\mathcal{S}}^\top$$

$\rightsquigarrow$ This is a rank K approximation of $\mathbf{X}$ of the data the information capture by the first K axes.

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$$\tilde{\mathbf{X}}^c = \mathbf{F}_\mathcal{S}\mathbf{U}_\mathcal{S}^\top = \mathbf{X}^c \mathbf{U}_\mathcal{S}\mathbf{U}_\mathcal{S}^\top$$

$\rightsquigarrow$ This is a rank K approximation of $\mathbf{X}$ of the data the information capture by the first K axes.

Remove size effect I

Carried by the 1st principal component

First component

$$\mathbf{f}_1 = \mathbf{X}^c \mathbf{u}_1.$$

We extract the best rank-1 approximation of $\mathbf{X}$ to remove the *size effect*, carried by the first axis, and return to the original space,

$$\tilde{\mathbf{X}}^{(1)} = \mathbf{f}_1 \mathbf{u}_1^\top.$$

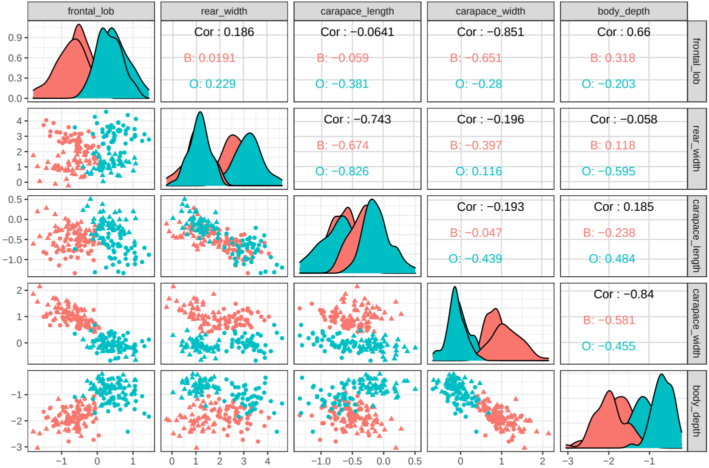
```
attributes <- select(crabs, -sex, -species) %>% as.matrix()
u1 <- eigen(cov(attributes))$vectors[, 1, drop = FALSE]
attributes_rank1 <- attributes %*% u1 %*% t(u1)
crabs_corrected <- crabs
crabs_corrected[, 3:7] <- attributes - attributes_rank1
```

$\rightsquigarrow$ Axis 1 explains a latent effect, here the size in the case at hand, common to all attributes.

Remove size effect II

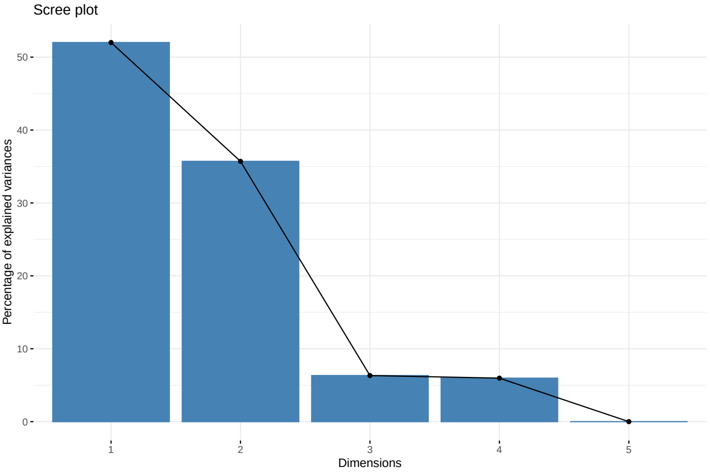
Carried by the 1st principal component

```r
ggpairs(crabs_corrected, columns = 3:7, aes(colour = species, shape = sex))
```



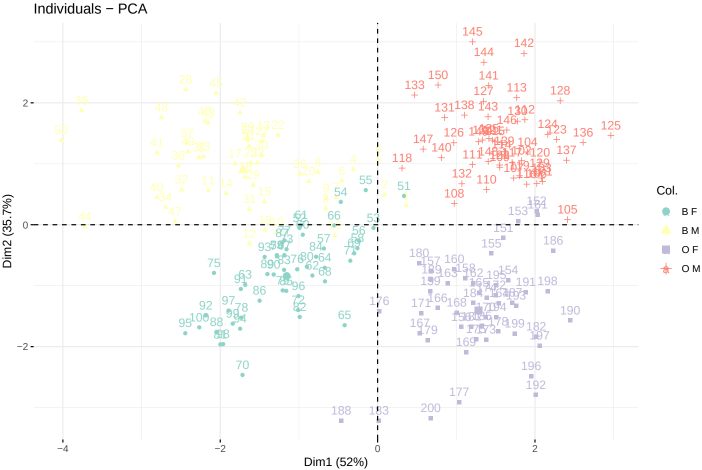
PCA on corrected data (1)

```
crabs_pca_corrected <- select(crabs_corrected, -species, -sex) %>% FactoMineR::PCA(
fviz_eig(crabs_pca_corrected)
```



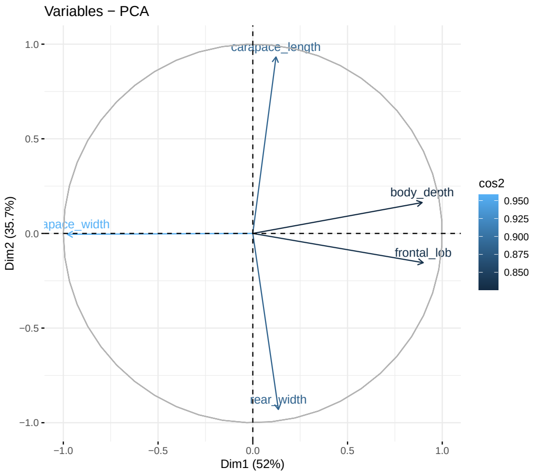
PCA on corrected data (2)

```
fviz_pca_ind(crabs_pca_corrected, col.ind = paste(crabs_corrected$species, crabs_co
```



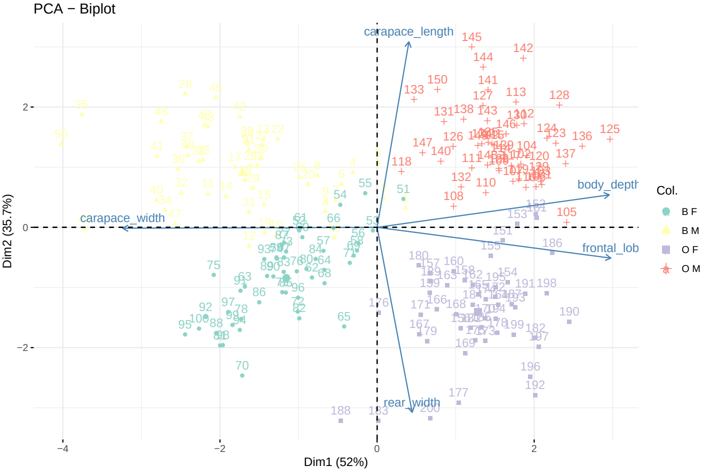
PCA on corrected data (3)

```
fviz_pca_var(crabs_pca_corrected, col.var = 'cos2')
```

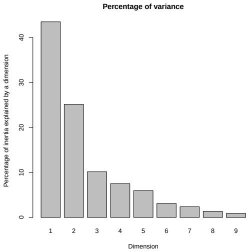


PCA on corrected data (3)

```
fviz_pca_biplot(crabs_pca_corrected, col.ind = paste(crabs_corrected$species, crabs
```



Choosing the number of components

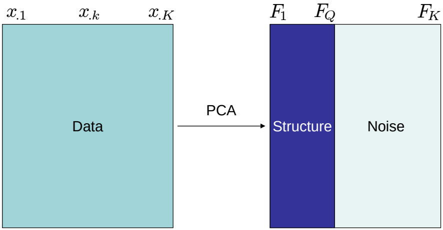


Various solutions, open question

Scree plot, test on eigenvalues, confidence interval, cross-validation, generalized cross-validation, etc.

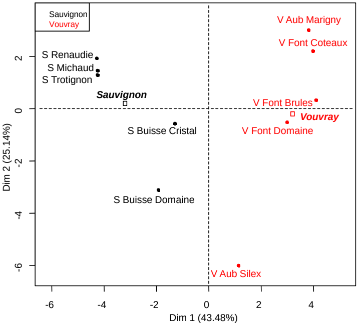
Objectives

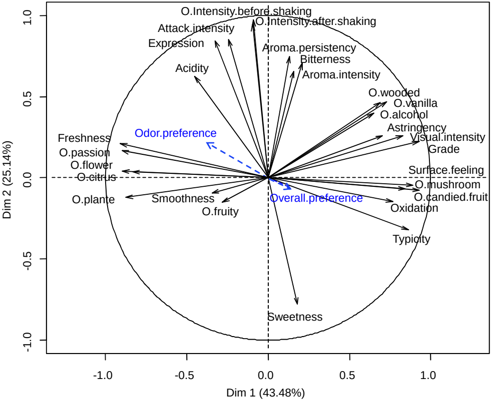
- Interpretation
- Separate structure and noise
- Data compression



Supplementary information

- continuous variables: projection (correlation with dimensions)
- observations: projection
- categorical variables: projection of the categories at the barycentre of the observations which take the categories





Outline

Outline

Principal Component Analysis

Reconstruction error approach

1. Construct a map Φ from the space $\mathbb{R}^d$ into a space $\mathbb{R}^{d'}$ of smaller dimension:

$$\begin{aligned}\Phi : \quad & \mathbb{R}^d \to \mathbb{R}^{d'}, d' \ll d \\ & \mathbf{x} \mapsto \Phi(\mathbf{x})\end{aligned}$$

2. Construct $\widetilde{\Phi}$ from $\mathbb{R}^{d'}$ to $\mathbb{R}^d$ (reconstruction formula)
3. Control an error between $\mathbf{x}$ and its reconstruction $\tilde{\Phi}(\Phi(\mathbf{x}))$, e.g

$$\sum_{i=1}^{n} \left\| \mathbf{x}_i - \tilde{\Phi}(\Phi(\mathbf{x}_i)) \right\|^2$$

Reconstruction error and PCA

PCA Model

Linear model assumption

$$\mathbf{x} \simeq \boldsymbol{\mu} + \mathbf{F}_{1:d'} \mathbf{U}_{1:d'}^{\top}$$

with $\mathbf{U}$ orthonormal and no constraint on $\mathbf{F}$

Reconstruction error

In the case of PCA, then

$$\Phi(\mathbf{x}) = (\mathbf{x} - \boldsymbol{\mu})^{\top}\mathbf{U} \quad \text{and} \quad \tilde{\Phi}(\mathbf{F}) = \boldsymbol{\mu} + \mathbf{F}\mathbf{U}^{\top}$$

$$\frac{1}{n}\sum_{i=1}^{n} \|\mathbf{x}_i - (\boldsymbol{\mu} + (\mathbf{x}_i - \boldsymbol{\mu})\mathbf{U}\mathbf{U}^{\top}\|^2$$

Explicit solution: $\boldsymbol{\mu} = \bar{x}$ the empirical mean and $\mathbf{U}$ is an orthonormal basis of the space spanned by the d' first eigenvectors of the empirical covariance matrix

Non linear extensions

Two directions

1. Non linear transformation of $\mathbf{x}$ before PCA: kernel-PCA
2. Other constrains on weigths $\mathbf{U}$ or loadings $\mathbf{F}$: ICA, NMF, ...

Kernel PCA

Linear assumption after transformation, with $\mathbf{U}$ orthonormal and no constraint on $\mathbf{F}$

$$\Psi(\mathbf{x} - \boldsymbol{\mu}) \simeq \mathbf{F}_{1:d'} \mathbf{U}_{1:d'}^{\top}$$

Non negative Matrix factorisation

Linear model assumption with $\mathbf{U}$ non-negative and $\mathbf{F}$ non-negative

$$\mathbf{x} \simeq \boldsymbol{\mu} + \mathbf{F}_{1:d'} \mathbf{U}_{1:d'}^{\top}$$

Auto-encoders Find Φ and $\tilde{\Phi}$ with a neural-network!

$\rightsquigarrow$ Fit $\mathbf{U}, \mathbf{F}$ with some optimization algorithms (much more complex!)

Outline

Principal Component Analysis

1. Background: high-school algebra
2. Geometric approach to PCA
3. Principal axes and variance maximization
4. Representation and interpretation
5. Additional tools and Complements
6. Beyond linear methods
   - Reconstruction error point of view
   - Relation preservation point of view

Pairwise Relation

Focus on pairwise relation $\mathcal{R}(\mathbf{x}_i, \mathbf{x}_{i'})$.

Distance Preservation

- Construct a map Φ from the space $\mathbb{R}^d$ into a space $\mathbb{R}^{d'}$ of smaller dimension:

$$\begin{aligned} \Phi : \quad & \mathbb{R}^d \to \mathbb{R}^{d'}, d' \ll d \\ & \mathbf{x} \mapsto \Phi(\mathbf{x}) \end{aligned}$$

$$\text{such that} \quad \mathcal{R}(\mathbf{x}_i, \mathbf{x}_{i'}) \sim \mathcal{R}'(\mathbf{x}'_i, \mathbf{x}'_{i'})$$

Multidimensional scaling

Try to preserve inner product related to the distance (e.g. Euclidean)

t-SNE – Stochastic Neighborhood Embedding

Try to preserve relations with close neighbors with Gaussian kernel