Prof. Dr. Bastian Amberg
School of Business & Economics
Department of Information Systems

Business Intelligence

06 Data Understanding & Data Visualization

Prof. Dr. Bastian Amberg

(summer term 2024)

22.5.2024

Schedule

Freie Universität Berlin

		Wed., 10:00-12:00		Fr., 14:00-16:00 (Start at 14:30)		Self-study		
	W1	17.4.	(Meta-)Introduction	19.4.		Python-Basics	Chap. 1	
	W2	24.4.	Data Warehouse – Overview & OLAP	26.4.	*[Blockveranstaltung SE Prof. Gersch]*		Chap. 2	
Basics	W3	1.5.		3.5.	Data Warehouse Modeling I		Chap. 3	
	W4	8.5.	Data Warehouse Modeling I & II	10.5.	Data Mining Introduction			
	W5	15.5.	CRISP-DM, Project understanding	17.5.	Python-Basics-Online Exercise	Python-Analytics	Chap. 1	
	W6	22.5.	Data Understanding, Data Visualization	24.5.	*No lectures, but bonus tasks* *1.) Co-Create your exam*		Chap. 2	
	W7	29.5.	Data Preparation	31.5.	*2.) Earn bonus points for the exam*			
Main Part	W8	5.6.	Predictive Modeling I	7.6.	Predictive Modeling II (10:00 -12:00)	BI-Project	Start	
	W9	12.6.	Fitting a Model I	14.6.	Python-Analytics-Online Exercise		|	
	W10	19.6.	*Guest Lecture*	21.6.	Fitting a Model II		|	Case Study
	W11	26.6.	How to avoid overfitting	28.6.	What is a good Model?		|	
	W12	3.7.	Project status update Evidence and Probabilities	5.7.	Similarity (and Clusters) From Machine to Deep Learning I		|	
Deep-ening	W13	10.7.		12.7.	From Machine to Deep Learning II		|	
	W14	17.7.	Project presentation	19.7.	Project presentation		End	
Ref.					*Klausur 1.Termin, 31.7.'24* *Klausur 2.Termin, 2.10.'24*	Projektbericht		

Note on Bonus tasks

Vom 24.5.‘24 bis spätestens 7.6.‘24

Bitte jeweils die genaue Aufgabenstellung inklusive Abgabeformalitäten beachten!
Diese ist ab Freitag, 24.5., 10 Uhr in Blackboard verfügbar.

1. **Co-Create your exam**

   Einzelleistung (bzw. Leistung des gesamten Kurses)

   - Zwei Aussagen im Kontext der Veranstaltungen 01 bis 04 formulieren (eine wahr, eine falsch)
   - Freitextaufgabe zu Veranstaltungen 01 bis 04 formulieren, die mit einem Wort (keine Aussage über wahr oder falsch!) beantwortet werden kann

   ➢ Falls bis zum 7.6.‘24 ≥ 84 (= 3 Fragen x 28 gemeldete Teilnehmer:innen) <u>unterschiedliche</u>, sinnvolle Fragen/Aussagen zusammen kommen, ist eine Teilmenge davon Bestandteil der Klausur

2. **Earn bonus points for the exam**

   Gruppenarbeit (min. 2 bis max. 3 Personen pro Gruppe)

   - Rechercheaufgabe zu Supervised, Unsupervised und Reinforcement Learning
   - Grafische Darstellung auf einer Folie inklusive Beschreibung und kritischer Würdigung
   - Dabei Einsatz von generativer KI möglich (z.B. ChatGPT, Bing AI),
     sofern die verwendeten Anfragen/Befehle nachvollziehbar dokumentiert werden

   ➢ Maximal drei Bonuspunkte, die auf die in der Klausur erreichte Punktzahl addiert werden (sofern die Klausur bestanden wurde)

Ref.

Last lesson

✓ From business problems to data mining tasks

✓ Supervised vs. unsupervised methods vs. reinforcement learning

- Demo Reinforcement Learning (from the last lesson)
- A.I. Learns to Drive From Scratch in Trackmania (very well explained youtube video)
- Optimization tasks in stochastic, dynamic environments (project example)

Learning Approach	Learn from…. (input? - output?)	Learn for…. (target?)	Example?

Kahoot-Fragen zu den Inhalten
www.kahoot.it
(über Smartphone oder Laptop)
PIN folgt

✓ The data mining process – CRISP-DM

○ Business / Project understanding

Ref.

Today's Agenda

First Part

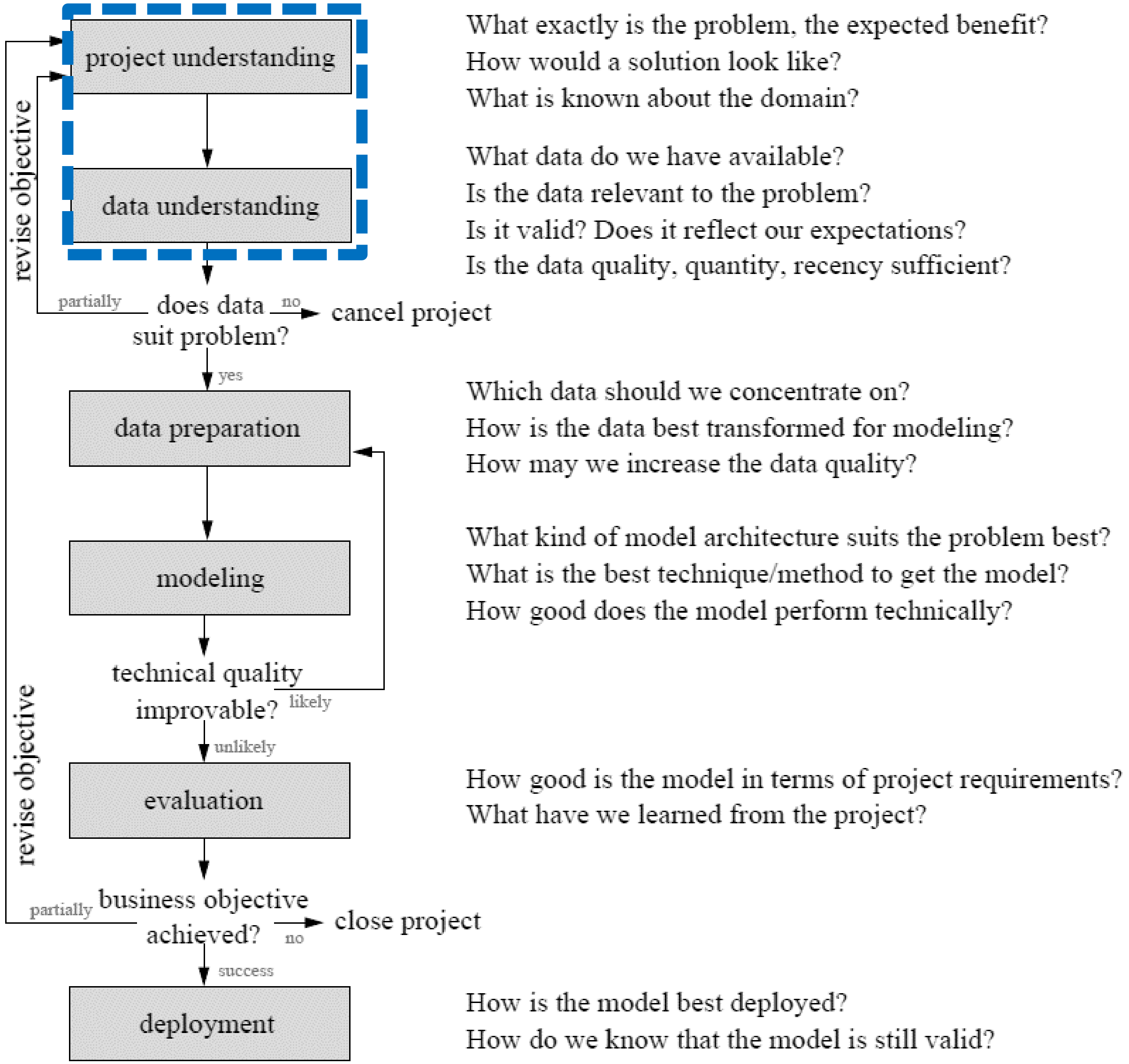
Project Understanding (continued)

See slides 5b from last week

Second Part

Data Understanding

This set of slides



Ref.

First Part

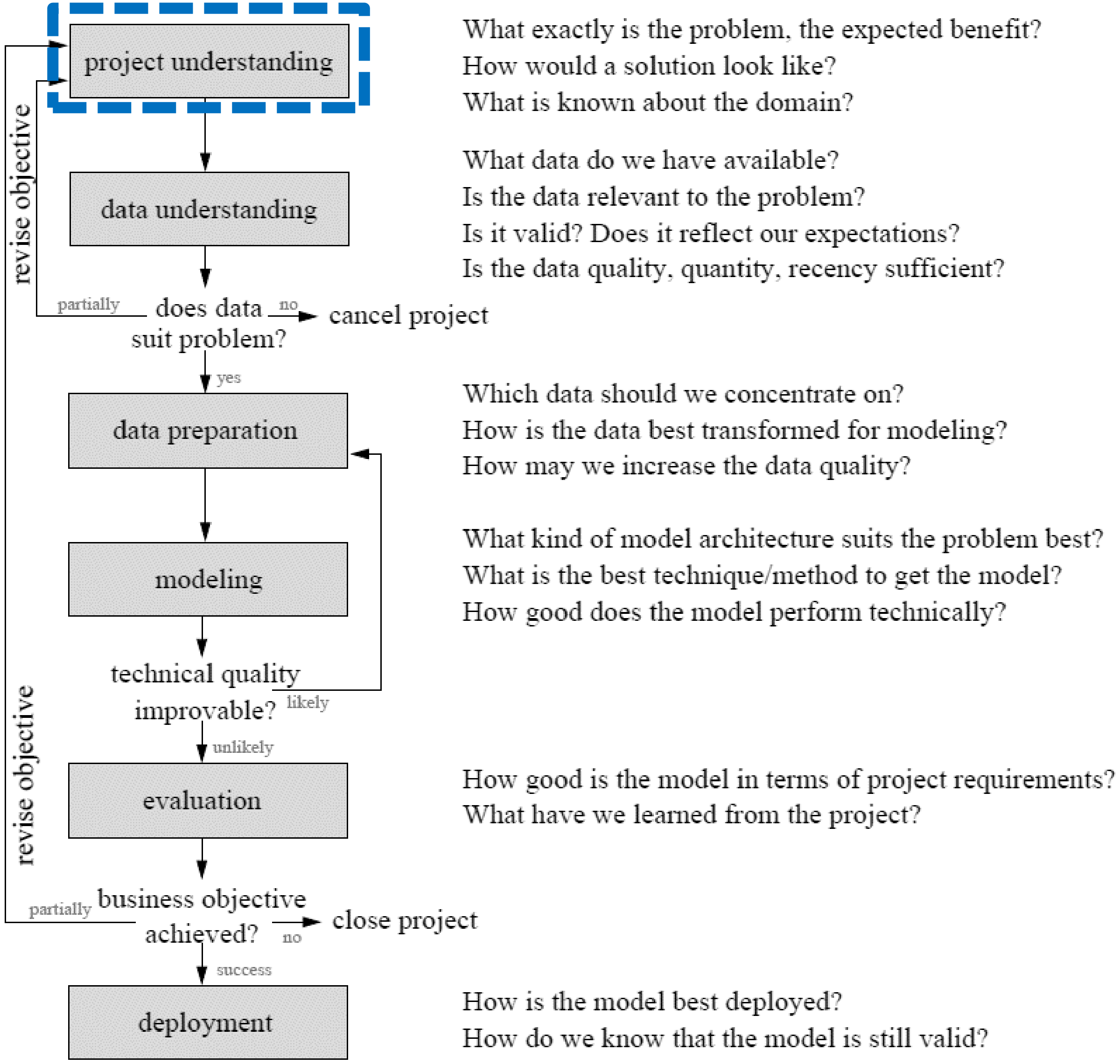
(see slides 10 to 18 from slide set 5b)

- ✓ The data mining process – CRISP-DM

- ✓ Business / Project understanding

Image: "Moneyball"/Columbia Pictures, Video

- ➢ Assess the situation
- ➢ Determine analysis goals



Ref.

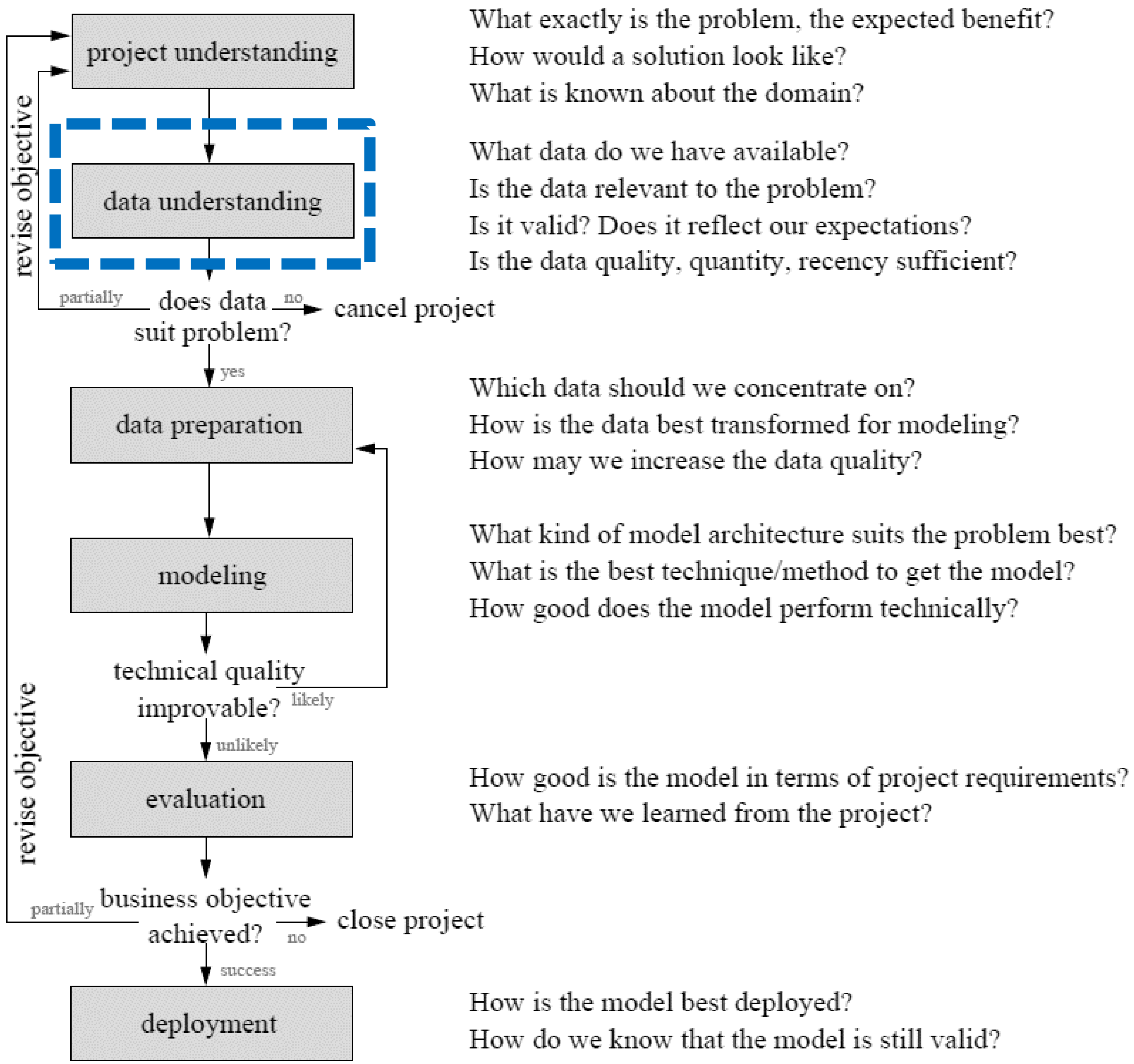
Second Part

Cross
Industry
Standard
Process for
Data
Mining

Iteration as
a rule

Process of data
exploration

Implementation of the
KDD Process



Ref. Wirth / Hipp (2000), Azevedo (2008)

Agenda for Data Understanding

Freie Universität Berlin

(1) Data Understanding

Attribute Understanding

Data Quality

(2) Data Visualization (= Data Understanding – Part 2)

Low-dimensional relationships

Univariate Analysis

Bivariate Analysis

Higher-dimensional relationships

Principal Component Analysis

Parallel Coordinates

Ref.

Goals of data understanding

Gain **general insights** about the data (independent of the project goal)

Check the assumptions made during the project understanding phase (representativeness, informativeness, data quality, presence/absence of external factors, dependencies, …)

Check the specified **domain knowledge**

Check suitability of the data for the project goals

Never trust any data as long as you have not carried out some simple plausibility checks!

Ref.

Attribute understanding

And types of attributes

We often assume that the data set is provided in form of a simple table

The rows of the table are called **instances, records or data objects**

The columns of the table are called **attributes, features or variables**

	Attribute 1	…	Attribute M
Record 1			
…			
Record n			

Categorical (nominal): finite domain. The values of a categorical attribute are often called classes or categories

Examples: [female, male, diverse], [ordered, received]

Ordinal: finite domain with a linear ordering on the domain.

Example: [B.Sc., M.Sc., Ph.D.], [Dawn, Noon, Afternoon, Evening, Night]

Numerical: values are numbers

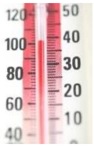
- **Discrete**: categorical attribute or numerical attribute whose domain is a subset of an integer number
- **Continuous**: numerical attribute with values in the real numbers or in an interval (float)

Ref.

Scales for numerical attributes

Interval scale: the definition of the value 0 is arbitrary. Ratios are meaningless.

Examples: date (Unix standard time: time point zero is in the year 1970), temperature (°C or °F)



Ratio scale: 0 has a canonical meaning

(none of the measured quality exists)

Ratios make sense.

Examples: distance, duration

Absolute scale: domain with a unique measurement unit.

Examples: any kind of counting process (number of children, number of visits to the doctor)

Specific problems of categorical attributes

Levels of granularity; Dynamic domains

Different **levels of granularity** might be definable.

Examples:

- product categories/types:
  - └ General category: drinks, food, clothes, …
    - └ More refined categories for drinks: water, beer, wine, …
      - └ Further refinement for water based on the producer.
        - └ Further refinement of the of each producer based on the bottle size (0.33 l, 0.5 l, 1 l, 1.5 l)

⇨ The most refined level provides the **most detailed information**, but will not help to discover general associations like “Wine and cheese are often bought together”

Dynamic domains: The possible values of the domain might change over time.

- Example: certain product categories or products might not be sold anymore. New product categories or products are introduced.

⇨ The analysis of such data will be **biased** to values (example: products) that have been in the domain for a long time.

Ref.

Data quality

Syntactic accuracy vs. Semantic accuracy

Syntactic accuracy is violated if an entry does not belong to the domain of the attribute

- The entry *fmale* for the categorical attribute *gender*
- Text entries for numerical attributes
- Values out of range for numerical attributes (negative numbers for weight, distance, counting process, …)

Syntactic accuracy can be checked quite easily

Semantic accuracy is violated if an entry is not correct although it belongs to the domain of the attribute

Name	Gender
John Smith	Female
Lisa McIntosh	Female
Rick Rickerton	Male
Jane Smith	Male
John Doe	Male

Semantic accuracy is more difficult to check than syntactic accuracy.

Can only be investigated based on “business rules” and plausibility checks.

Ref.

Data quality

Completeness, Unbalanced data and timeliness

complete **attribute values**:
fraction of “null” entries for an attribute.

Note that missing values are not always marked explicitly as missing, for instance in the case of *default entries*!

e.g., Time: 12 o'clock
Birthday: 01.01.xxxx

complete **records**: complete records might be missing.

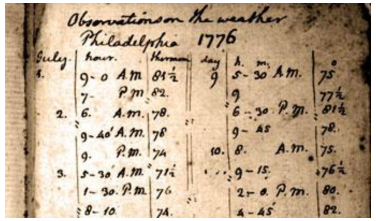
Example 1: Three years ago, a new system was introduced and not all customer data were transferred to the new system.
Example 2: The data set is biased, e.g., a bank might have rejected customers with no income, but they did not protocol it.

Unbalanced data:
the data set might be biased extremely to one type of records

Production line for goods including quality control → defective goods will be a very small fraction of all records!

e.g., 99.9% (+)
0.01% (–)

Timeliness:
is the available data up to date to be considered to be representative?



Ref.

Images: NCDC (Weather data from Thomas Jefferson)

Agenda

Data Visualization (= Data Understanding – Part 2)

Low-dimensional relationships

Univariate Analysis

Bivariate Analysis

Higher-dimensional relationships

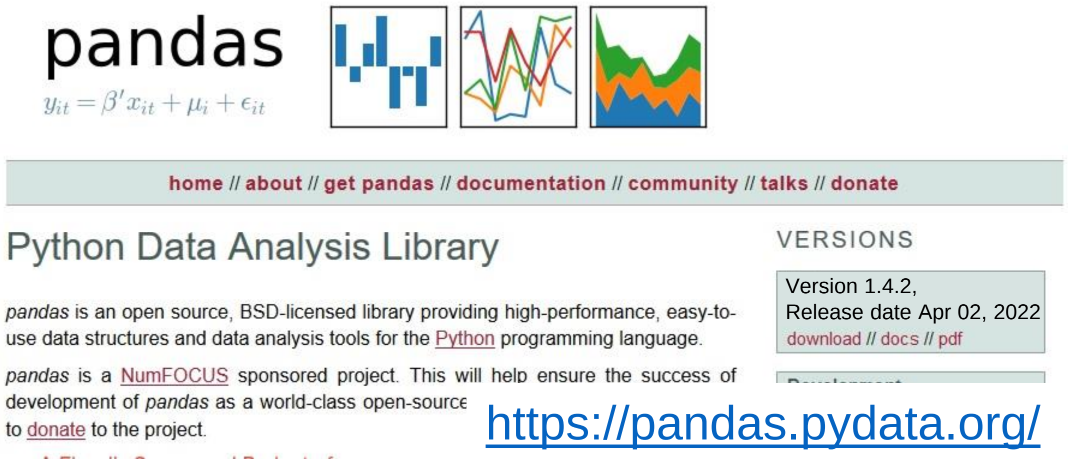
Principal Component Analysis

Parallel Coordinates

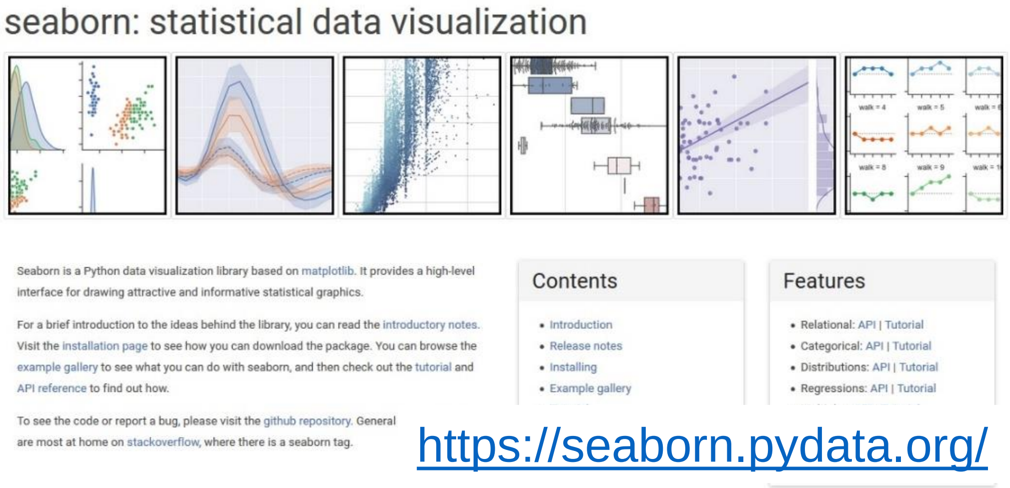
Ref.

First: Python libraries for data visualization

used libraries…
(among others)



https://pandas.pydata.org/



https://seaborn.pydata.org/

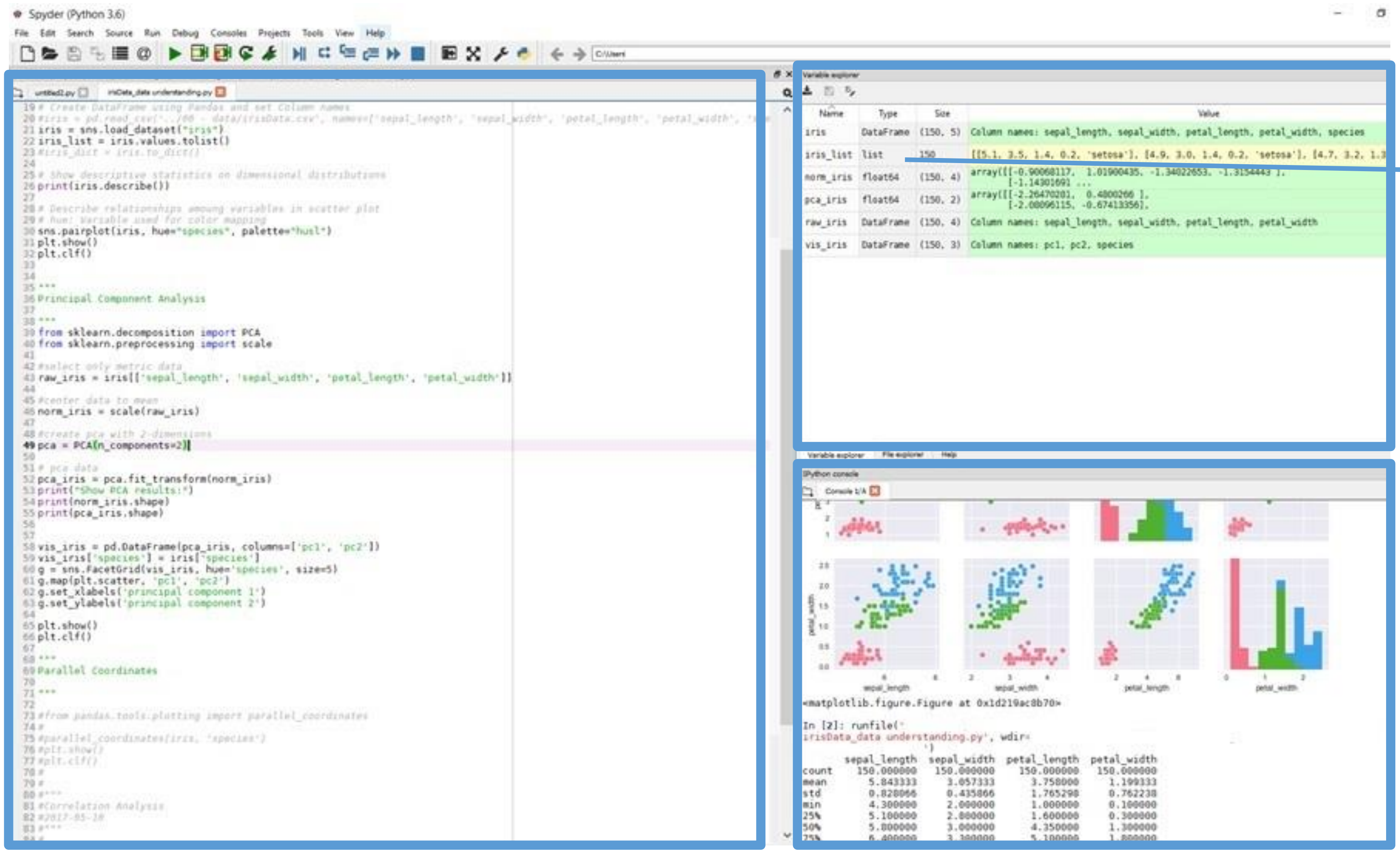
How to use?
>> See sample code on the slides.

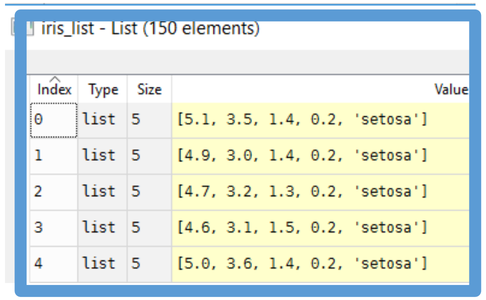
Ref.

First: Getting started with a Python-IDE

Anaconda Spyder

Code





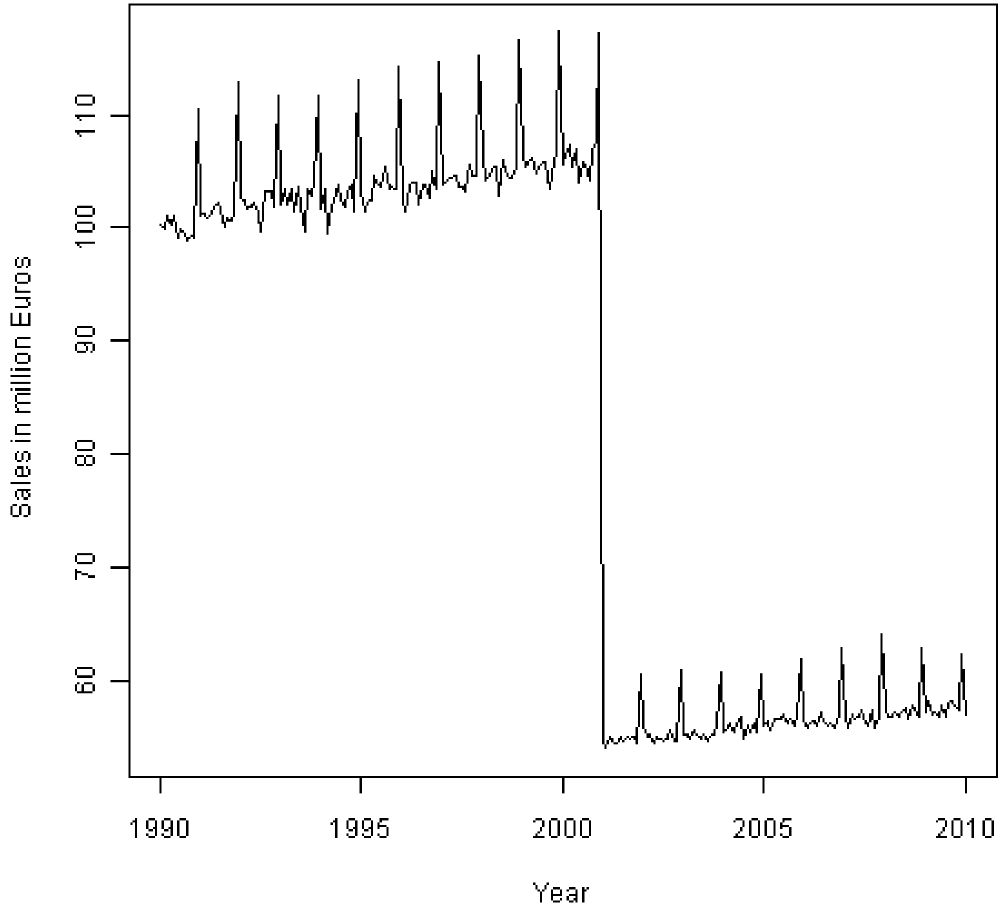
Variable Explorer

iPython Console (input/output)

Ref.

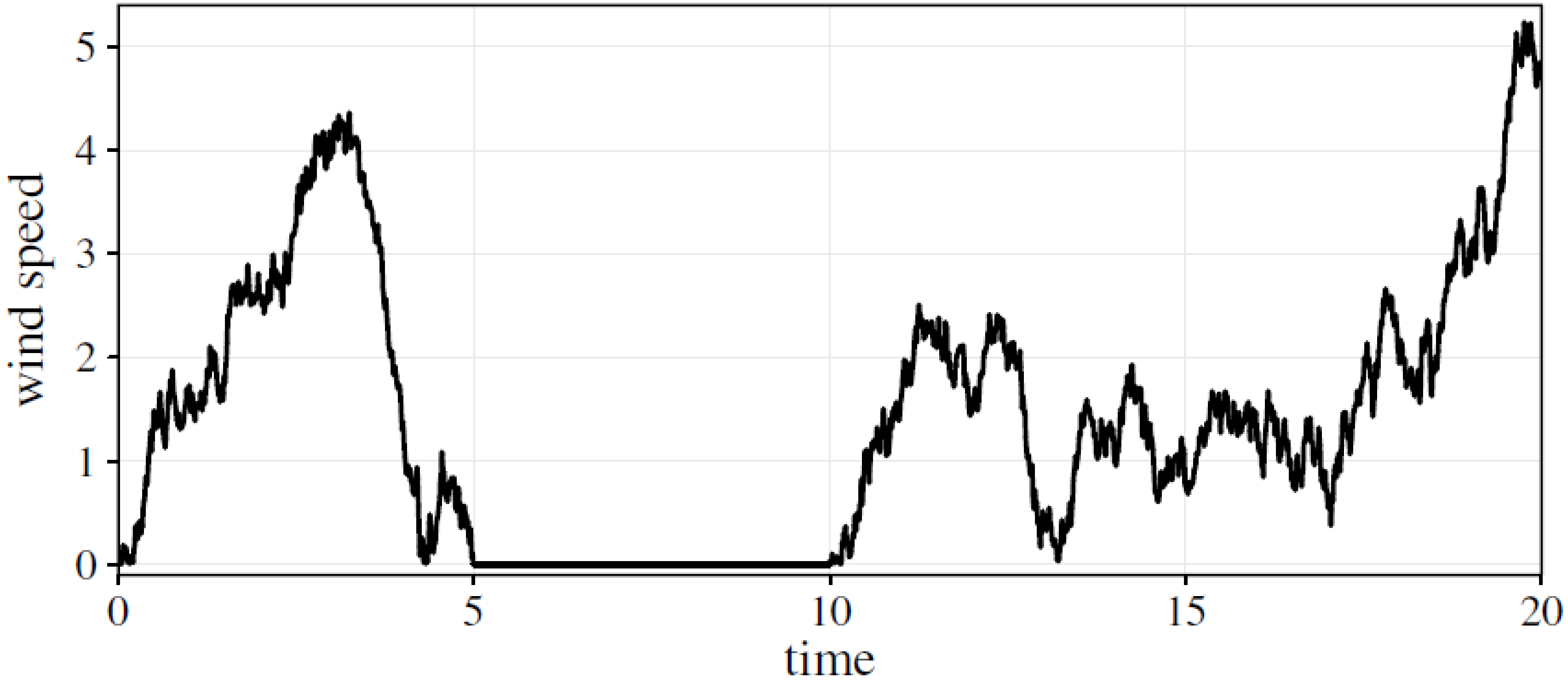
Data visualization

“There is no excuse for failing to plot and look”.
Tukey (1977)



Ref. Tukey (1977)

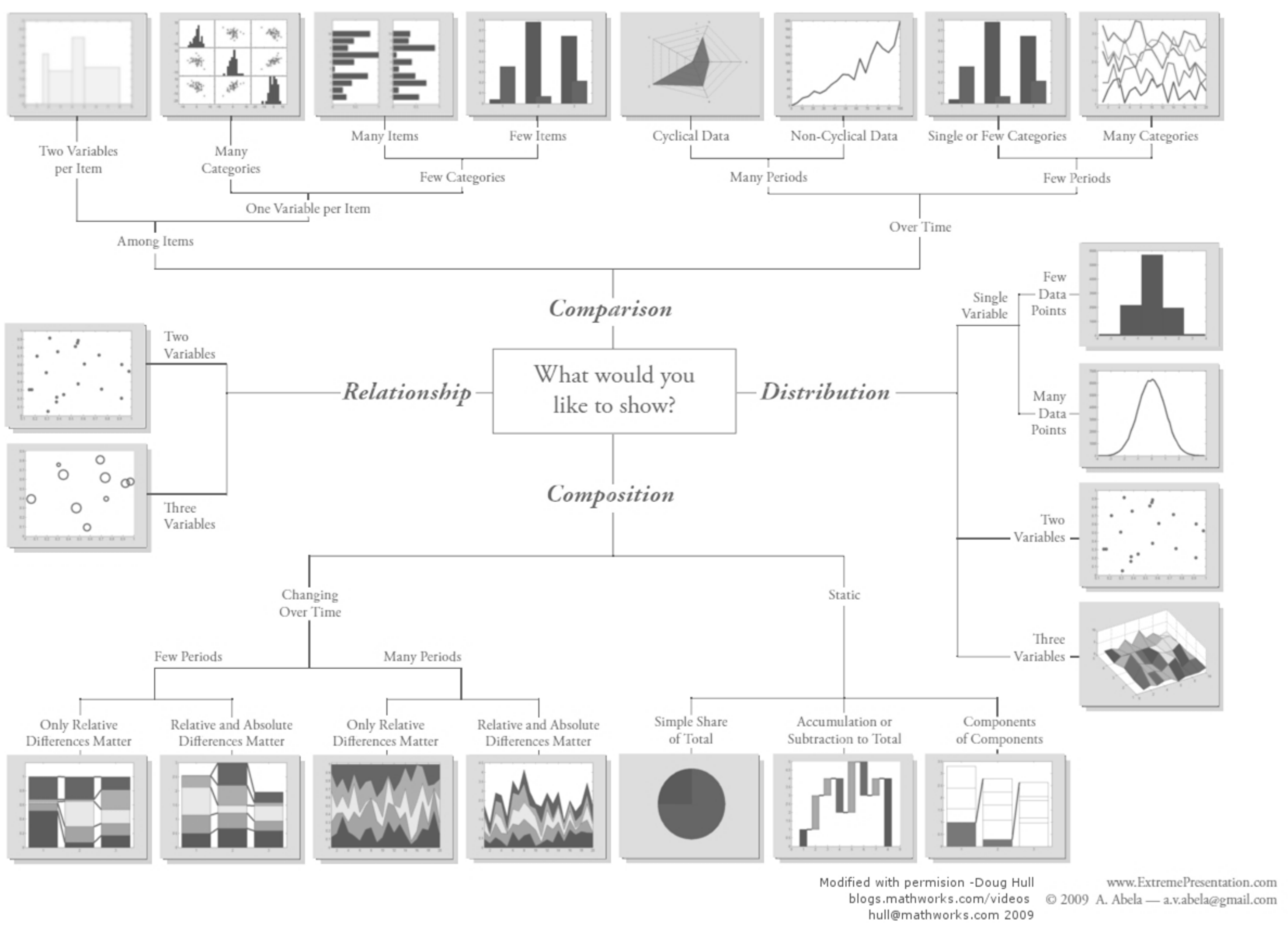
Hidden missing values



Ref.

Visualization Types

Selecting the 'right' visualization



Graphic representation constitutes one of the ***basic sign-systems*** *conceived by the human mind for the purposes of* ***storing***, ***understanding***, *and* ***communicating*** *essential* ***information***. *As a "language" for the eye, graphics benefits from the ubiquitous properties of visual perception. As a monosemic system, it forms the rational part of the world of images.*
(Bertin, 1983)

"They must ***make sense to the user*** *and require a* ***visual language system*** *that uses colour, shape, line, hierarchy and composition to communicate clearly and appropriately, much like the alphabetic and character-based languages used worldwide between humans."*
(Woolman, 2002)

A good infographic should be ***functional*** *as a hammer,* ***multilayered*** *as an onion, and* ***beautiful*** *and* ***true*** *as an equation (or as a scientific theory). An information graphic must be precise, accurate, efficient, and deep before the designer can apply his or her own visual style or typographical and color preferences to the display.*
(Alberto Cairo, 2012)

Ref. http://extremepresentation.typepad.com, Bertin (1983), Woolman (2002), Cairo (2012),

Agenda

Low-dimensional relationships

Univariate Analysis

Bivariate Analysis

Higher-dimensional relationships

Principal Component Analysis

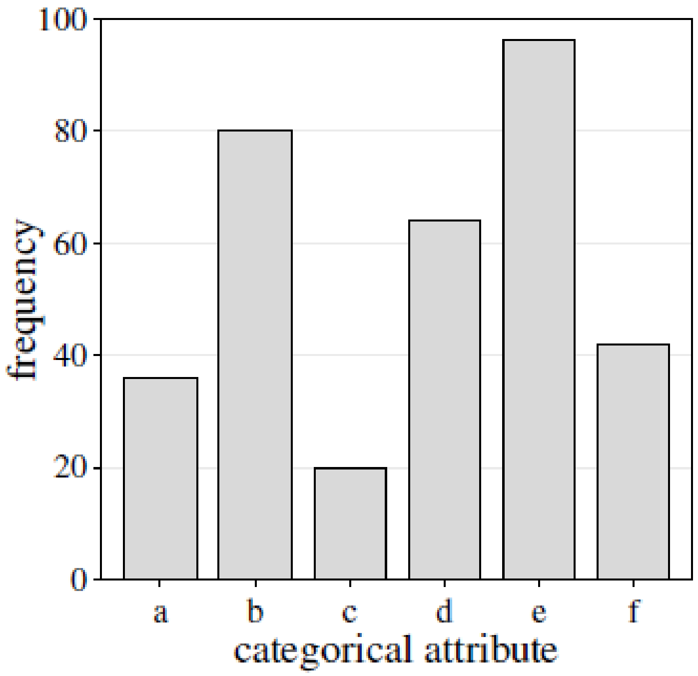
Parallel Coordinates

Ref.

Common visualizations

Bar charts and Histograms

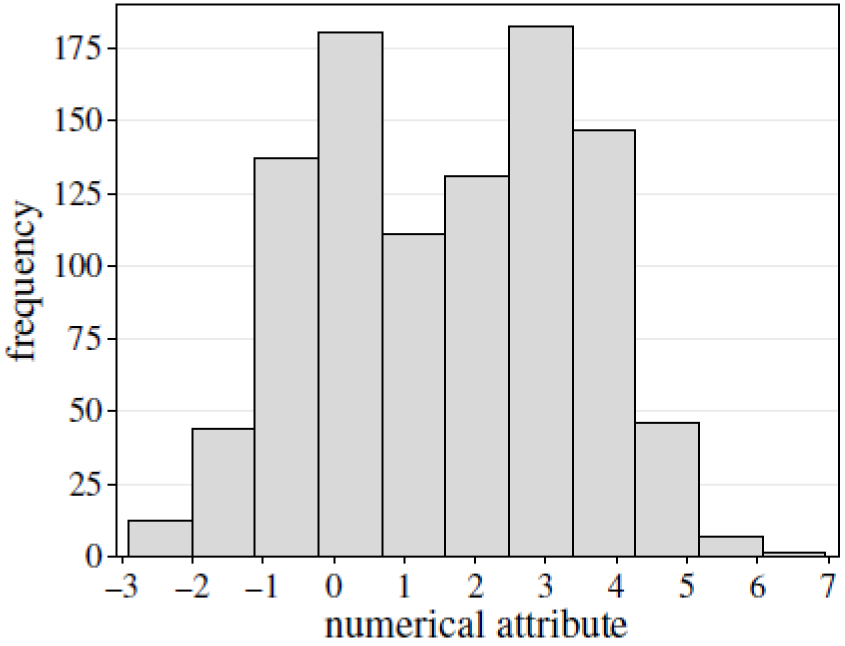
A **bar chart** is a simple way to depict the frequencies of the values of a categorical attribute.



A **histogram** shows the frequency distribution for a numerical attribute.

The range of numerical attribute is discretized into a fixed number of intervals (“bins”), usually of equal length.

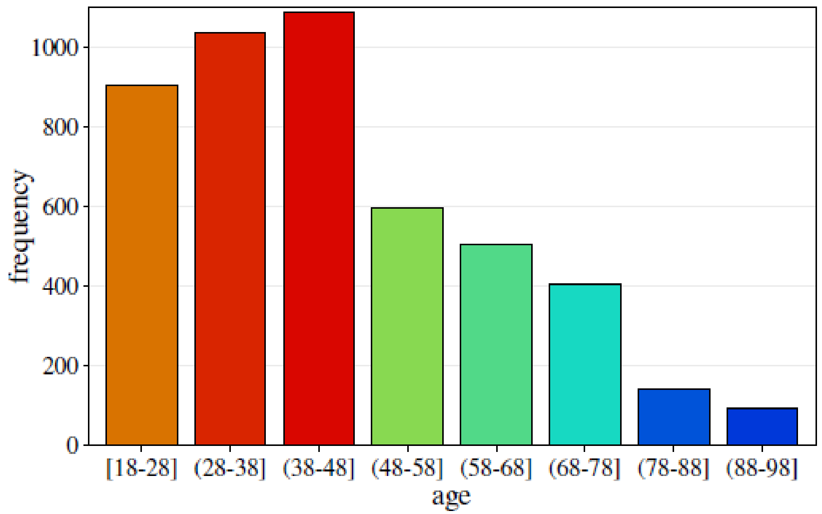
For each interval, the (absolute) frequency of values falling into it is indicated by the height of a bar.

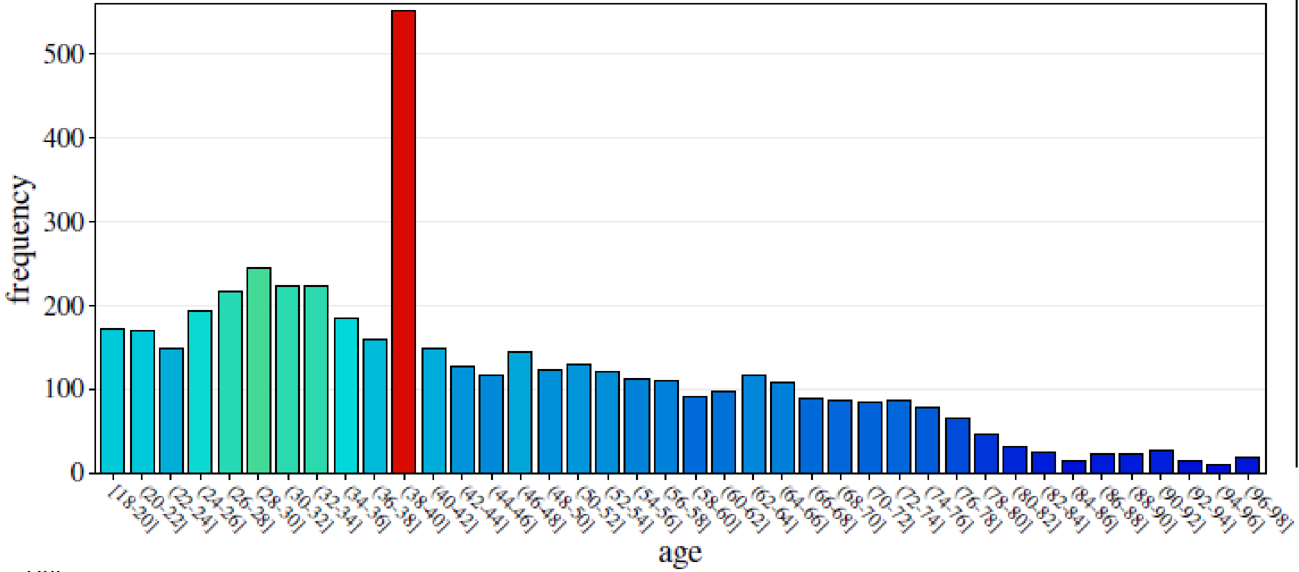


Ref.

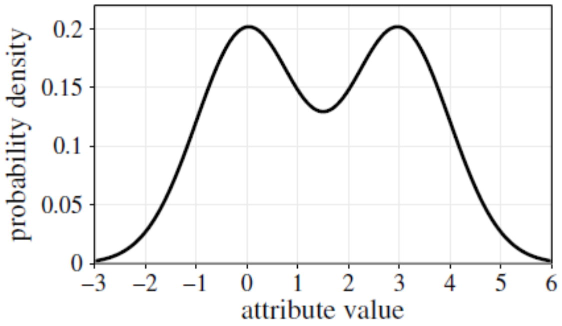
Common visualizations

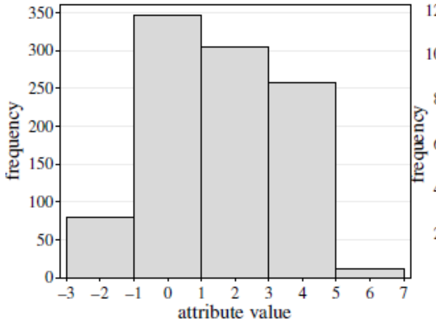
Histograms: The number of bins is very important.

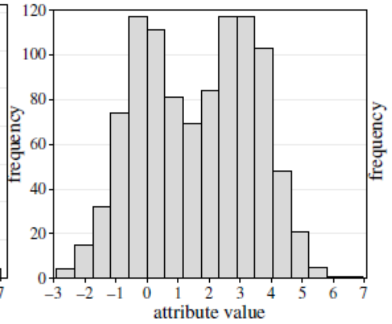


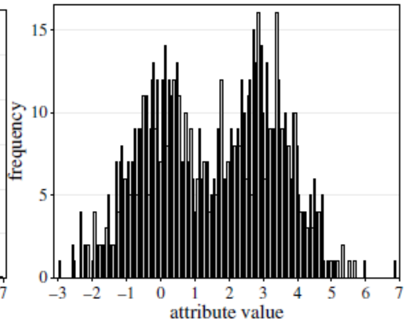


Three histograms with 5, 17 and 200 bins for a sample from the same bimodal distribution. Sample size is n = 1000.









Rel.

Example data set

Iris data

Collected by E. Anderson in 1935

Contains measurements of four real-valued variables of 150 **iris flowers** of types Iris Setosa, Iris Versicolor, Iris Virginica

- Sepal length [Kelchblatt]
- Sepal widths
- Petal lengths [Blütenblatt]
- Petal widths

The fifth attribute is the name of the flower type

Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
5.1	3.5	1.4	0.2	Iris-setosa
...				
...				
5.0	3.3	1.4	0.2	Iris-setosa
7.0	3.2	4.7	1.4	Iris-versicolor
...				
...				
5.1	2.5	3.0	1.1	Iris-versicolor
5.7	2.8	4.1	1.3	Iris-virginica
...				
...				
5.9	3.0	5.1	1.8	Iris-virginica

Ref.

Iris Setosa

Borsten-Schwertlilie

Iris Versicolor

Versch-f. Schwertl.

Iris Virginica

Sumpf-Schwertlilie

```
import pandas as pd
# Create DataFrame using Pandas and set Column names
iris = pd.read_csv('irisData.csv', names=['sepal_length','sepal_width','petal_length','petal_width','species'])
# Show descriptive statistics on dimensional distributions
print(iris.describe())
# Show histogram
iris.hist(column='sepal_length', bins = (4.0,4.5,5.0,5.5,6.0,6.5,7.0,7.5,8))
```

Iris data set: boxplots

Boxplots are a very compact way to visualize and summarize main characteristics of a sample from a numerical attribute

Line in the middle = median

Box = interquartile range

Whiskers = 1.5 x interquartile range

```
import pandas as pd
import seaborn as sns

iris = pd.read_csv('irisData.csv', names=['sepal_length','sepal_width','petal_length','petal_width','species'])

sns.boxplot(x="species", y="sepal_length", data=iris, notch=True)
```

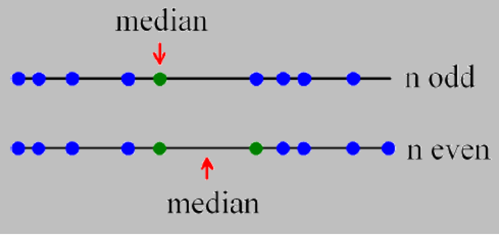
Reminder:

Median:
the value in the middle (for the values given in increasing order)

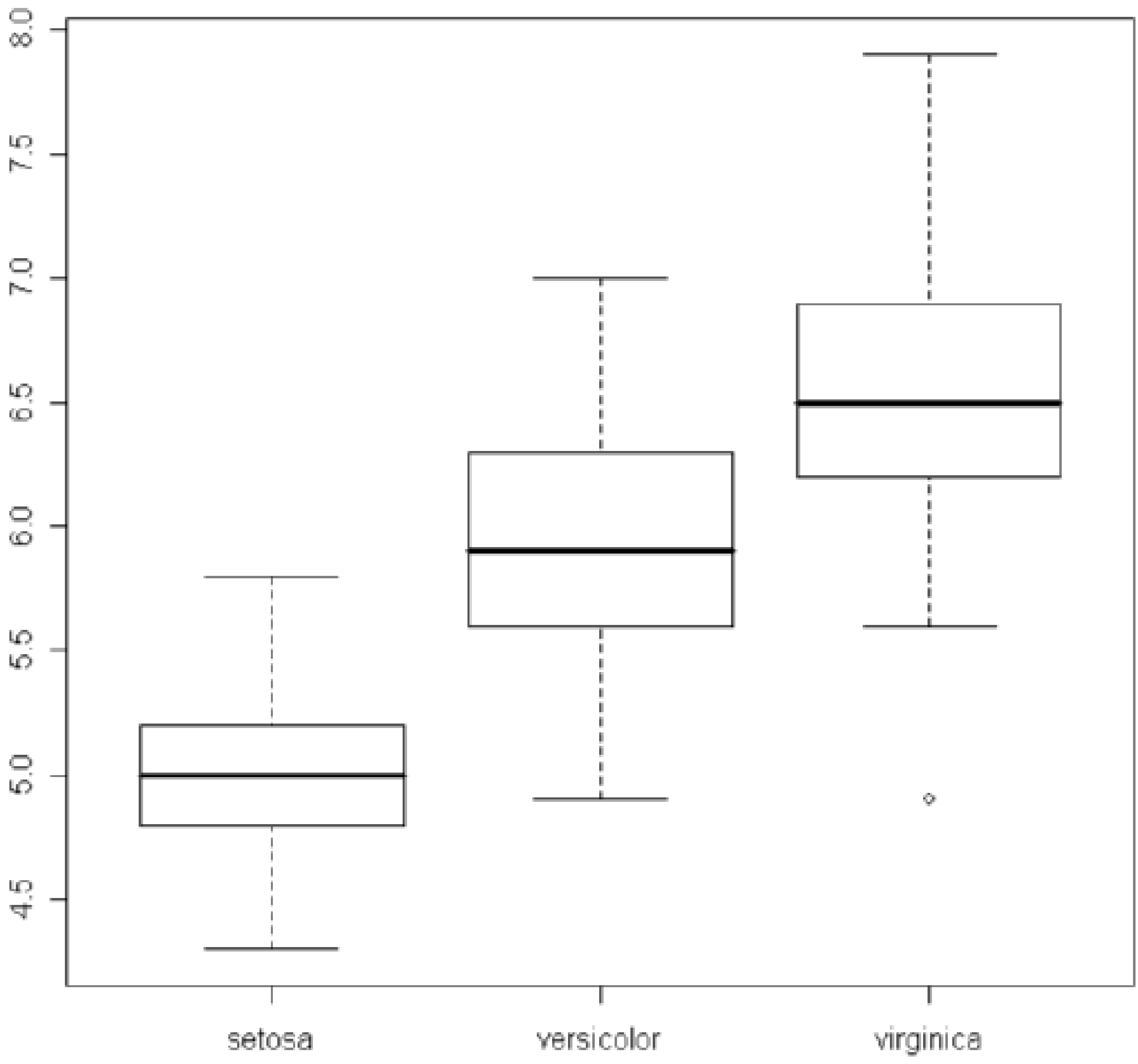
q%-quantile (0<q<100):
The value for which q% of the values are smaller and 100-q% are larger. The median is the 50%-quantile.

Quartiles:
25%-quantile (1st), median (2nd), 75%-quantile (3rd)

Interquartile range:
3rd quantile – 1st quantile



Sepal length (Kelchblattlänge)



Agenda

Low-dimensional relationships

Univariate Analysis

Bivariate Analysis

Higher-dimensional relationships

Principal Component Analysis

Parallel Coordinates

Ref.

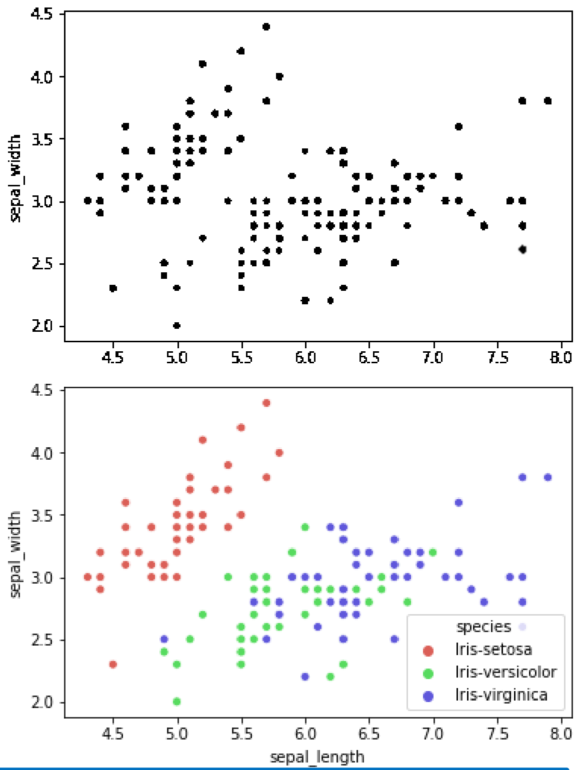
Common visualizations

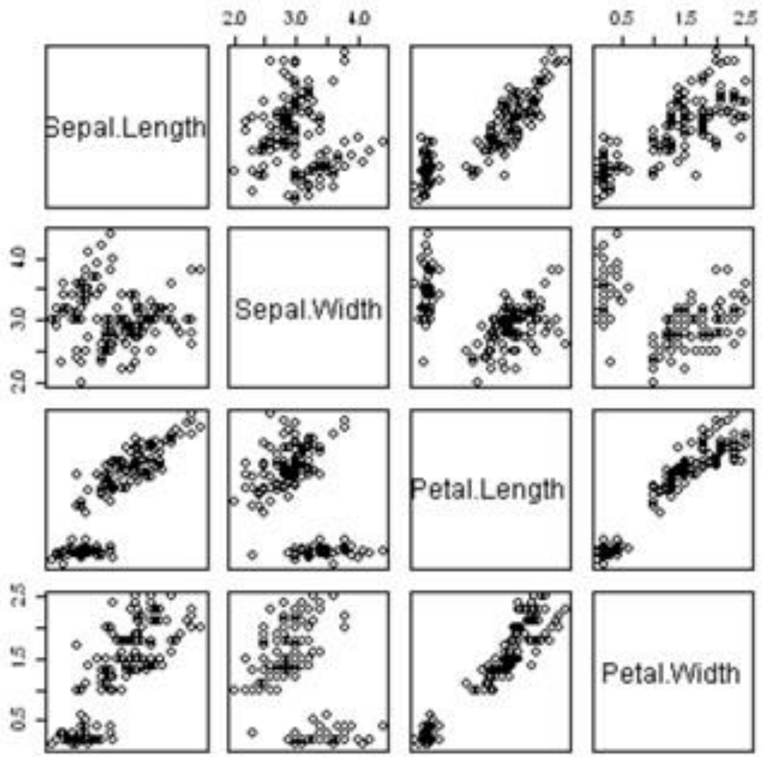
Scatter plots

Scatter plots visualize two variables in a two-dimensional plot

Each axes corresponds to one variable

Not suited for larger data sets



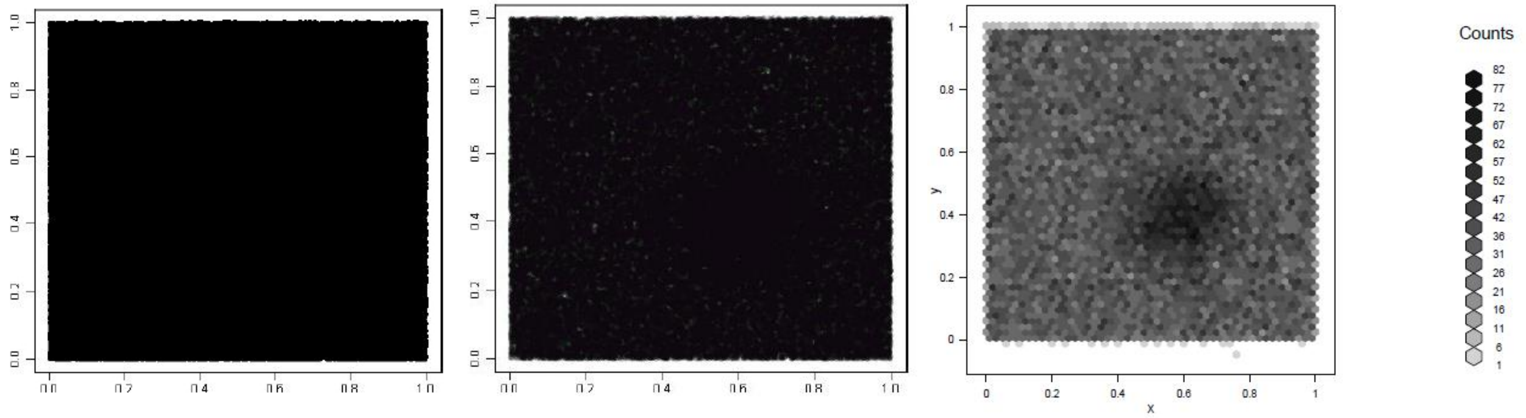



```
import pandas as pd
import seaborn as sns

iris = pd.read_csv('irisData.csv', names=['sepal_length','sepal_width','petal_length','petal_width','species'])

# Describe relationships amoung variables in scatter plot
# hue: Variable used for color mapping
sns.scatterplot(data=iris, x="sepal_length", y="sepal_width", hue="species", palette="hls")

# Plot pairwise relationships in a dataset.
sns.pairplot(iris, hue="species", palette="hls")
# see https://seaborn.pydata.org/generated/seaborn.pairplot.html
```

Common visualizations

Scatter plots: density

For large data sets, points are plotted over each other and density information is lost.



Left:
1000000 objects

Middle:
Instead of solid points, semitransparent points are plotted

Right:
hexagonal binning. Grey intensity denotes number of points

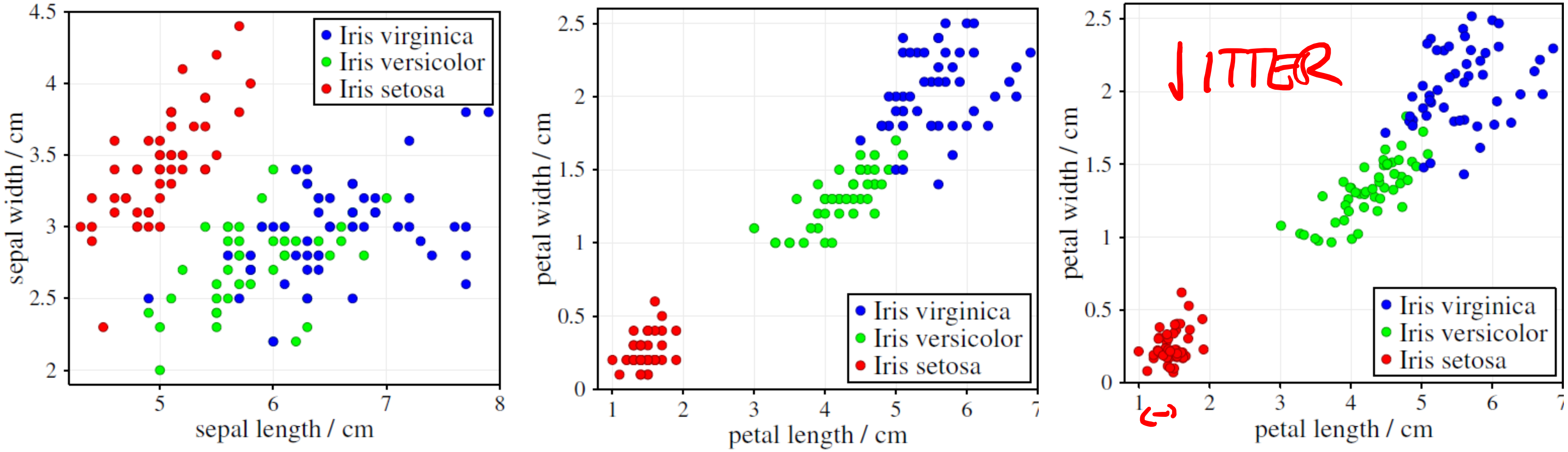
Iris Data Set Example

```
import pandas as pd
import seaborn as sns

iris = pd.read_csv('irisData.csv', names=['sepal_length','sepal_width‘,
'petal_length','petal_width','species'])

iris.plot.hexbin(x="sepal_length", y="sepal_width", gridsize=20)
sns.jointplot(data=iris, x="sepal_length", y="sepal_width", kind="hex",
color="k",joint_kws=dict(gridsize=20), marginal_kws=dict(bins=15, rug=True))
```

Ref.

Common visualizations

Scatter plots: further elaboration



Scatter plots can be **enriched** with additional information:
color or different symbols incorporate **a third attribute** in the scatter plot.

What differences does this reveal?

Data objects with the same values cannot be distinguished in a scatter plot → **jitter** (adding random noise)

Ref.

Correlation analysis

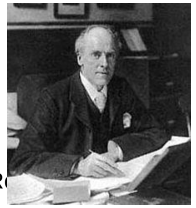
Freie Universität Berlin

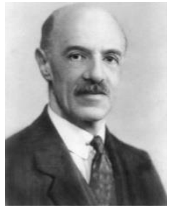
Scatter plots can **“visually” reveal correlations** or dependencies between two attributes.

Statistical measures for correlation are a more formal approach to correlation analysis and can be carried out automatically.

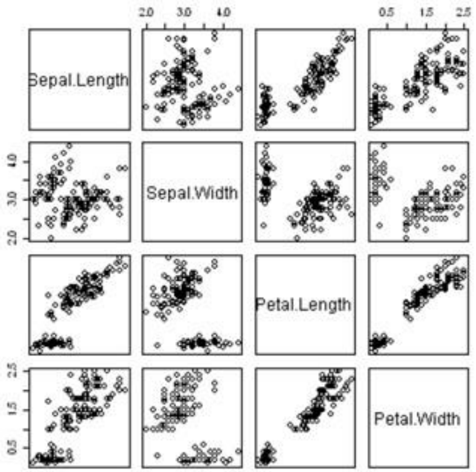
We briefly sketch…

- Pearson’s correlation coefficient
  - >> video for explanation
- Rank correlation coefficients
  - >> video for explanation
  - Spearman’s rho
  - Kendall’s tau





R




```
import pandas as pd

iris = pd.read_csv('irisData.csv', names=….)

print("Show Pearson's correlation:")
print(iris.corr())
#
print()
print("Show Spearman's rho correlation:")
print(iris.corr('spearman'))
#
print()
print("Show Kendal's tau correlation:")
print(iris.corr('kendall'))
```

python

Show Pearson's correlation:

	sepal_length	sepal_width	petal_length	petal_width
sepal_length	1.000000	-0.109369	0.871754	0.817954
sepal_width	-0.109369	1.000000	-0.420516	-0.356544
petal_length	0.871754	-0.420516	1.000000	0.962757
petal_width	0.817954	-0.356544	0.962757	1.000000

Show Spearman's rho correlation:

	sepal_length	sepal_width	petal_length	petal_width
sepal_length	1.000000	-0.159457	0.881386	0.834421
sepal_width	-0.159457	1.000000	-0.303421	-0.277511
petal_length	0.881386	-0.303421	1.000000	0.936003
petal_width	0.834421	-0.277511	0.936003	1.000000

Show Kendal's tau correlation:

	sepal_length	sepal_width	petal_length	petal_width
sepal_length	1.000000	-0.072112	0.717624	0.654960
sepal_width	-0.072112	1.000000	-0.182391	-0.146988
petal_length	0.717624	-0.182391	1.000000	0.803014
petal_width	0.654960	-0.146988	0.803014	1.000000

Pearson's correlation coefficient

The (sample) Pearson's correlation coefficient is a measure for a linear relationship between two numerical attributes X and Y and is defined as

$$r_{xy} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{(n-1)s_x s_y}$$

where $\bar{x}$ and $\bar{y}$ are the mean values of the attributes X and Y, respectively. s_x and s_y are the corresponding (sample) standard deviations.

The larger the absolute value of the Pearson correlation coefficient, the stronger the **linear relationship** between the two attributes.

$$-1 \leq r_{xy} \leq 1$$

Pearson's corrrellation assumes normal distribution (vulnerable to skewed data) and linear relationships.

Applicable to continuous variables.

Ref.

Rank correlation coefficient

Please read on your own

Pearson's correlation coefficient measures linear correlation.

Even for monotone functional, but non-linear relationship Pearson's correlation coefficient will not be -1 or 1. It can even be close to zero despite a monotone functional relationship.

Rank correlation coefficients avoid this by ignoring the exact numerical values of the attributes and *considering only the ordering* of the values.

They intend to measure monotonous correlations between attributes, where the monotonous function does not have to be linear.

Example: Aggregate Single Sales (US)

Pos	Artist and Title	Sales estimate	This year
1	Mark Ronson - Uptown Funk	7,470,000	120,000
2	Pharrell Williams - Happy	7,280,000	40,000
3	Katy Perry - Dark Horse	6,230,000	20,000
4	Taylor Swift - Shake It Off	5,840,000	60,000
5	Meghan Trainor - All About That Bass	5,710,000	20,000
ordinal		continuous	

Rank correlation coefficients

Spearman’s rho

Please read on your own

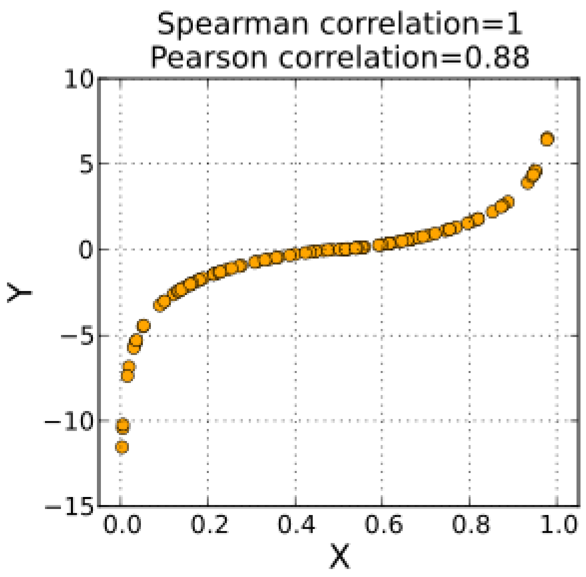
Spearman‘s rank correlation coefficient (**Spearman‘s rho**) is defined as

$$\rho = 1 - 6\,\frac{\sum_{i=1}^{n}\left(r(x_i)-r(y_i)\right)^2}{n(n^2-1)},$$

where we sum the deviations between $r(x_i)$ – the rank of value x_i when we sort the list $(x_1, \ldots, x_n)$ in increasing order – and $r(y_i)$.

When the rankings of the x- and y-values are exactly in the same order, Spearman‘s rho will yield the value 1.

If they are in reverse order, we will obtain the value -1.



Spearman‘s rho makes no assumption on the distribution and is applicable to continuous and discrete (ordinal) variables.

It is sensitive to large deviations.

Ref.

Image: Skbkekas (2009) | Wikimedia

Rank correlation coefficients

Kendall’s tau

Kendall‘s tau rank correlation coefficient (Kendall‘s tau) is defined as

$$\tau_a = \frac{C-D}{\frac{1}{2}n(n-1)}$$

where C and D denote the numbers of concordant (similar rank order) and discordant pairs with similar ranks, respectively.

$$C = \left|\left\{(i,j) \middle| x_i < x_j \text{ and } y_i < y_j\right\}\right|$$

$$D = \left|\left\{(i,j) \middle| x_i < x_j \text{ and } y_i > y_j\right\}\right|$$

Kendall‘s tau makes no assumption on the distribution.
Kendall‘s tau_a is applicable to continuous and discrete (incl. ordinal) variables

Less sensitive to errors and discrepancies in the data as Spearman.

Ref.

Agenda

Next Lesson

Low-dimensional relationships

Univariate Analysis

Bivariate Analysis

Higher-dimensional relationships

Principal Component Analysis

Parallel Coordinates

Ref.

Outlook I:
Methods for higher-dimensional data

(and an introductory example about the main idea of **Principal Component Analysis**)

Next Lesson

Freie Universität Berlin

General approach for incorporating all attributes in a plot:

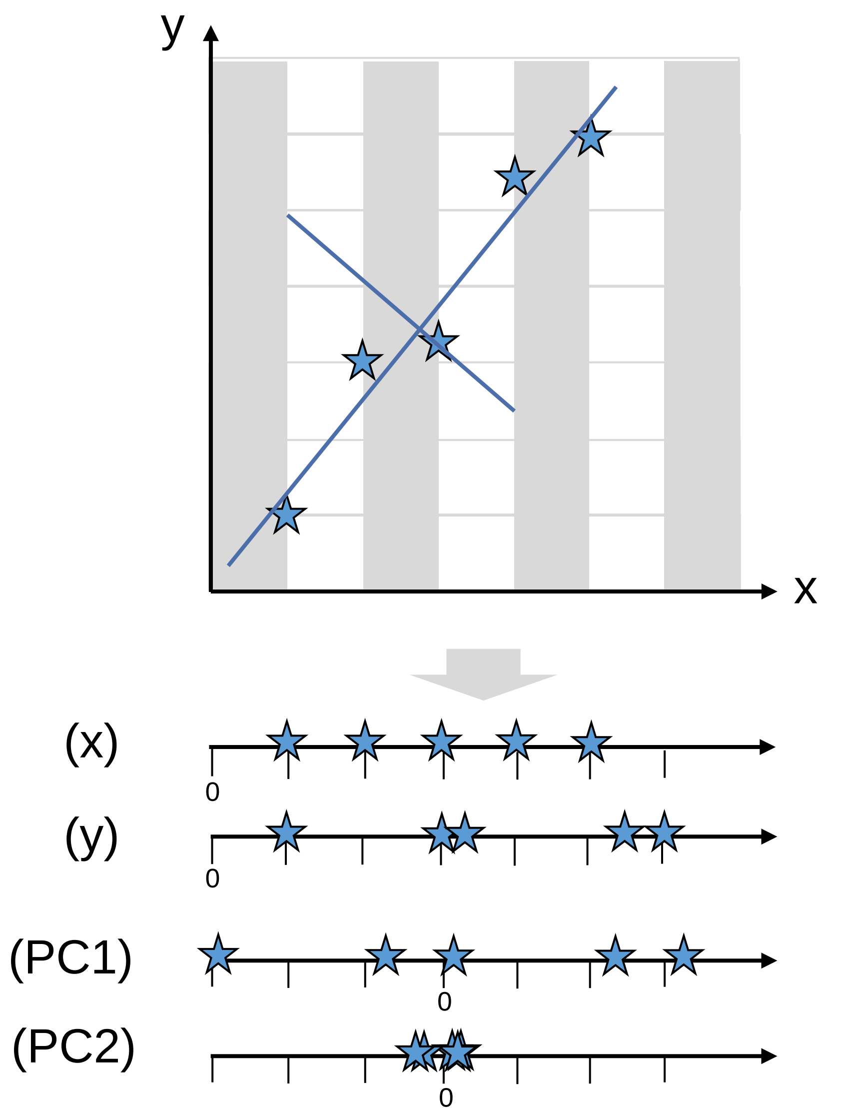
There is no unique measure for structure preservation.

Try to preserve as much of the “structure” of the high-dimensional data set when **representing (plotting) the data in two (or three) dimensions**

Define a measure that evaluates lower-dimensional representations (plots) of the data in terms of **how well a representation preserves the original “structure”** of the high-dimensional data set.

Find the representation (plot) that gives the best value for the defined measure.

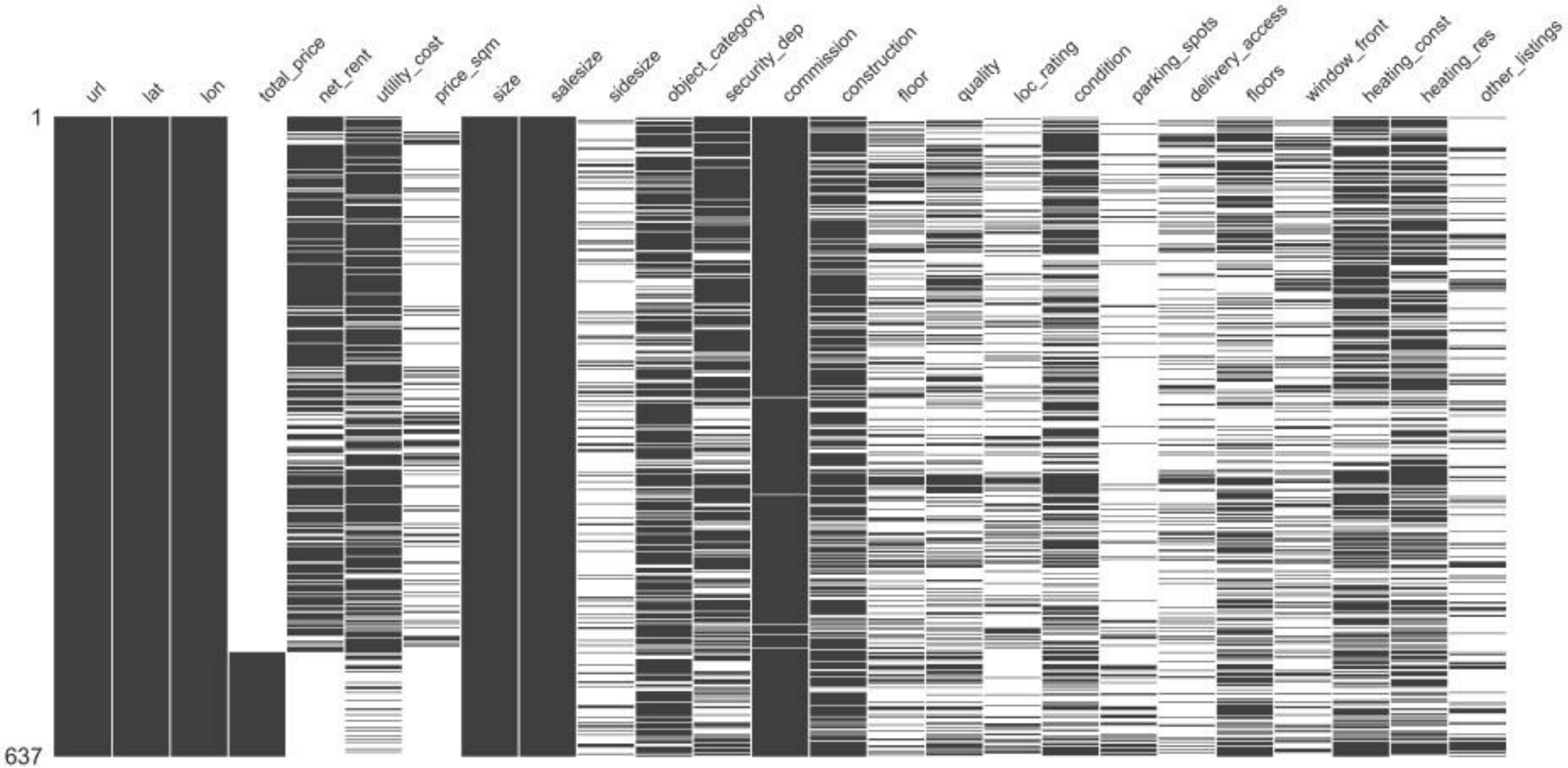
From $\mathbb{R}^2$ to $\mathbb{R}^1$



Next Lesson: More details about PCA

Outlook II:
Data understanding vs. Data preparation

Example: Which attributes should be selected?



Ref. Master Thesis Konrad (2019)

Fragen?

- ✓ Data understanding I
  - ✓ Attribute Understanding
  - ✓ Data Quality

- ✓ Data visualization, correlation analysis (Data understanding II)

- ✓ Low-dimensional relationships
  - ✓ Univariate Analysis
  - ✓ Bivariate Analysis
- o Higher-dimensional relationships
  - o Principal Component Analysis
  - o Parallel Coordinates

Recommended reading

Berthold et al. Chapter 4

Han, J., Kamber, M., Pei, J.: Data Mining: Concepts and Techniques. Morgan Kaufmann, 2011

Ref.

Todos for next Week

- Python-Analytics – Chapter 2
  Kursmaterial > Readings/Übungen > Python Übungen – Jupyter

- Please try the sample code on the Iris dataset on your own.

- Please get familiar with the PCA (incl. excursus) on the following slides.

Ref.

Principal Component Analysis (PCA)

Structure preservation through variance in data set

Next Lesson

PCA compresses a large data set to capture the *essence of the original data* through linear transformation

PCA constructs **a projection** from the high-dimensional space to a lower-dimensional space (plane or hyperplane) using only the most relevant dimensions

PCA uses the **variance in the data** set as the structure preservation criterion.

Assumption: Large variances describe interesting dynamics, smaller noise.

PCA preserves as much of the original variance of the data when projected to a lower-dimensional space

(Sample) variance for a numerical attribute:

$$s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2 = \frac{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}{n(n-1)}$$

Ref. e.g., Kristensen & Terje (2016, p. 81 ff.)

Principal Component Analysis

Procedure: Objective

Next Lesson

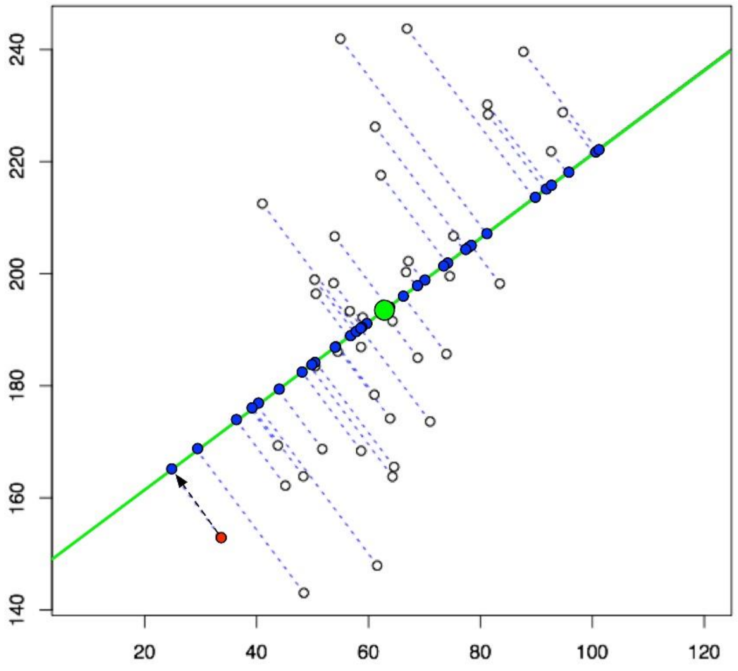
The data points are first **centered around the origin** by subtracting the mean values

Objective:

find a projection in the form of a linear mapping given by $\boldsymbol{y} = \boldsymbol{M}(\boldsymbol{x} - \overline{\boldsymbol{x}})$, where M is a $q \times m$ matrix such that the **variance** of the projected data $y_i = M(x_i - \bar{x})$ is **maximized**

($2 \times m$ for projections to a plane)

Projecting 2 dimensions on 1



PCA uses the covariance matrix which holds information on spread (variance) and orientation (covariance)

$$\Sigma = \begin{bmatrix} \sigma(x,x) & \sigma(x,y) \\ \sigma(y,x) & \sigma(y,y) \end{bmatrix}$$

See excursus for in-depth information

Ref. e.g., Kristensen & Terje (2016, p. 81 ff.)

Image: Pachter (2014)

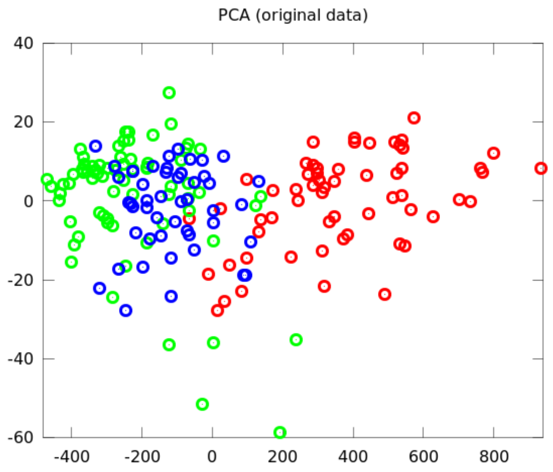
Principal Component Analysis

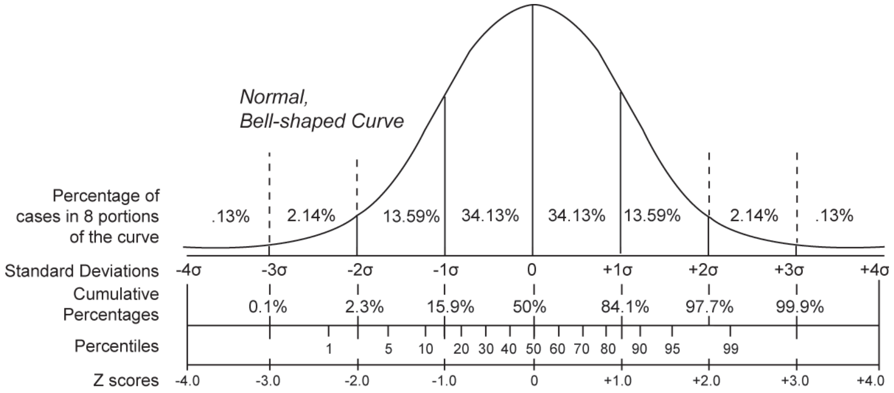
Procedure: Problem

Problem:
Without restriction for the matrix M, the entries in M can be chosen arbitrary large so that the data are not only projected, but also scaled, leading to an arbitrary large variance of the projected data.

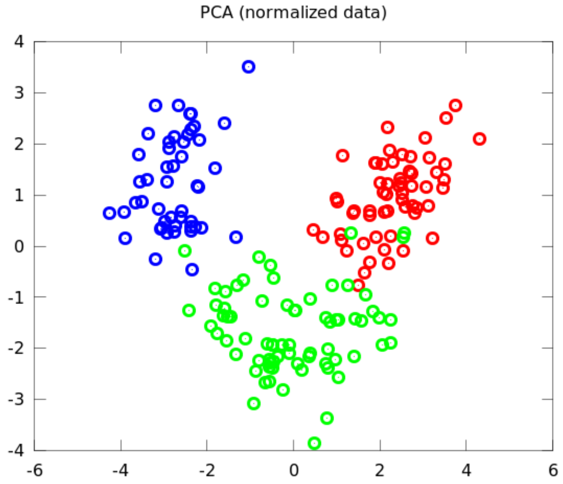
We introduce **constraints** such that the matrix M is only a projection:

The row v_i of the matrix $M = (v_1, \ldots, v_q)$ must be normalized, i.e., $||v_i|| = 1$.





Usually, the data should be **zero-score standardized** ($x \rightarrow \frac{x-\hat{\mu}_x}{\hat{\sigma}_x}$) to ensure that all attributes contribute equally to the overall variance
(with $\hat{\mu}_x$ being the mean value and and $\hat{\sigma}_x$ the sample standard deviation of attribute X, z-score: numeric distance of x in standard deviations from mean)



Ref. e.g., Kristensen & Terje (2016, p. 81 ff.)

Images: Wagner (2011)

Principal Component Analysis

Choosing principal components

Next Lesson

Freie Universität Berlin

Excursus

Solution of the constraint optimization problem:

The projection matrix M is given by $M = (v_1, \ldots, v_q)$,

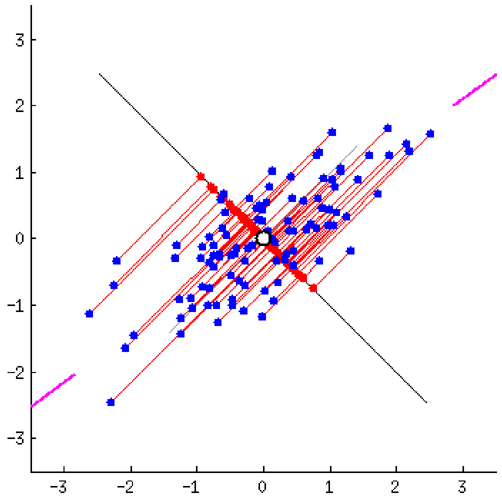
where the **principal components** $v_1, \ldots, v_q$

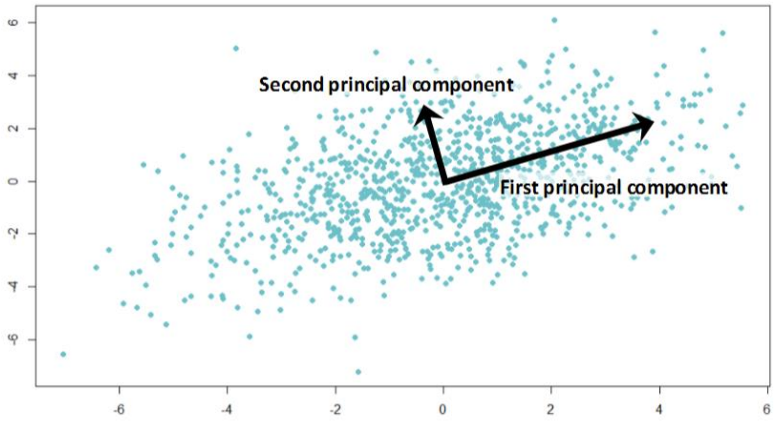
are the *normalized eigenvectors of the covariance matrix* of the attributes in the data set

$$\sigma_{jk} = \frac{1}{n-1}\sum_{i=1}^{n}(x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k)^T$$

for the q **largest eigenvalues** $\lambda_1 \geq \cdots \geq \lambda_q$.

λ is called an eigenvalue of a matrix A, if there is a non-zero vector $\boldsymbol{v}$ such that $A\boldsymbol{v} = \lambda\boldsymbol{v}$ holds. The vector v is called eigenvector (direction of the data) to the eigenvalue λ (magnitude of its spread).





Ref. e.g., Kristensen & Terje (2016, p. 81 ff.), An illustrative explanation for Eigenvalue/Eigenvectors (in German)

Image. Gabasova (2014)

Principal Component Analysis

Excursus

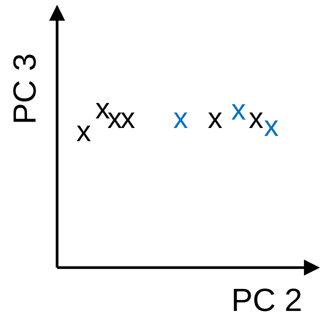
Dimension reduction

Let $\lambda_1 \geq \cdots \geq \lambda_m$ be the eigenvalues of the covariance matrix.

When we project the data to the first q principal components $v_1, \ldots, v_q$ corresponding to the eigenvalues $\lambda_{1,} \ldots, \lambda_q$, this projection will preserve a fraction of of the variance of the original data.

$$\frac{\lambda_1 + \cdots + \lambda_q}{\lambda_1 + \cdots + \lambda_m}$$

Omid principal components which explain little variance in the data, like…



Iris data set:

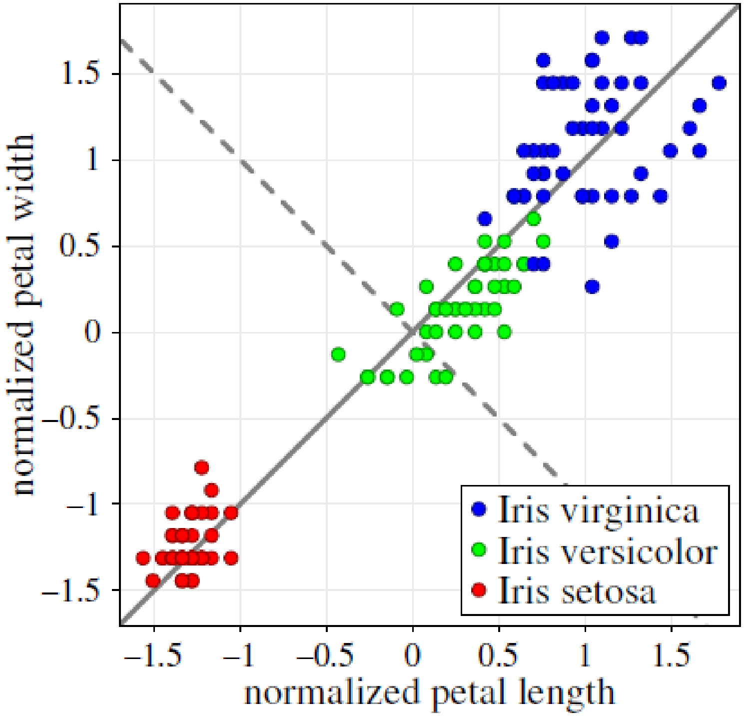
	PC1	PC2	PC3	PC4
Proportion of variance	0.73	0.229	0.0367	0.00518
Cum. proportion	0.73	0.958	0.9948	1.00000

Ref.

PCA – Iris data set example (1/2)

Next Lesson

PCA applied to the **Iris data set** restricted to the (normalized) petal length and width



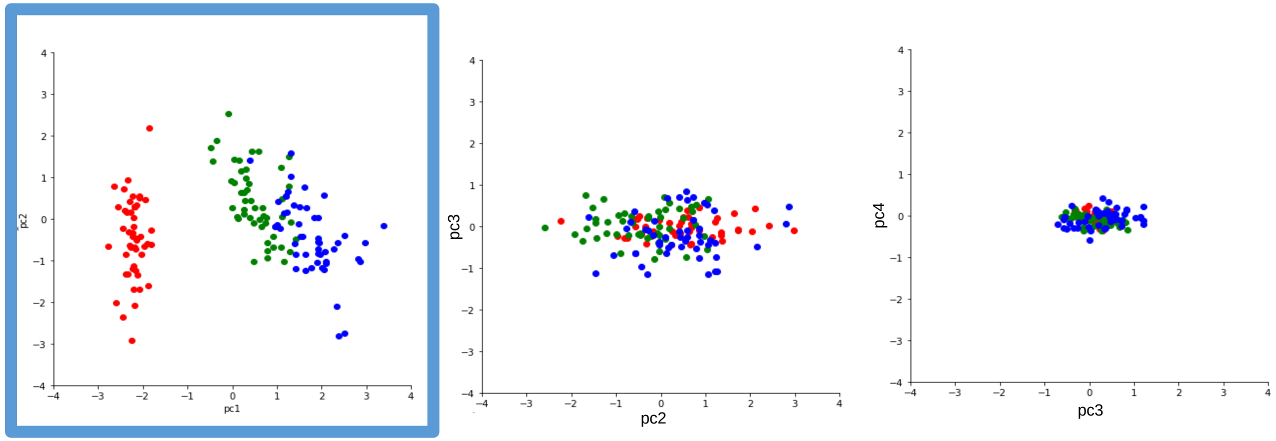
The principal components are always *orthogonal*

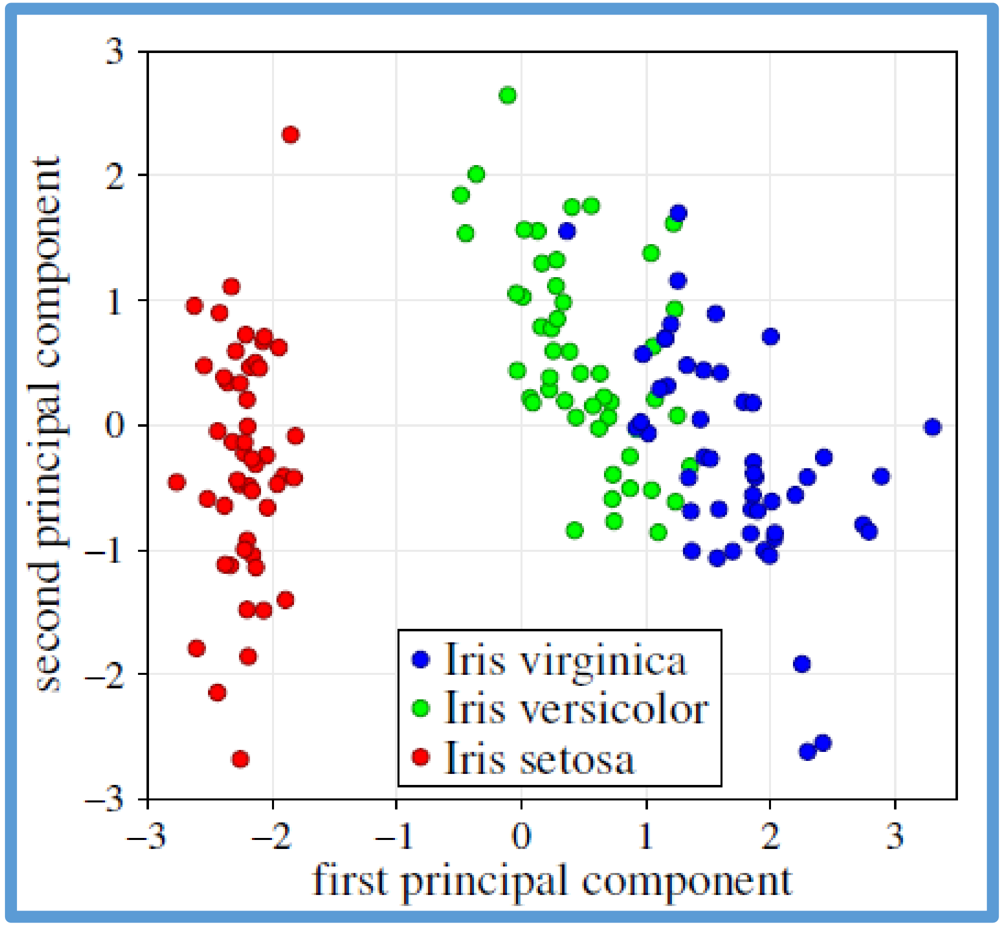
Ref.

PCA – Iris data set example (2/2)

Freie Universität Berlin

Projection to the first two principal components of PCA taking all four numerical attributes into account





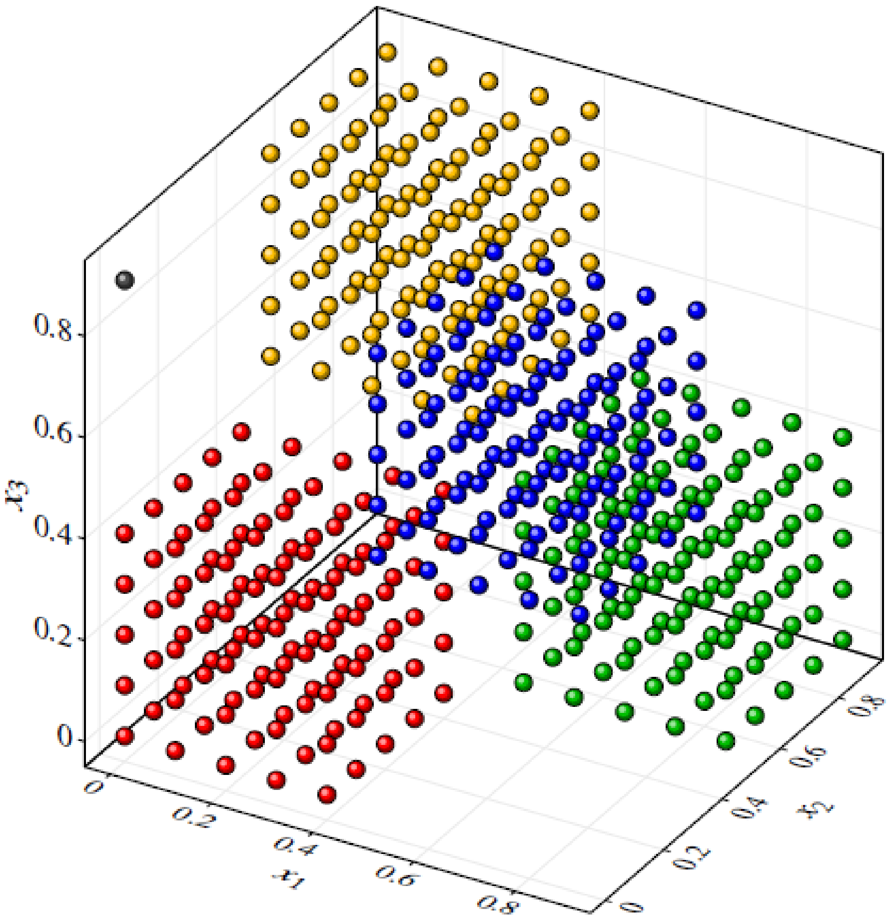
Original data is **reconstructable** from the principal components

Ref.

PCA – Chessboard example (1/2)

Next Lesson

An artificial data set filling a cube in a chessboard-like manner



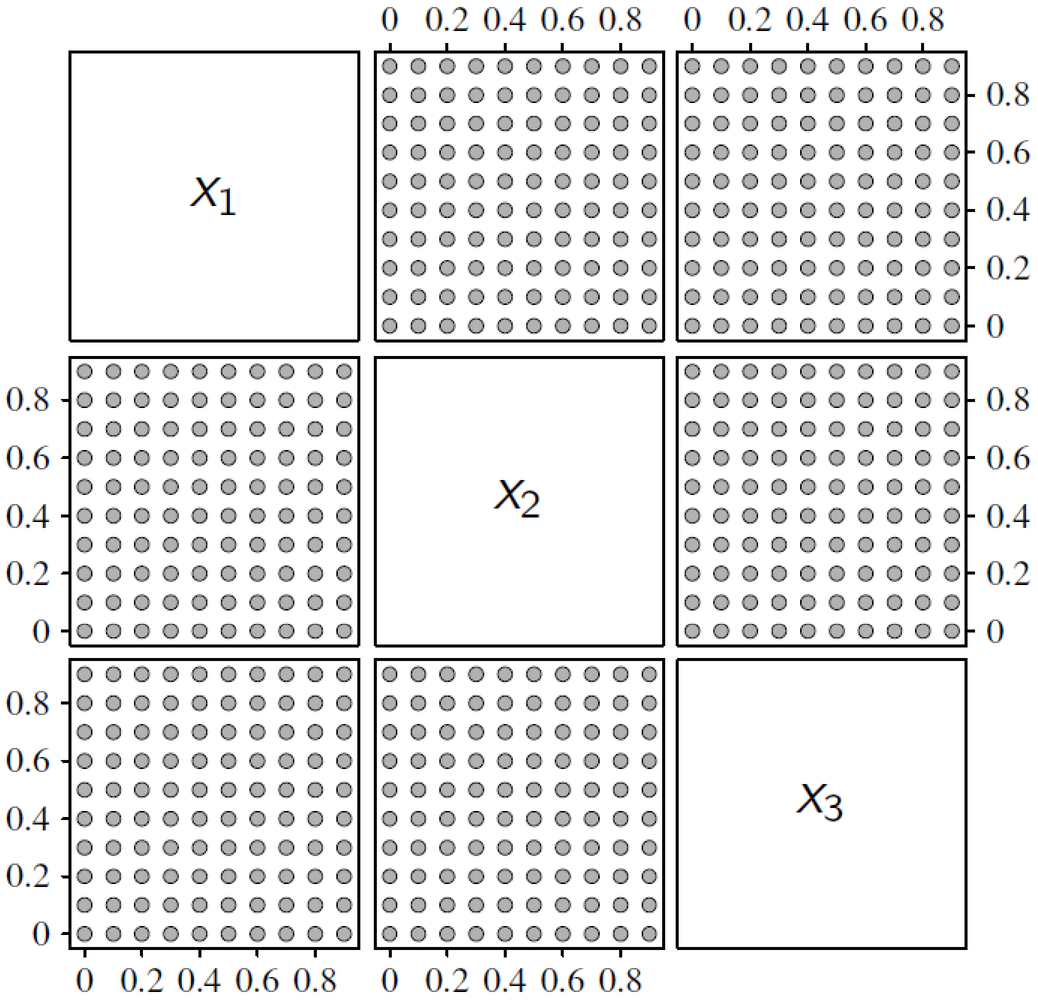
Ref. Berthold et al. (2010)

PCA – Chessboard example (2/2)

Next Lesson

Scatter plots

Is data uniformly distributed over the grid?



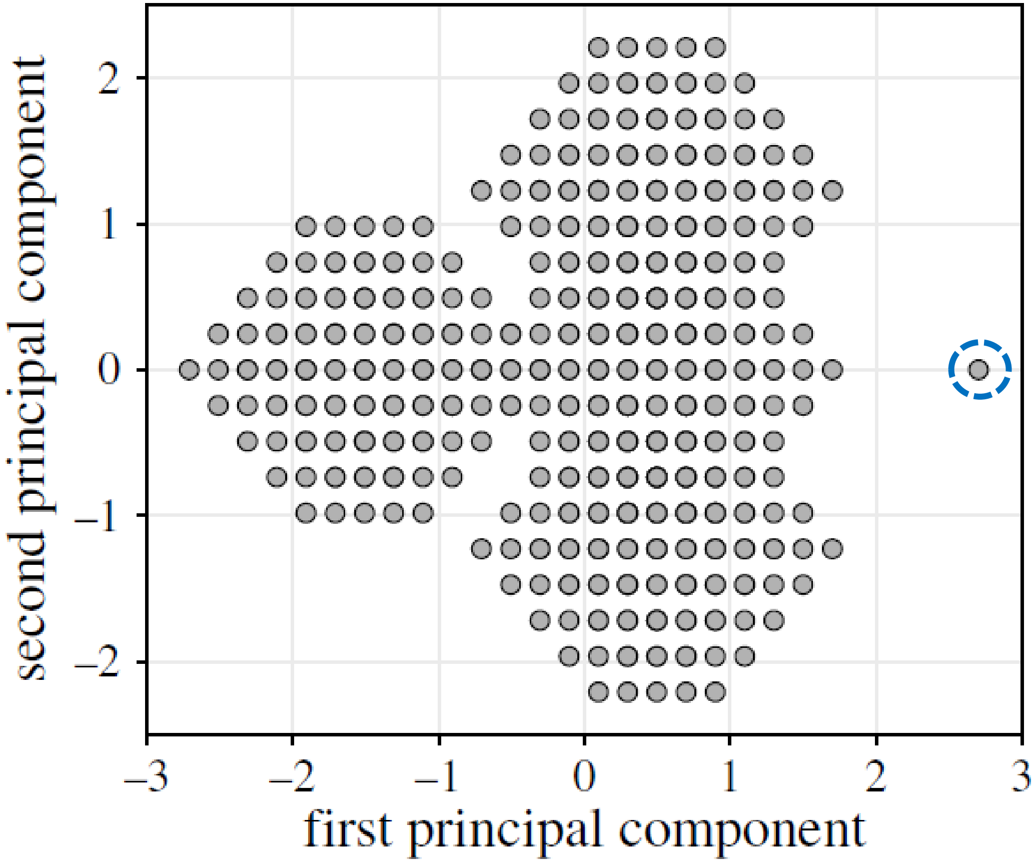
Ref. Berthold et al. (2010)

Projection to the first two **principal components**

Data is not uniformly distributed.

There is a pattern in the data set.

Data can be recreated from PCA.



Principal Component Analysis – Iris Data Set

Python Example

```
from sklearn.decomposition import PCA
from sklearn.preprocessing import scale

iris = pd.read_csv('irisData.csv', names=['sepal_length', 'sepal_width', 'petal_length', 'petal_width', 'species'])
#select only metric data
raw_iris = iris[['sepal_length', 'sepal_width', 'petal_length', 'petal_width']]

#center data to mean
norm_iris = scale(raw_iris)

#create pca with 4-dimensions
pca = PCA(n_components=4)
#pca data
pca_iris = pca.fit_transform(norm_iris)

print(pca.explained_variance_)
print(pca.explained_variance_ratio_)
print(pca.explained_variance_ratio_.cumsum())

#visualize pcas
vis_iris = pd.DataFrame(pca_iris, columns=['pc1', 'pc2', 'pc3', 'pc4'])
vis_iris['species'] = iris['species']
g = sns.FacetGrid(vis_iris, hue='species', palette=['r','g','b'], ylim=(-4,4), xlim=(-4,4), height = 6)
g.map(plt.scatter, 'pc1', 'pc2')
plt.show()

g = sns.FacetGrid(vis_iris, hue='species', palette=['r','g','b'], ylim=(-4,4), xlim=(-4,4), height = 6)
g.map(plt.scatter, 'pc2', 'pc3')
plt.show()

g = sns.FacetGrid(vis_iris, hue='species', palette=['r','g','b'], ylim=(-4,4), xlim=(-4,4), height = 6)
g.map(plt.scatter, 'pc3', 'pc4')
plt.show()
```

Example in Python

Ref.