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About Data, Preparation, PCA

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Data Mining (praktisch) SoSe 2025

Datum	Thema
01.04.25	Einführung ins Modul und Thema
08.04.25 (flex)	Python Einführung via Data Camp (Zeitlich frei einteilbarer Onlinekurs)
15.04.25	V&Ü Business Understanding und wirtschaftliche Grundlagen
22.04.25	Online Sprechstunde
29.04.25	Online Einzelabnahme Business Understanding Meilenstein
06.05.25	V&Ü Data Understanding and Visualization
13./14.05.25	Probelehrveranstaltungen für Statistische Methoden in der KI – DataCamp
20.05.25	Online Einzelabnahme Data Understanding Meilenstein
27.05.25	V&Ü Data Distributions and Transformations
03.06.25	Online Gruppenabnahme Data Preparation Meilenstein
10.06.25	V&Ü Clustering algorithms and evaluation
17.06.25	Online Sprechstunde
24.06.25	Online Gruppenabnahme Modeling and Evalation Meilenstein
01.07.25	Online Sprechstunde
08.07.25	Finale Projekt-Präsentationen (alle Gruppen durchgängig anwesend)

Goals today

- Learn some data preprocessing / preparation

- Get to know dimension reduction methods

RECAP OF LAST WEEK

…to remember the most important concepts / ideas

Other Categorization: Discrete & Continuous Attributes

- Discrete Attribute
  - Has only a finite or countable infinite set of values
    - Examples: zip codes, counts or the set of words in a collection of documents
  - Often represented as integer variables.
  - Note: binary attributes are a special case of discrete attributes
- Continuous Attribute
  - Has real numbers as attribute values
    - Examples: temperature, height, or weight.
  - Practically, real values can only be measured and represented using a finite number of digits.
  - Continuous attributes are typically represented as floating-point variables.

1. Excercise about different types of attribute values

Which operations are allowed ?

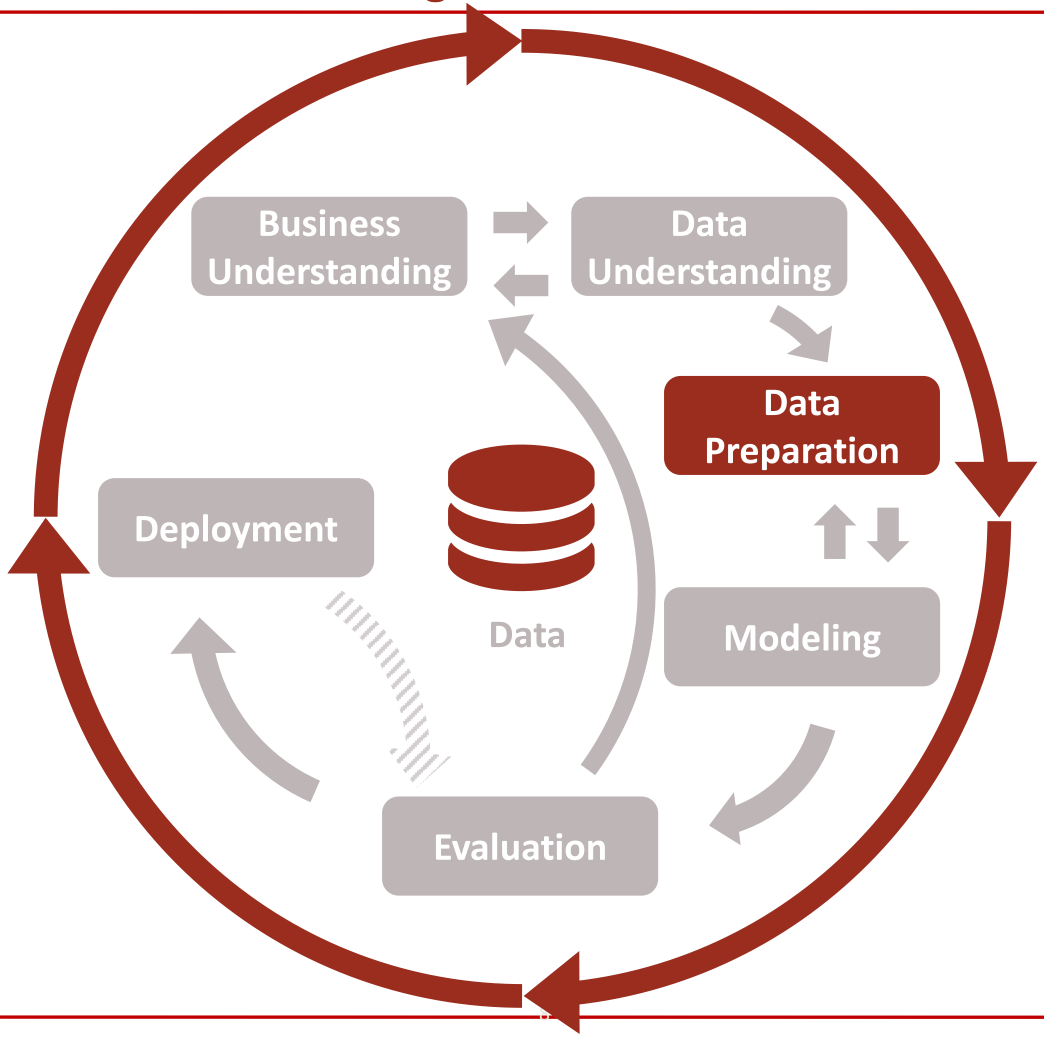
Attribut Type	Mathem. Operation (two values)	Aggregation (many values)
nominal	= ≠	Mode, count
ordinal	all from nominal & <>	Median, count
interval	all from ordinal & +, -	Mean, sum
ratio	all from intervall & *, /	Mean, sum, division

DATA PREPARATION

…how to get more value to the data

CRISP-DM

Cross-Industry Standard Process for Data Mining



Why Data Preprocessing is Crucial

- The problem: all data analysis approaches are dumb. They rely on statistics, but
  - they do not understand data
  - they can not be creative
- Data pre-processing is the step where the data scientist tells the algorithm what it needs to know about the data

Coding of the Application Domain – Mapping of Real World Objects

- Real world objects / real world context
- **Instance**, example, sample, object
- Coding is composed of **attributes** (features, characteristics)
- Different possible types of attributes
  - Numerical (age: 10, 50, 100)
  - Ordinal - ordered categories (weight: underweight, normal weight, overweight, very overweight)
  - Nominal - categories (profession: computer scientist, analyst, teacher, …)

An Explanatory Example

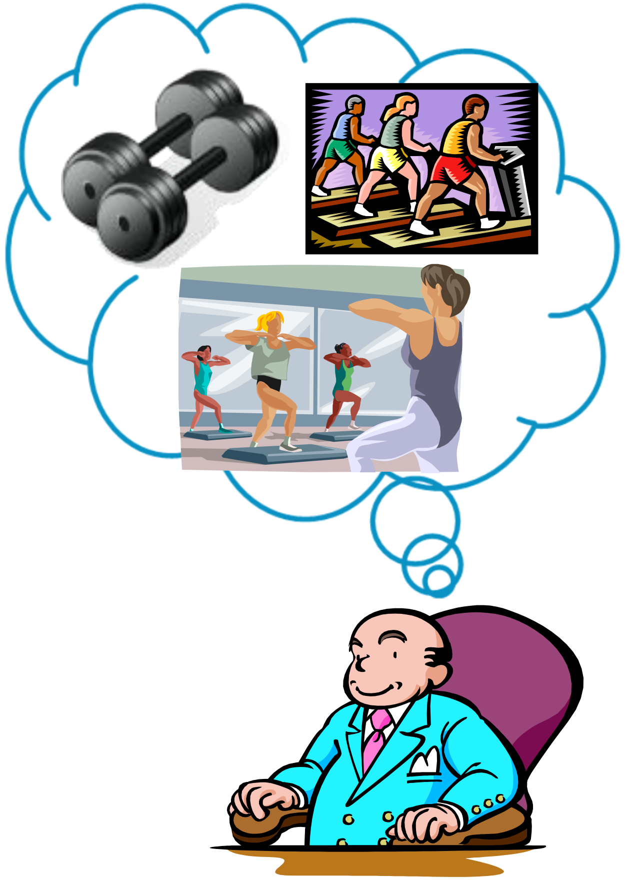
Manager of gym chain

Goals:

- New members
- Less contract cancellations

The road to success:

- New individual pricing structure
- More targeted advertising and offers



How to Code the Members?

ID - key

attribute

effect variable/ label

Effect variable (label) for advertising in example: stated goal of fitness

ID	gender	age	weight	running contract?	contract period (until today)	stated goal of fitness
1	F	51	normal	yes	5	general fitness
7	F	16	over	no	1	loss of weight
D1	M	26	normal	yes	0.5	muscle growth
19	M	60	under	yes	4	muscle growth
93	M	40	very over	yes	8	loss of weight
46	F	37	normal	no	6	general fitness
56	M	50	over	yes	12	?
4	F	19	under	yes	3	?
58	F	29	normal	yes	0.2	?

labelled data

unlabelled data

A few more words about attributes

Naming attributes

Descriptive attributes

Referential attributes

ID	gender	age	weight	running contract?	contract period (until today)	stated goal of fitness	Studio ID
1	F	51	normal	yes	5	general fitness	1
7	F	16	over	no	1	loss of weight	2
11	M	26	normal	yes	0.5	muscle growth	2
19	M	60	under	yes	4	muscle growth	1
93	M	40	very over	yes	8	loss of weight	3
46	F	37	normal	no	6	general fitness	3

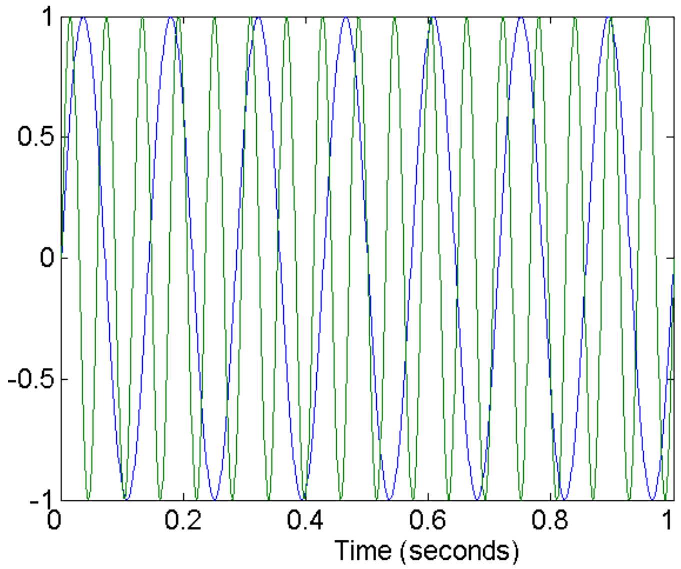
Derived attributes

Data Quality

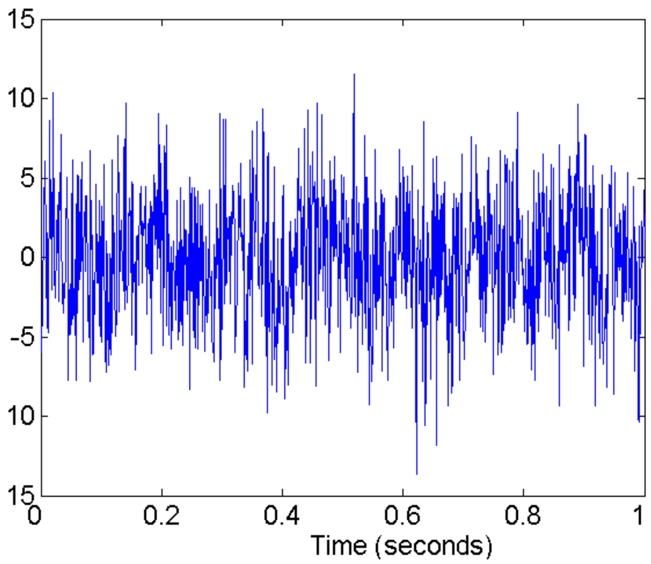
- What kinds of data quality problems exist?
- How can we detect problems with the data?
- What can we do about these problems?
- Examples of data quality problems:
  - Noise and outliers
  - missing values
  - duplicate data

Noise

- Noise refers to modification of original values
  - Examples: distortion of a person's voice when talking on a poor phone and "snow" on television screen



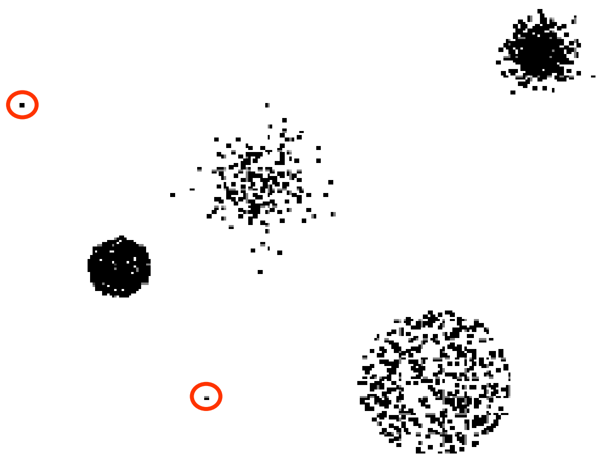
Two Sine Waves



Two Sine Waves + Noise

Outliers

- Outliers are data objects with characteristics that are considerably different than most of the other data objects in the data set



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Missing Values

- Reasons for missing values
  - Information is not collected
    - e.g., people decline to give their age and weight
  - Attributes may not be applicable to all cases
    - e.g., annual income is not applicable to children
- Handling missing values
  - Eliminate Data Objects
  - Estimate missing values
  - Ignore the missing value during analysis
  - Replace with all possible values
    - weighted by their probabilities

How do I Cope with Missing Data?

- Delete instance
- Delete attribute
- Insert standard value
- „Mean“value
- Striking value
- Use suitable model-building

– Frequent problems

- Sometimes a missing value has been replaced with a hard-coded value („9999“).
- But sometimes a missing value also has a meaning

ID	gender	age	weight	running contract?	contract period (until today)	stated goal of fitness
1	F	51	normal	yes	5	general fitness
7	F	16	?	no	1	loss of weight
11	F	26	normal	yes	0.5	muscle growth

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Duplicate Data

- Data set may include data objects that are duplicates or almost duplicates of one another
  - Major issue when merging data from heterogeneous sources
- Examples:
  - Same person with multiple email addresses
- Data cleaning
  - Process of dealing with duplicate data issues
  - Sea Thomas Krause, Entwurf und Implementierung einer effizienten Dublettenerkennung für große Adressbestände in http://epb.bibl.fh-koeln.de/frontdoor/index/index/docId/270

Derived Features

- The algorithm does not know about attribute dependencies
  - Construct quotients, differences, etc. of attributes
- The algorithm does not know about meaning of data
  - Date → weekday, holiday, …
- Also: joining with external data, e.g. ZIP code → population, location & day → weather, …
- Construct meaningful attributes by hand
- Also remove unnessary attributes, e.g. identifiers

Note: different philosophy between database as archive and analytical database!

Special case: Time-dependent Data

- Many data mining algorithms work only with spreadsheet data
- Connections between rows – as with time-dependent data – are usually not made automatically
- Construct meaningful attributes
  - Time since last visit
  - Number of visits in last month
  - Average number of visits per week
  - Weight difference since last visit
  - …

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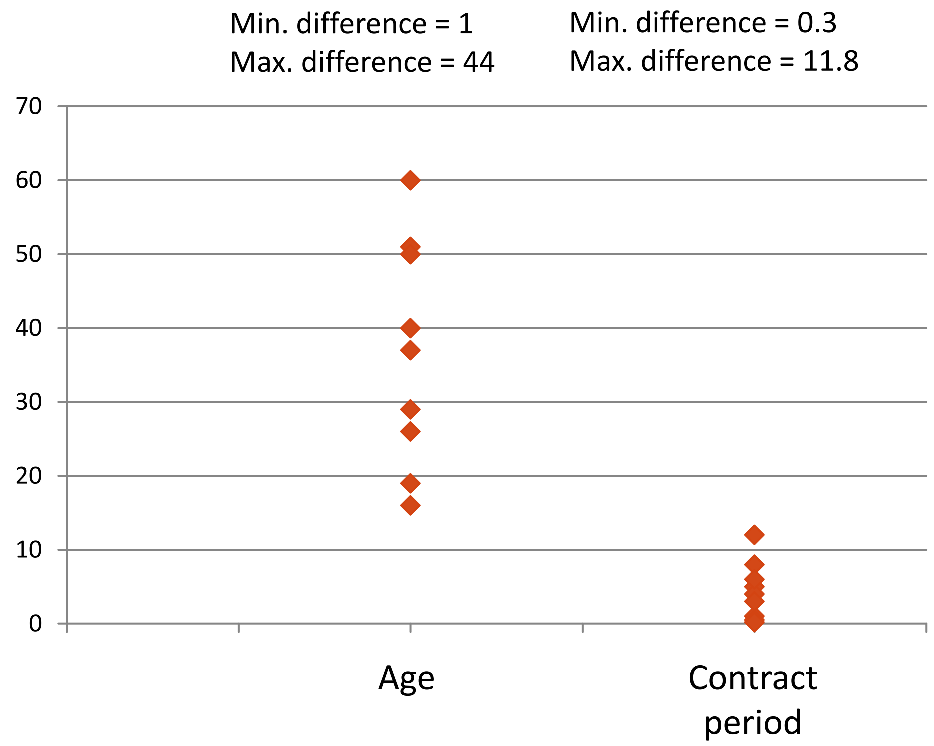
Standardization / Normalization

Numerical attributes may be in different intervals

→ varying influence on model

age	contract period (until today)
51	5
16	1
26	0.5
60	4
40	8
37	6
50	12
19	3
29	0.2



Standardization / Normalization

- Numerical attributes maybe in different intervals → varying influence on model
- Harmonization by standardization
- Z-Transformation (mean value to 0, standard deviation to 1)

$$\tilde{a}_i = \frac{a_i - \mu_a}{\sigma_a}$$

- Linear normalization (values between 0 (-1) and 1)

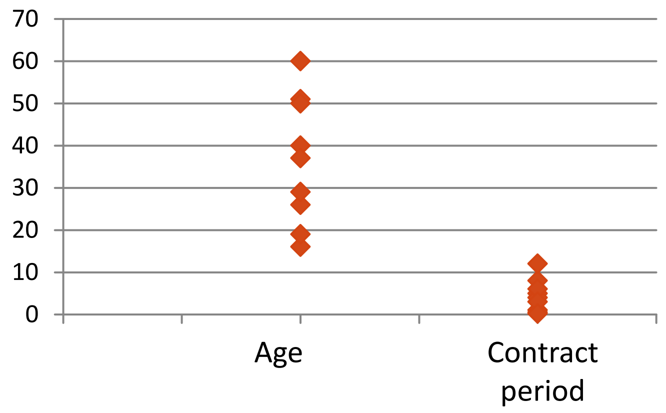
$$\tilde{a}_i = \frac{a_i - \min(a)}{\max(a) - \min(a)}$$

Gym Example – Z-Transformation

age	contract period (until today)
51	5
16	1
26	0.5
60	4
40	8
37	6
50	12
19	3
29	0.2

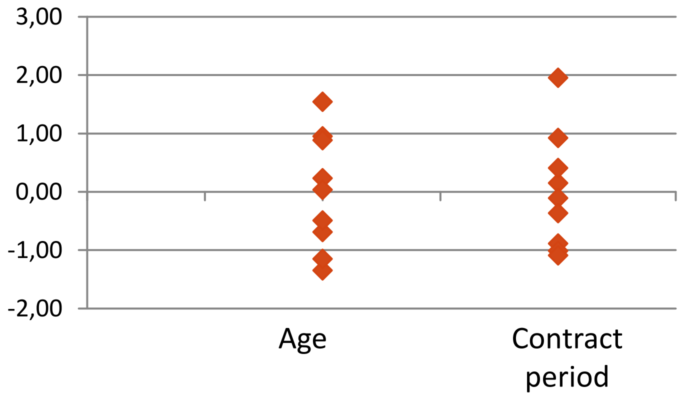
$$\tilde{a}_i = \frac{a_i - \mu_a}{\sigma_a}$$

age	contract period (until today)
0.96	0.15
-1.34	-0.88
-0.69	-1.01
1.55	-0.11
0.23	0.93
0.04	0.41
0.89	1.96
-1.15	-0.36
-0.49	-1.09



Min. difference = 0.07
Max. difference = 2.89

Min. difference = 0.08
Max. difference = 3.04

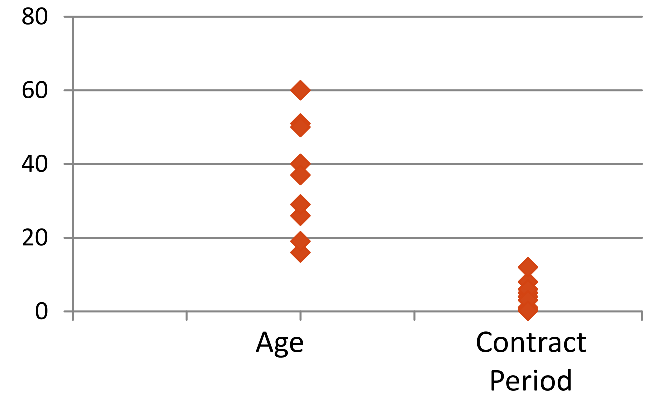


Gym Example – Linear Standardization

age	contract period (until today)
51	5
16	1
26	0.5
60	4
40	8
37	6
50	12
19	3
29	0.2

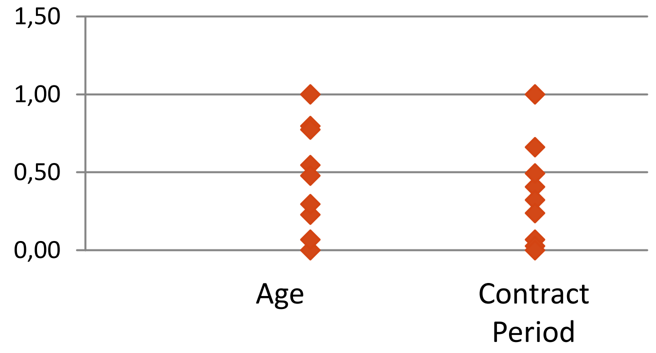
$$\tilde{a}_i = \frac{a_i - \min(a)}{\max(a) - \min(a)}$$

age	contract period (until today)
0.80	0.41
0.00	0.07
0.23	0.03
1.00	0.32
0.55	0.66
0.48	0.49
0.77	1.00
0.07	0.24
0.30	0.00



Min. difference = 0.02
Max. difference = 1.00

Min. difference = 0.03
Max. difference = 1.00



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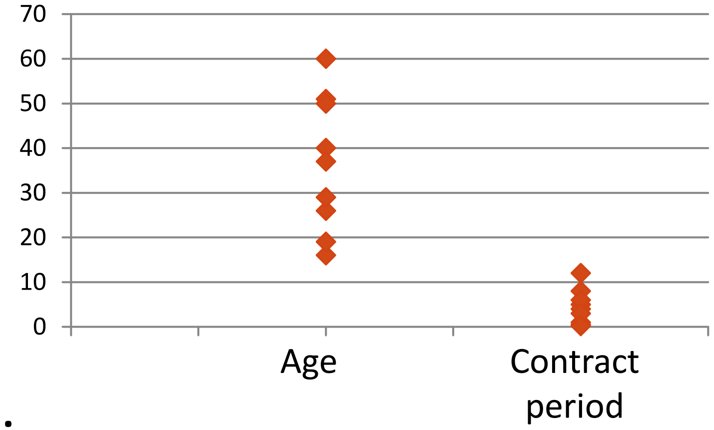
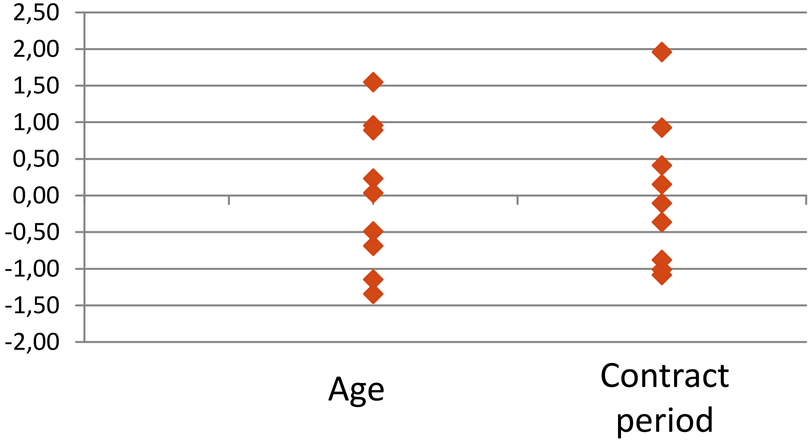
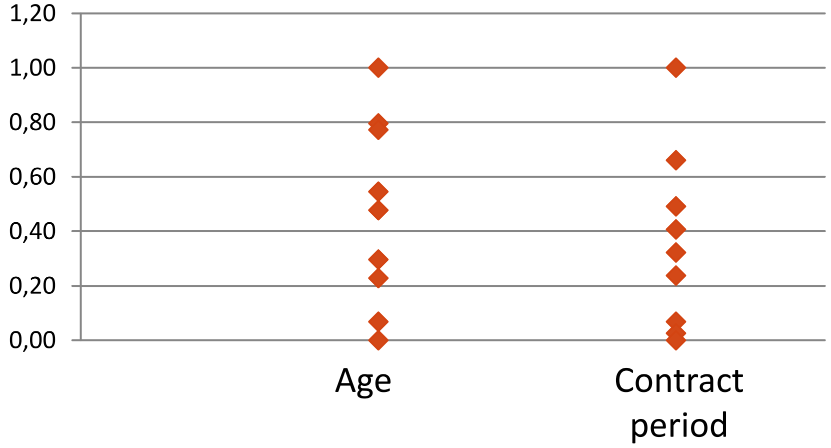
Gym Example – Standardization Comparisons



Z-Transformation



Linear Standardization



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Most algorithms assume data to be normal-distributed

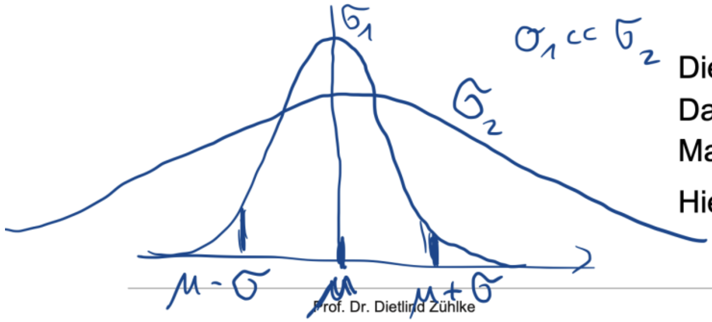
- Normal distribution – recap from mathematics 2

Normalverteilung = Gaußverteilung

Eine stetige Zufallsvariable $X\colon \Omega\colon \mathbb{R}$ heißt normalverteilt mit Mittelwert μ und der Standardabweichung σ oder kurz $N(\mu,\sigma)$-verteilt, wenn ihre Dichtefunktion lautet

$$\omega(t) = \frac{1}{\sigma \cdot \sqrt{2\pi}} \cdot \exp\left(-\frac{(t-\mu)^2}{2\sigma^2}\right)$$

Die Normalverteilung hat die typische Form der Gauß'schen Glockenkurve.

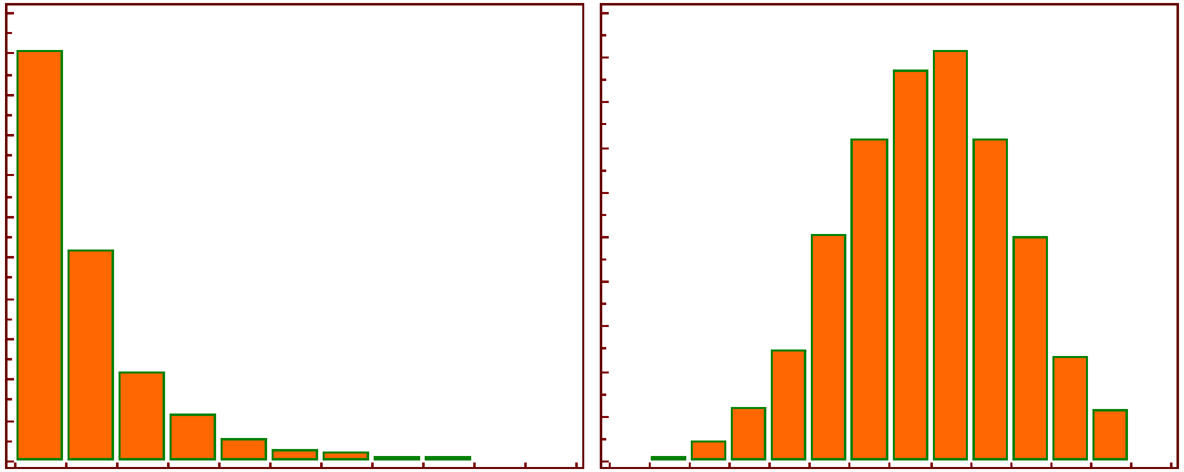


Die Parameter μ und σ lassen sich unmittelbar aus der grafischen Darstellung der Dichtefunktion ablesen: Die Gaußglocke hat ihr Maximum bei $t = \mu$ und ihr Wendepunkt bei $\mu - \sigma$ und $\mu + \sigma$.

Hier liegen 68,2% der Daten im Intervall $[\mu - \sigma, \mu + \sigma]$.

Log-transformation to help with skewed data

- Skewed data means a lot of small values and a long „tail“ of larger ones
- Log-transformation makes data more similar to normal-distributed data
  - Original number = x
  - Transformed number $x'=\log_{10}(x)$
  - Back-transformed number = $10^{x'}$
- For zeros or negative numbers log is not defined
  - Add a constant to each number to make them positive and non-zero.



https://www.medcalc.org/manual/log-transformation.php

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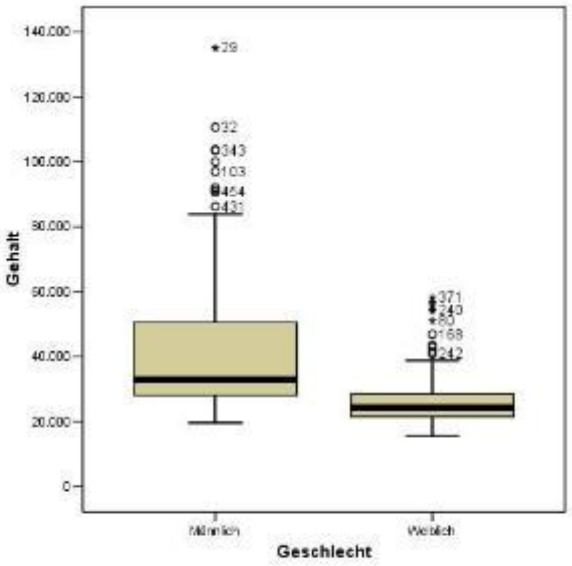
Exploratory Data Analysis

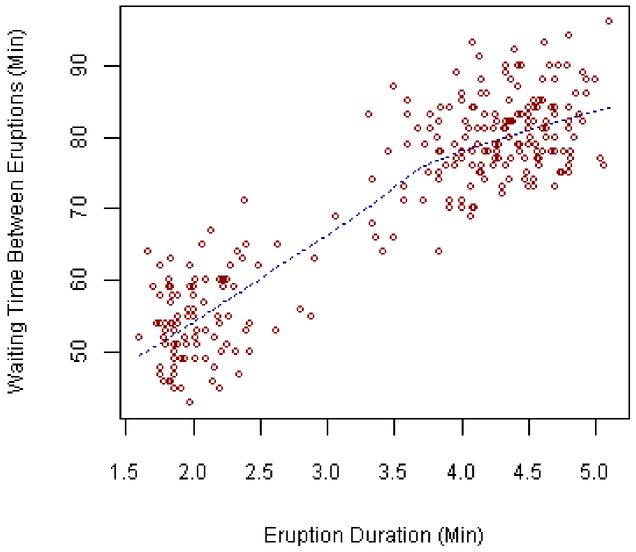


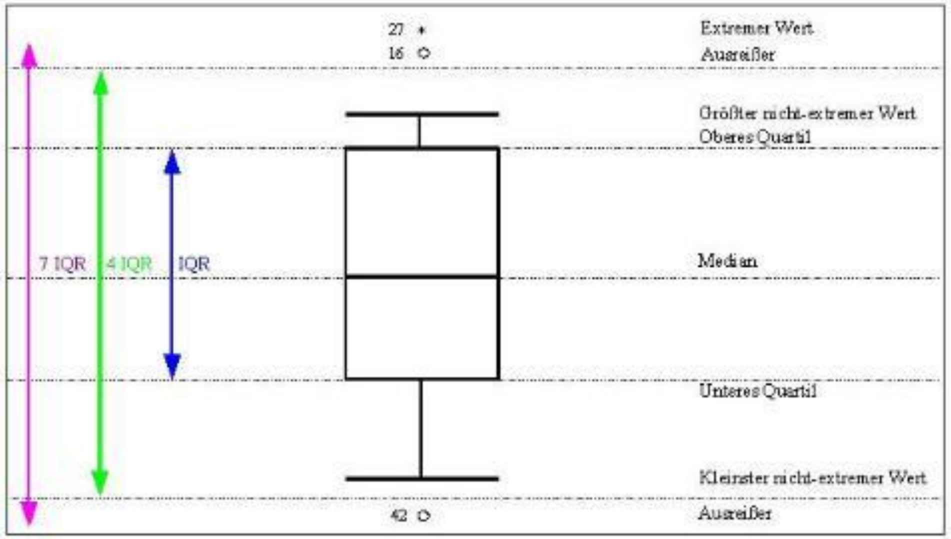
Boxplots

- Categorical target attributes

Scatterplots

- Numerical target attributes
- Suspected correlation





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Re-Use of Pre-Processing
Making your life easier in the long run

- Data preprocessing is a manual, time-consuming process, but it can often be reused for new projects
- Report quality problems!
- If possible, turn off the root cause
- Add pre-processing to data warehouse, e.g. derived features
- Document insights

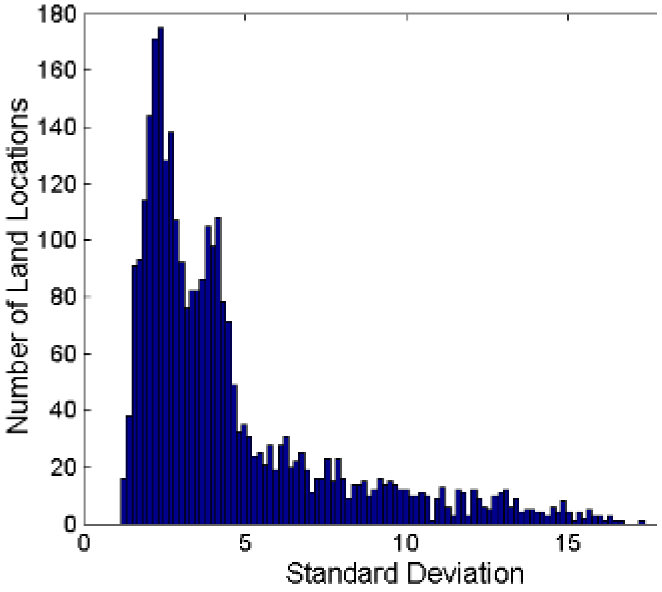
Aggregation

- Combining two or more attributes (or objects) into a single attribute (or object)
- Purpose
  - Data reduction
    - Reduce the number of attributes or objects
  - Change of scale
    - Cities aggregated into regions, states, countries, etc
  - More “stable” data
    - Aggregated data tends to have less variability

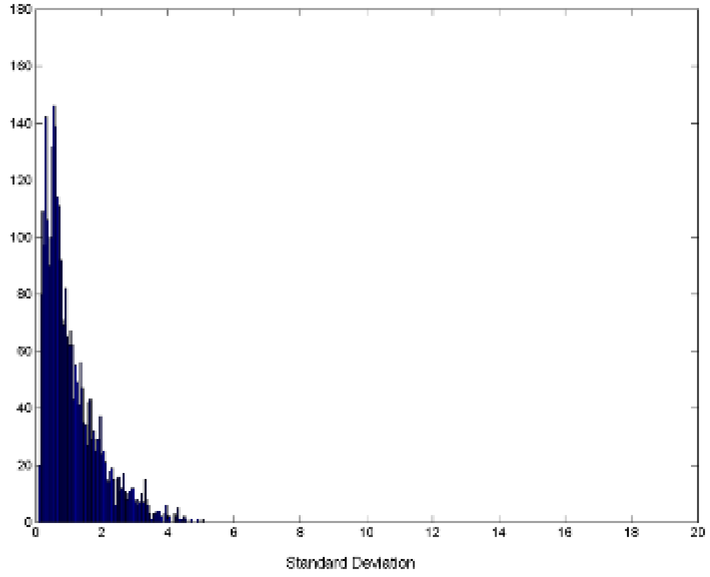
SQL:
Group By

Aggregation

Variation of precipitation (of rain) in Australia



Standard Deviation of Average Monthly Precipitation



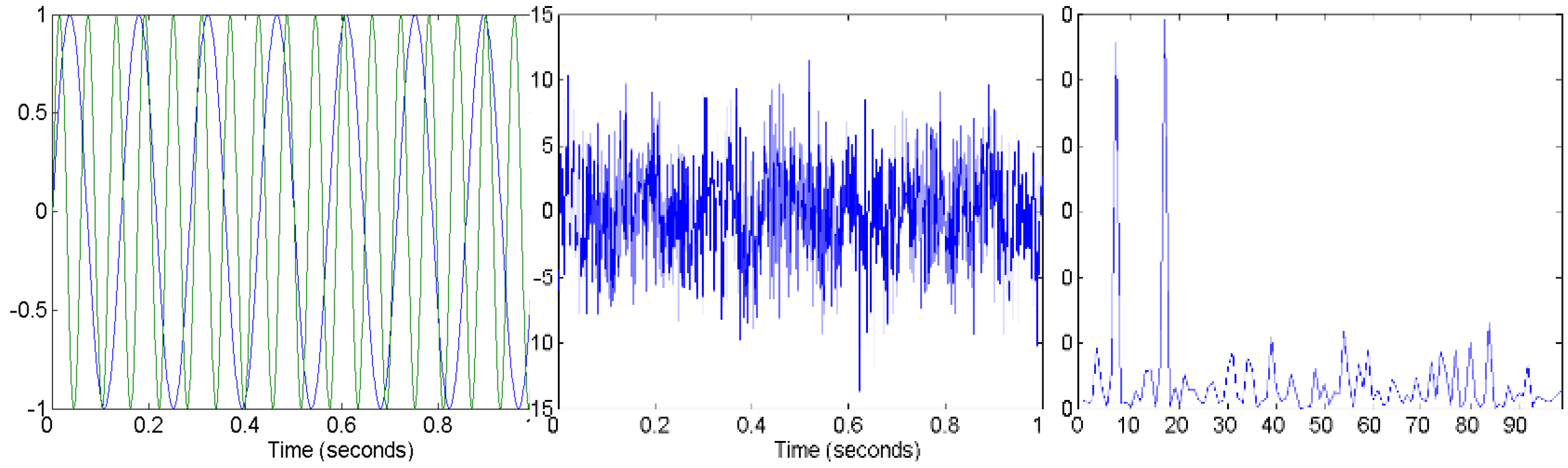
Standard Deviation of Average Yearly Precipitation

Feature Creation

- Create new attributes that can capture the important information in a data set much more efficiently than the original attributes
- Three general methodologies:
  - Feature Extraction
    - domain-specific
  - Mapping Data to New Space
  - Feature Construction
    - combining features

Mapping Data to a New Space

- Fourier transform



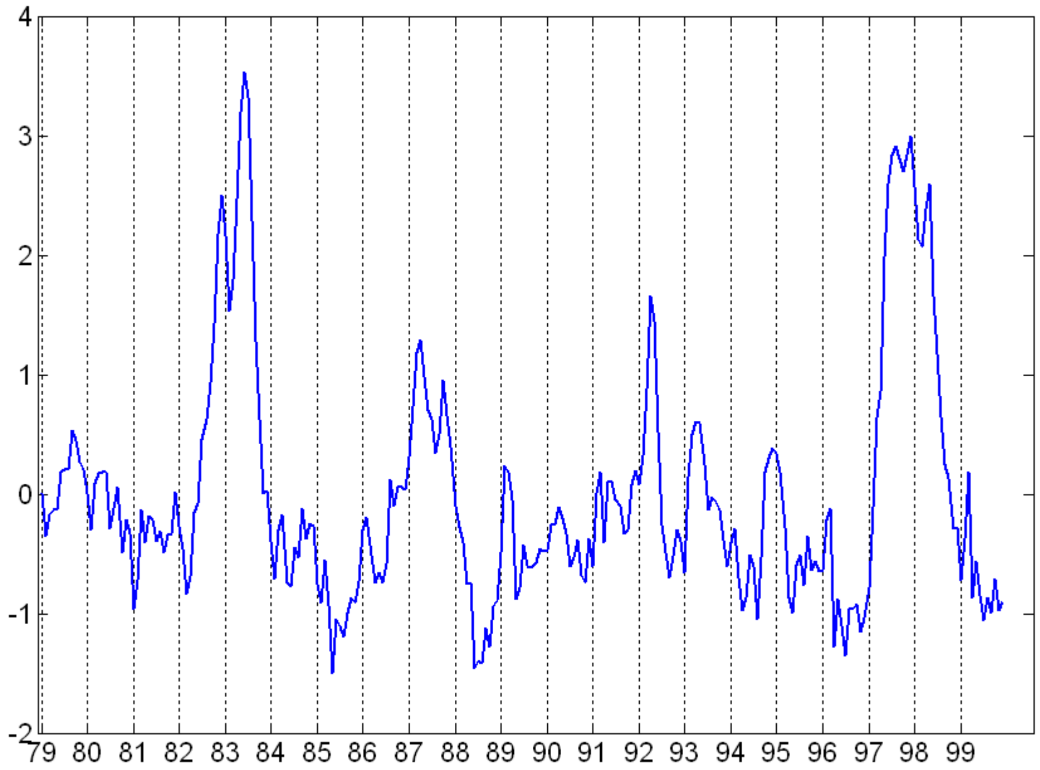
Two Sine Waves

Two Sine Waves + Noise

Frequency

Attribute Transformation

- A function that maps the entire set of values of a given attribute to a new set of replacement values such that each old value can be identified with one of the new values
  - Simple functions: x^k, $\log(x)$, e^x, $|x|$
  - Standardization and Normalization



Why dimensionality reduction?

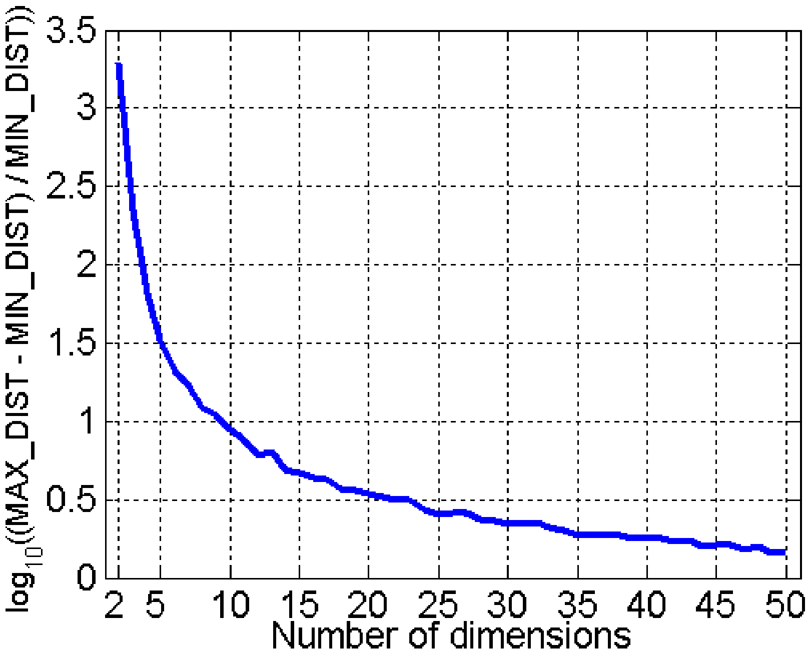
- Some features may be irrelevant
- We want to visualize high dimensional data
- “Intrinsic” dimensionality may be smaller than the number of features
- Applications
  - Digital image and speech processing
  - Gene expression
  - Visualization of large networks

Curse of Dimensionality

- When dimensionality increases, data becomes increasingly sparse in the space that it occupies

- Definitions of density and distance between points, which is critical for clustering and outlier detection, become less meaningful

- Term "Curse of Dimensionality" was introduced by Richard E.Bellmann,
  - https://en.wikipedia.org/wiki/Curse_of_dimensionality



- Randomly generate 500 points
- Compute difference between max and min distance between any pair of points

Dimensionality Reduction

- Purpose:
  - Avoid curse of dimensionality
  - Reduce amount of time and memory required by data mining algorithms
  - Allow data to be more easily visualized
  - May help to eliminate irrelevant features or reduce noise
- Techniques
  - Principle Component Analysis
  - t-SNE
  - UMAP
  - Others: e.g. supervised

Feature Subset Selection

- Another way to reduce dimensionality of data
  - Redundant features
    - duplicate much or all of the information contained in one or more other attributes
    - Example: purchase price of a product and the amount of sales tax paid
  - Irrelevant features
    - contain no information that is useful for the data mining task at hand
    - Example: students-ID is often irrelevant to the task of predicting students-GPA (Grade Point Average)

Feature Subset Selection

- Techniques:
  - Brute-force approach:
    - Try all possible feature subsets as input to data mining algorithm
  - Embedded approaches:
    - Feature selection occurs naturally as part of the data mining algorithm
  - Filter approaches:
    - Features are selected before data mining algorithm runs
  - Wrapper approaches:
    - Use the data mining algorithm as a black box to find best subset of attributes

Unsupervised feature selection – dimensionality reduction

- Idea:
  - Given data points in n-dimensional space,
  - Project into lower dimensional space while preserving as much information as possible
  - In particular, choose projection that minimizes the squared error in reconstructing original data

PCA

…how to boil it down to lower dimensionality

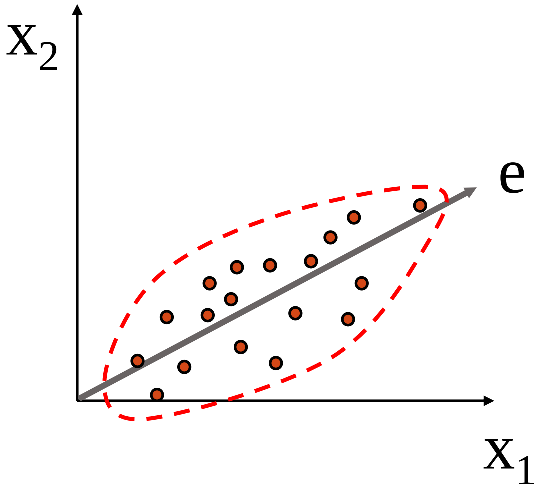
Principle Component Analysis

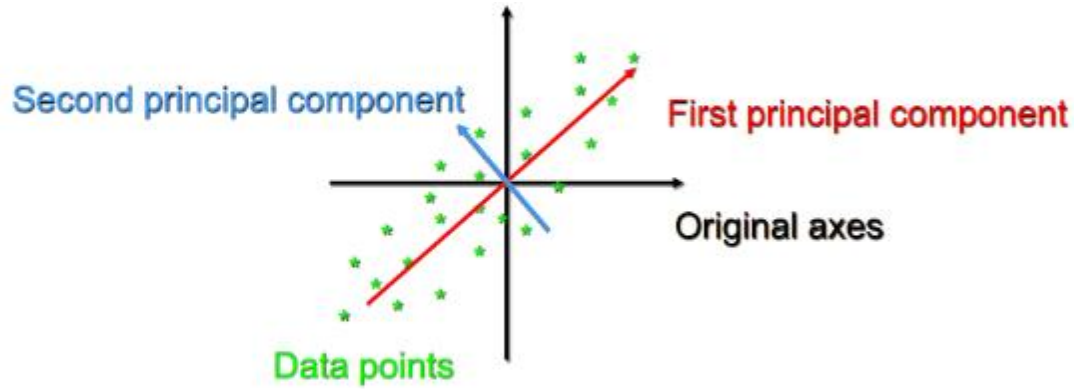
- Type: **Linear method**
- Aim: Projection of the data onto orthogonal axes (principal components) that explain maximum variance
- Preservation: Preserves global structures (variance)
- Computational effort: Very efficient, can handle large data sets and high dimensionality
- Deterministic: Always the same result (if no random component)
- Interpretability: Each component is a linear combination of the original characteristics → easy to interpret

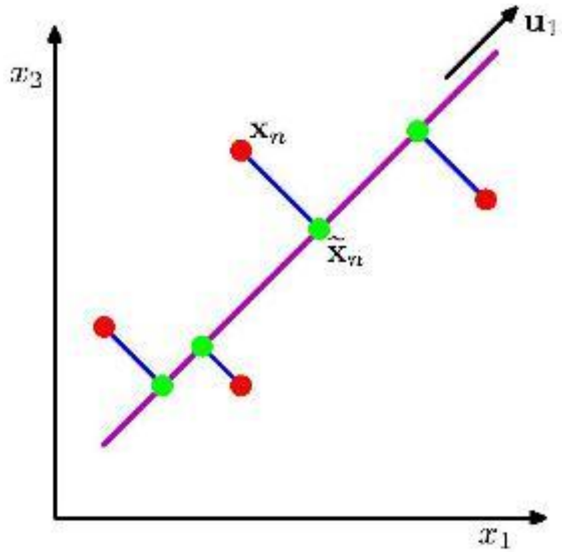
- Use: First choice when the relationship between variables is predominantly linear and fast, reproducible results are required.

Principle Component Analysis

- Goal is to find a projection that captures the largest amount of variation in data
- Approximating a high-dimensional data set with a lower-dimensional linear subspace
- Orthogonal projection of data into lower-dimension linear space that
  - minimizes mean squared distance between
    - data point and
    - projections (sum of blue lines)







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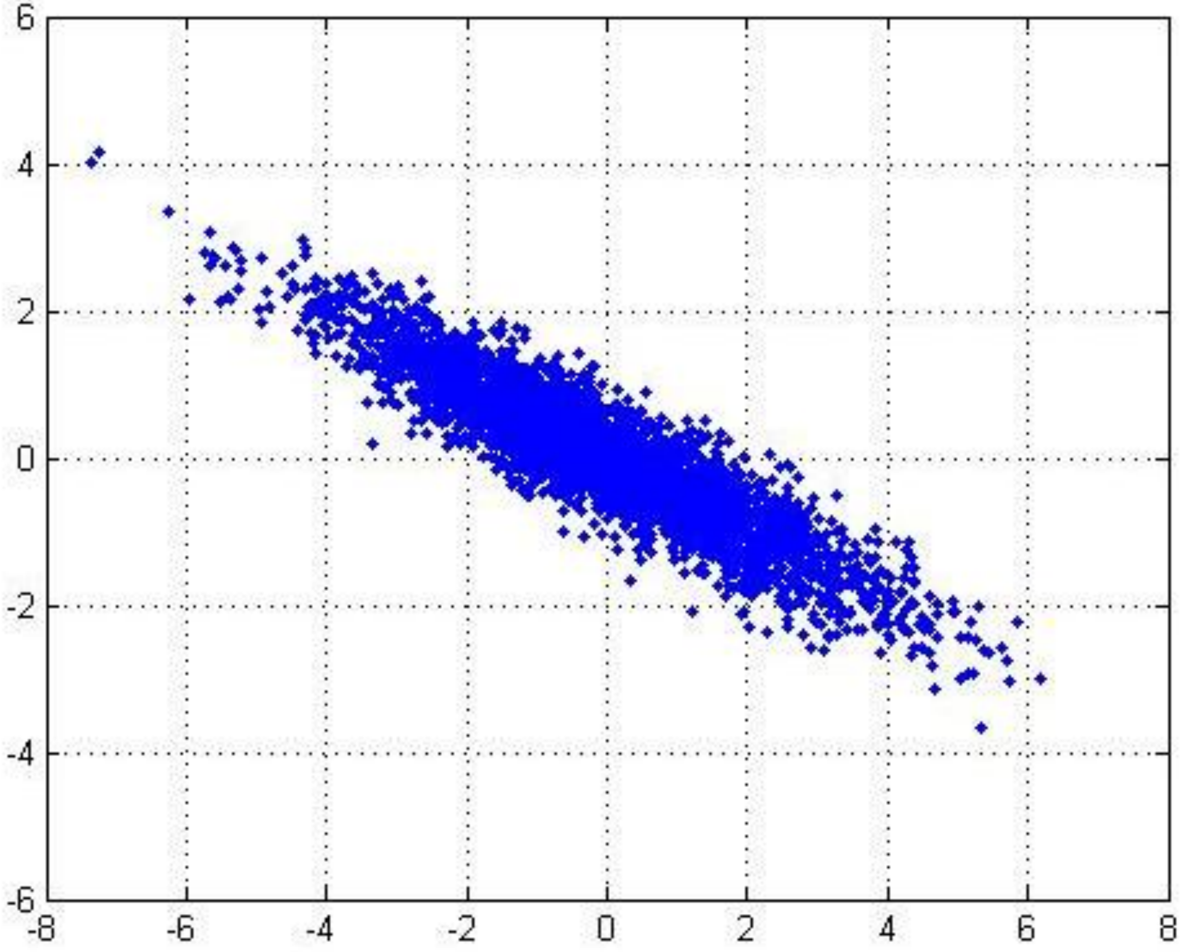
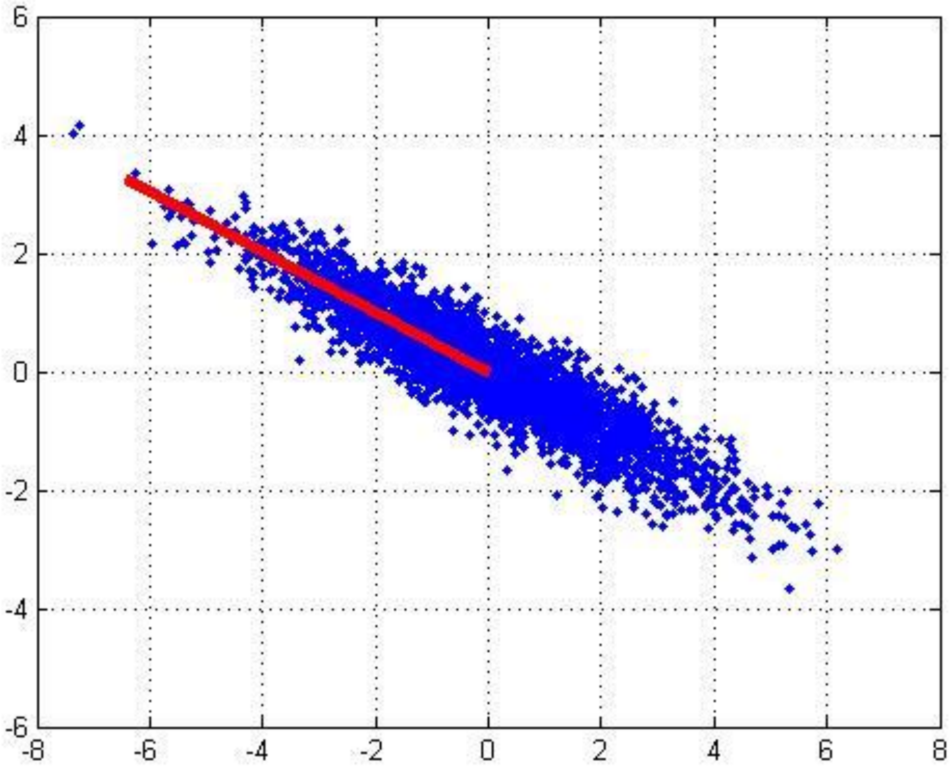
PCA: Two dimensional Values

2D Gaussian dataset



1st PCA axis



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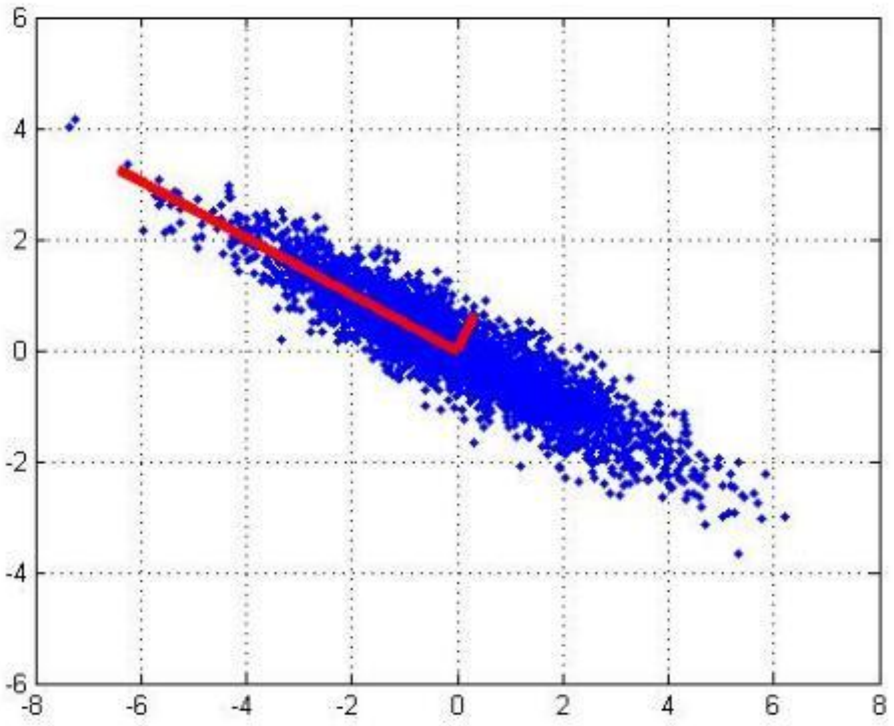
2^{nd} PCA axis



PCA algorithm: Covariance Matrix

- Given vectors {$\mathbf{x}_1$, …, $\mathbf{x}_n$}, compute covariance matrix Σ

$$\Sigma_{j,k} = \frac{1}{n-1}\sum_{i=1}^{n}(X_{ij} - \overline{X}_j)(X_{ik} - \overline{X}_k)$$

for j, k = 1..n and $\overline{\mathbf{x}}_k = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_{k,i}$

- **PCA** basis vectors = the eigenvectors of Σ
- Larger eigenvalue $\Rightarrow$ more important eigenvectors

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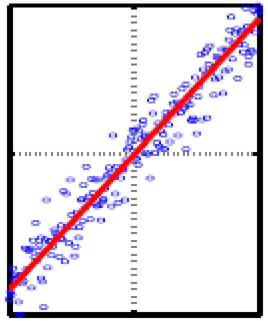
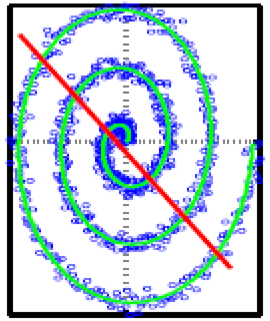
PCA Algorithm

1. Create n x m data matrix X, with one row vector x_k per each data point
2. Subtract mean $\bar{\mathbf{x}}$ from each row vector x_k in X
3. compute Σ the covariance matrix of X
   - Σ is square and symmetrical, grade m
4. Find all eigenvectors and eigenvalues of Σ
5. PCA‘s are the eigenvectors with the largest eigenvalues

Properties of PCA

- Strengths
  - Eigenvector method
  - No tuning parameters
  - Non-iterative
  - No local optima
- Weaknesses
  - Limited to linear projections





PCA is for linear, fast analyses.

Dimensionality Reduction: PCA

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Dimensions = 206

T-SNE

…when the local similarity of data is important

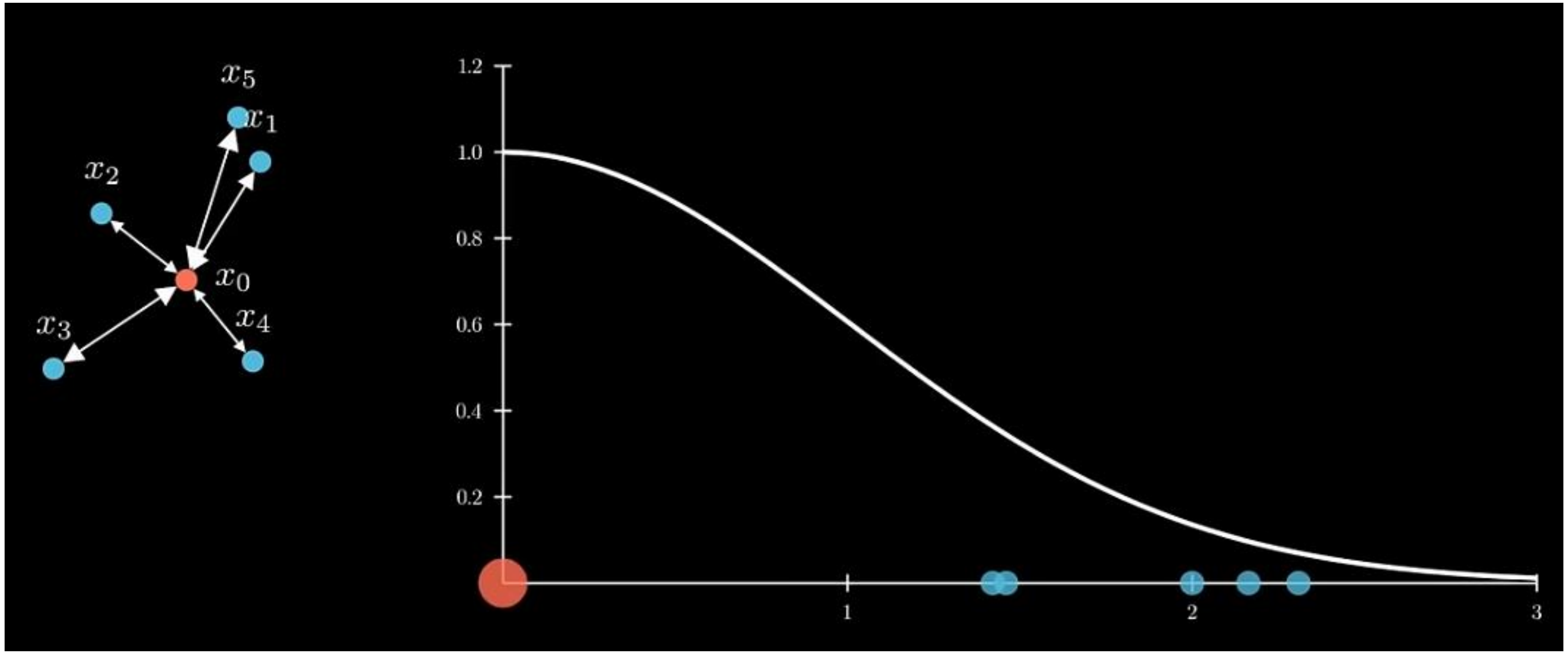
t-distributed Stochastic Neighbor Embedding

- Type: **Non-linear, probabilistic method**
- Goal: Preservation of local neighborhoods; similar points in the original space remain close in the 2D/3D projection space
- Preservation: **Strong local focus** (clusters become clearly visible), global structure usually distorted
- Computational effort: Relatively high ($O(N^2)$), scales poorly to very large data sets
- Stochastic: Results vary slightly with different initializations
- Parameters: "Perplexity", learning rate, etc., must be fine-tuned

- Use: Ideal for explorative data analysis when the focus is on cluster structures. Not suitable for directly interpreting distances between distant clusters.

t-SNE is excellent for detecting fine clusters but is computationally intensive and not globally accurate.

t-distributed Stochastic Neighbor Embedding



UMAP

…when the global structure of data is important

Uniform Manifold Approximation and Projection

- Type: **Non-linear, graph-based method**
- Goal: Reconstruction of a weighted graph of the data and optimization of a low-dimensional embedding
- Conservation: Balances local and global structures better than t-SNE
- Computational effort: Significantly faster than t-SNE, scales up to millions of points
- Deterministic (with fixed random seed): Reproducible with the same seed
- Parameters: n_neighbors (local vs. global focus), min_dist (cluster density)

- Use: If you want to see both cluster structures and rough global relationships and need to process large data sets efficiently.

UMAP combines the strengths of both approaches: fast calculation, good cluster representation and at the same time a certain global coherence

Sampling

- Sampling is the main technique employed for data selection.
  - It is often used for both the preliminary investigation of the data and the final data analysis.
- Statisticians sample because obtaining the entire set of data of interest is too expensive or time consuming.
- Sampling is used in data mining because processing the entire set of data of interest is too expensive or time consuming.

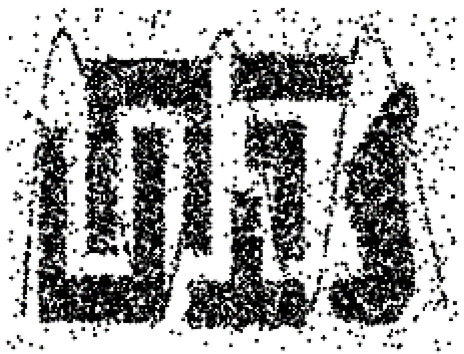
Sampling …

- The key principle for effective sampling is the following:
  - using a sample will work almost as well as using the entire data sets, if the sample is representative
  - A sample is representative if it has approximately the same property (of interest) as the original set of data
- Example:
  - Extrapolation in political votings

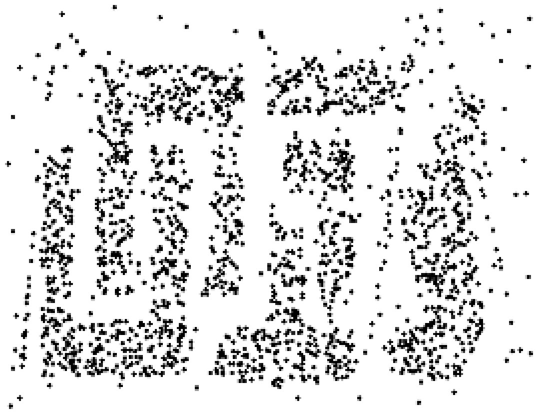
Types of Sampling

- Simple Random Sampling
  - There is an equal probability of selecting any particular item
- Sampling without replacement
  - As each item is selected, it is removed from the population
- Sampling with replacement
  - Objects are not removed from the population as they are selected for the sample.
    - In sampling with replacement, the same object can be picked up more than once
- Stratified sampling
  - Split the data into several partitions;
  - then draw random samples from each partition

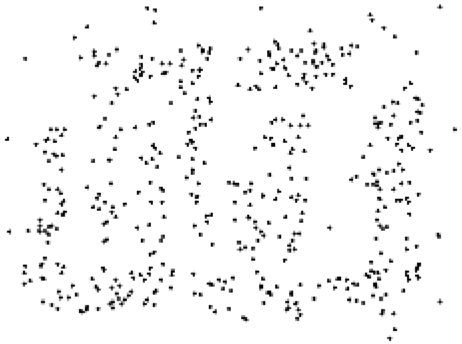
Sample Size: Patterns



8000 points



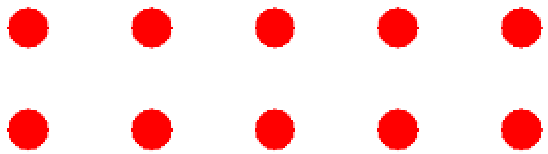
2000 Points

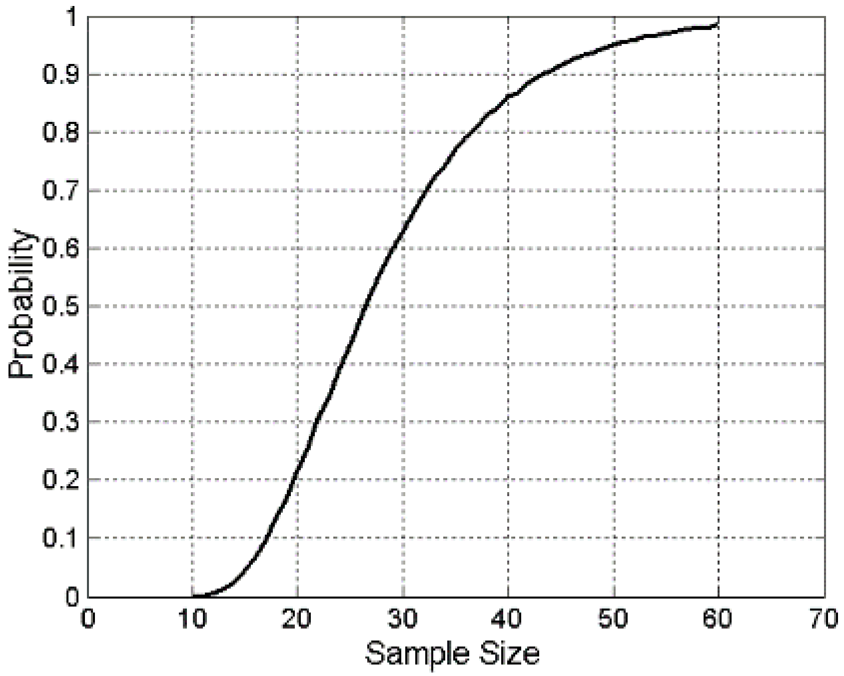


500 Points

Sample Size

- What sample size is necessary to get at least one object from each of 10 groups?





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Literature

1. Bing, Liu, Web Data Mining, Springer, 2008.
2. Han, J. und Kamber, M. "Data Mining. Concepts and Techniques", Morgan Kaufmann, 2011.
3. Smith, L.I,: A tutorial on Principal Components Analysis, 2002 in http://www.cs.otago.ac.nz/cosc453/student_tutorials/principal_components.pdf
4. Tan, Steinbach, Kumar: „Introduction to Data Mining", Pearson Education Limited, 2013.
5. Witten I.H., Eibe, F., Data Mining, Practical Machine Learning Tools and Techniques, Morgan Kaufmann, 2011.
6. https://scikit-learn.org/stable/modules/decomposition.html