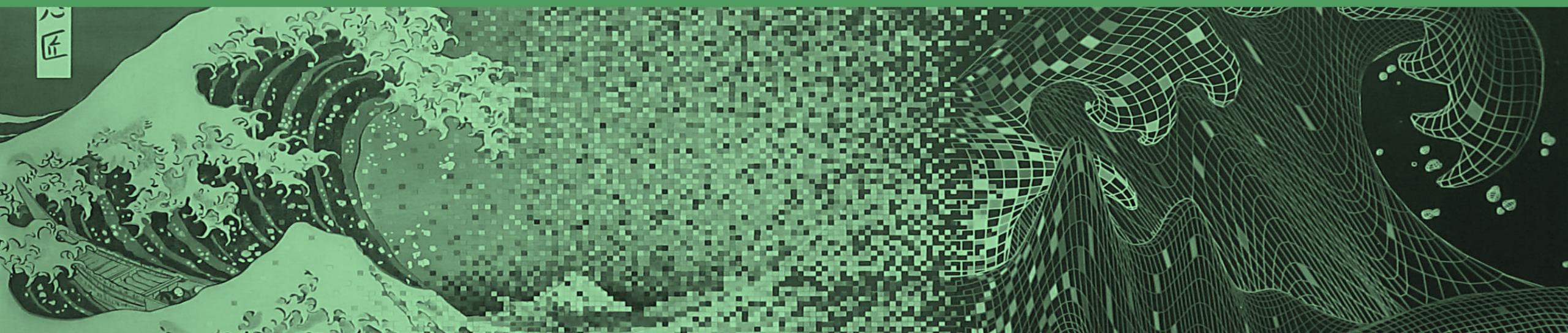
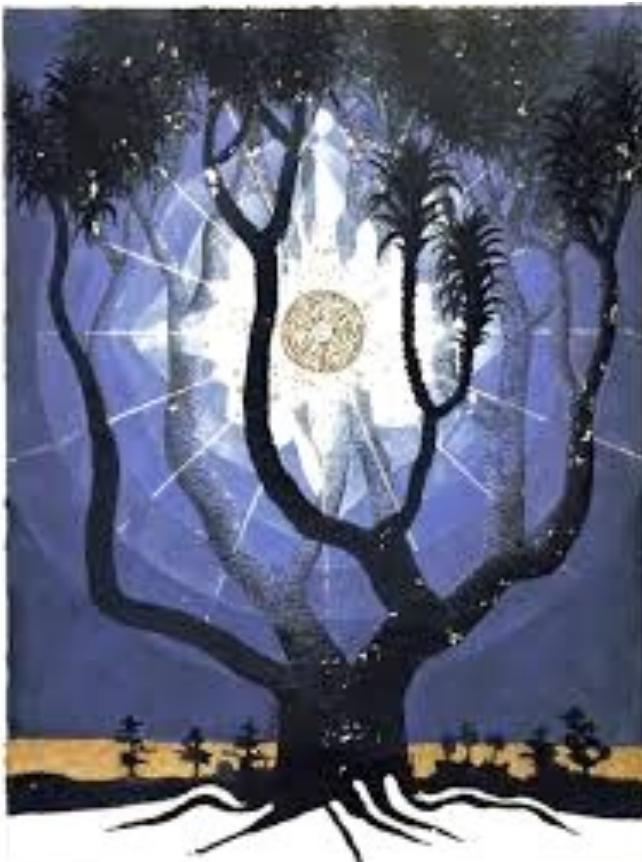


# Introduction to Machine Learning

## Learning and Univariate Data Analysis

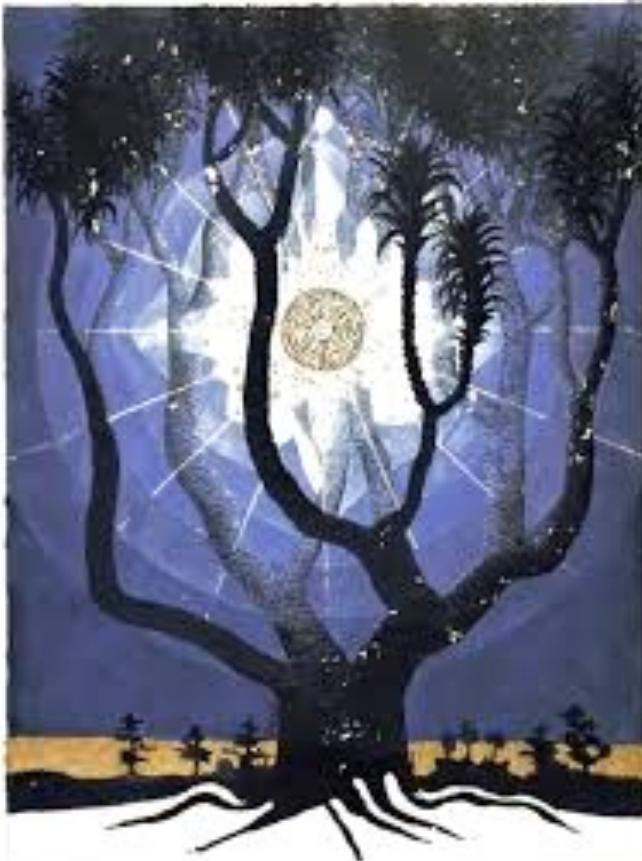


# Outline



- **Machine learning**
  - intelligence and learning
  - data science and AI
  - symbolic learning
  - terminology
  - descriptive and predictive tasks
- **Univariate data analysis**
  - numeric and categoric variables
  - empirical and theoretical distributions
  - summary statistics
  - outlier removal
  - discriminant analysis
  - correlation

# Outline



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# Intelligence

- **Rationality** ⇐
  - ability to act in a way that maximizes some utility function
- **Adaptability** ⇐
  - ability learn from experience
  - make abstractions (patterning)
  - deal with novelty and change
- **Curiosity**
  - ability to engage creative imaginative or inquisitive reasoning



# What is machine learning?

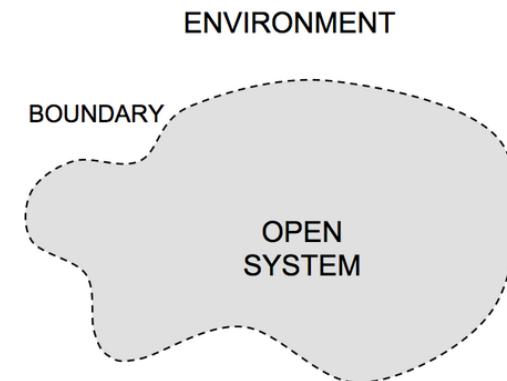
- **Artificial Intelligence (AI)** emulates **qualities of human intelligence** to answer real-world problems
  - parallels between human and artificial intelligence?
  - many AI techniques inspired from human psychology, biology, behavior
- **Learning** is a fundamental quality intelligence
  - “*learning is any process by which a system improves performance from experience*”  
(by Herbert Simon)
- **Machine learning (ML) as a subfield of AI**
  - AI with a focus on rationality => optimization, planning, reasoning, ...
  - AI with a focus on curiosity => autonomous agents, affective computing, ...
  - AI with a focus on adaptability from experience (data records) => ML

# Systemic world view

- **system**
  - set of elements organized with a shared purpose
  - (open) surrounded and influenced by its environment
  - described by its structure, purpose and functioning

- *open systems evolve*

- Universe → galaxy → solar system
  - Earth → societies → individuals
  - organs → cells → atoms



# Systemic world view

- Everything is systemic:
  - **biological** systems
  - **ecological** systems
  - **societal** systems
  - **mechanical** systems
  - **digital** systems
  - **quantum** systems
  - **hybrid** systems
  - **astrophysical** systems

By monitoring systems (e.g. sensorization, observation)...

- **data** ⇒ information (descriptive learning) ⇒ **knowledge**
- **data** ⇒ **decision support** system (predictive learning)

*“we contain, are, interact and move within systems”*

Psychoanalyst: *Know the influence of systems in our life and be free!*

# Data everywhere!

Sensorization examples:

- **biological** systems
  - physiological signals from biosensors, molecular signals using multi-omic high-throughput technologies
  - health records (diagnostics, prescriptions, undertaken surgeries), exposomics, demographics
- **knowledge** systems
  - corpora from digital libraries and the Web
- **ecological** systems
  - biodiversity, plant health, crop and livestock conditions, water quality, food nutrition, forestry and fishery surveillance from remote vision (satellite, drones), physical sensors, acoustic sensors, citizen notifications
- **societal** systems
  - social interactions via social networks, telecom and messaging apps
  - commerce and finance via transaction records
- **urban** systems
  - traffic records from mobile phones, smart card validations, inductive loop counters, privacy-preserving
  - water and energy supply via telemetry (flowrate, pressure, smart sensors)
- ... [*complete the list*]

# From experience to learning

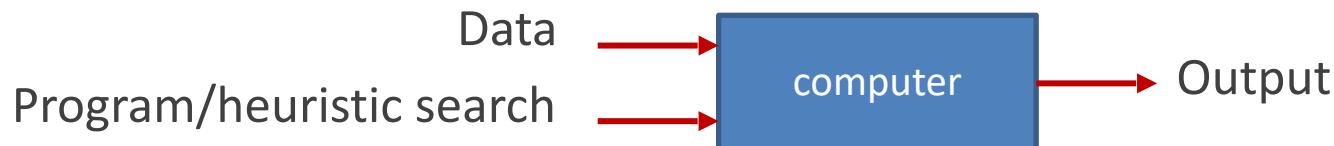
- Data records acquired from:
  - multiple systems of the same type
    - e.g. different individuals, vehicles, computers, organizations
  - single system under different conditions
    - e.g. brain under different stimuli, crop under different weather conditions, e-commerce along time
- Multiple data records... statistics!
  - discover of relevant relations/associations (patterning)
- Pattern recognition aids us in:
  - understanding systems' behavior (descriptive learning)
  - supporting decisions (predictive learning)

# Machine Learning

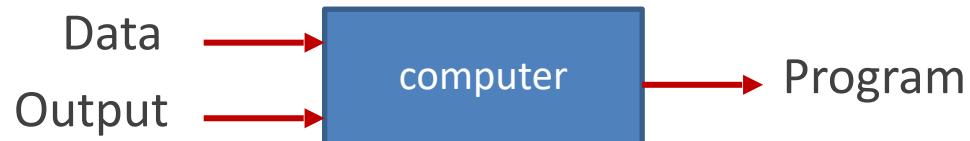
- Machine Learning *versus Artificial Intelligence*
  - recall: ML is a subfield of the larger AI field
- Machine Learning *versus Data Science*
  - ML as a set of concepts, principles and computational methods to aid decisions and accomplish other digital tasks from available data
    - grounded on statistical, algebraic, mathematical and algorithmic foundations
  - Data Science has been termed the art of discovering what we don't know from data
    - the non-trivial extraction of implicit, previously unknown, and potentially useful knowledge from data
    - ML provides the foundational concepts and algorithmic means for Data Science

# The ML stance

- Traditional programming and classic AI



- Machine learning

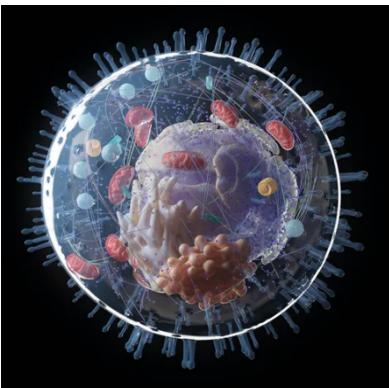


*“Machine Learning: field of study that gives computers the ability to learn without being explicitly programmed”*

Arthur Samuel (1959)

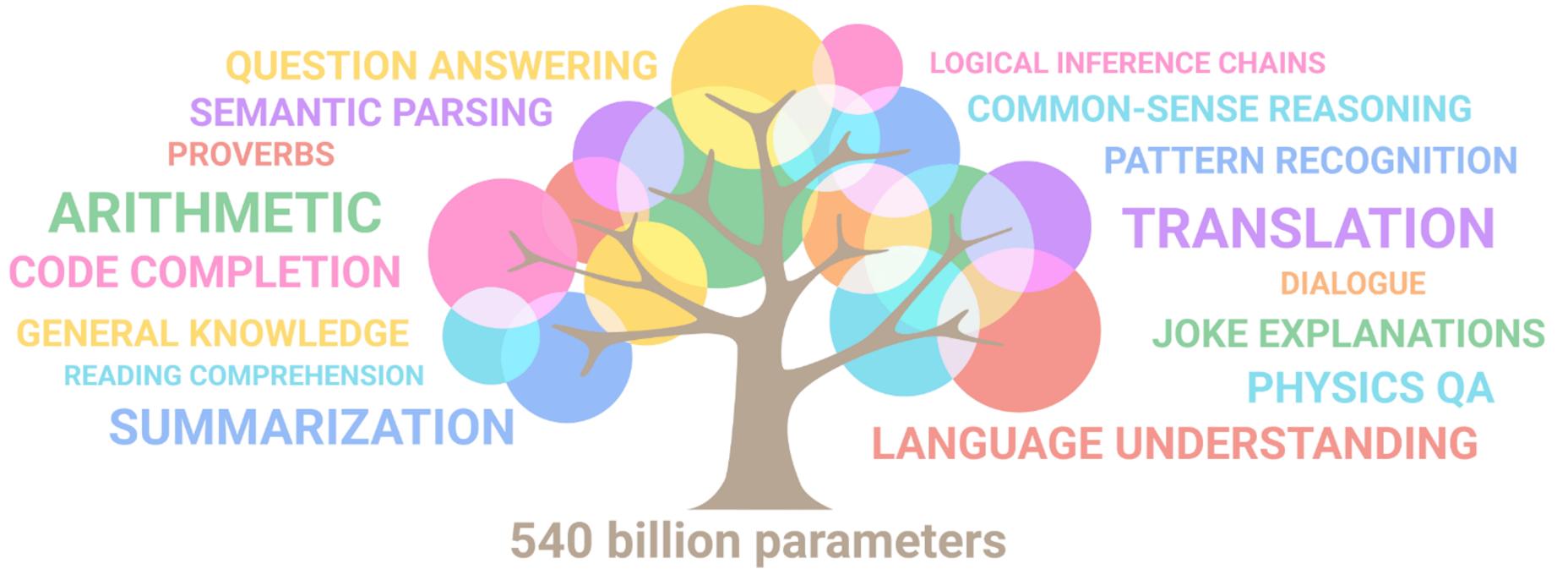
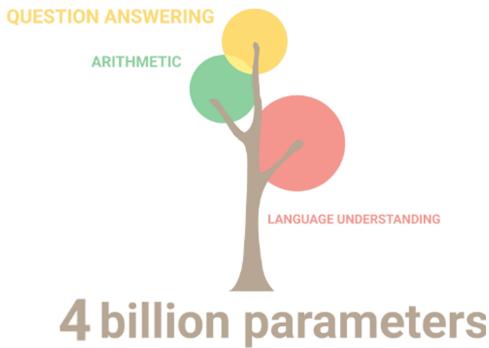
# When?

- Human expertise does not exist (e.g. navigating on Mars)
- Humans cannot explain their expertise (e.g. speech recognition)
- Models must be customized (e.g. personalized medicine)
- Models are based on huge amounts of data (e.g. genomics)



- Learning isn't always useful: there is no need to learn to calculate payroll!

# When?



- Task-specific *versus* multi-task/purpose learning – the era of Large Language-and-Vision Models

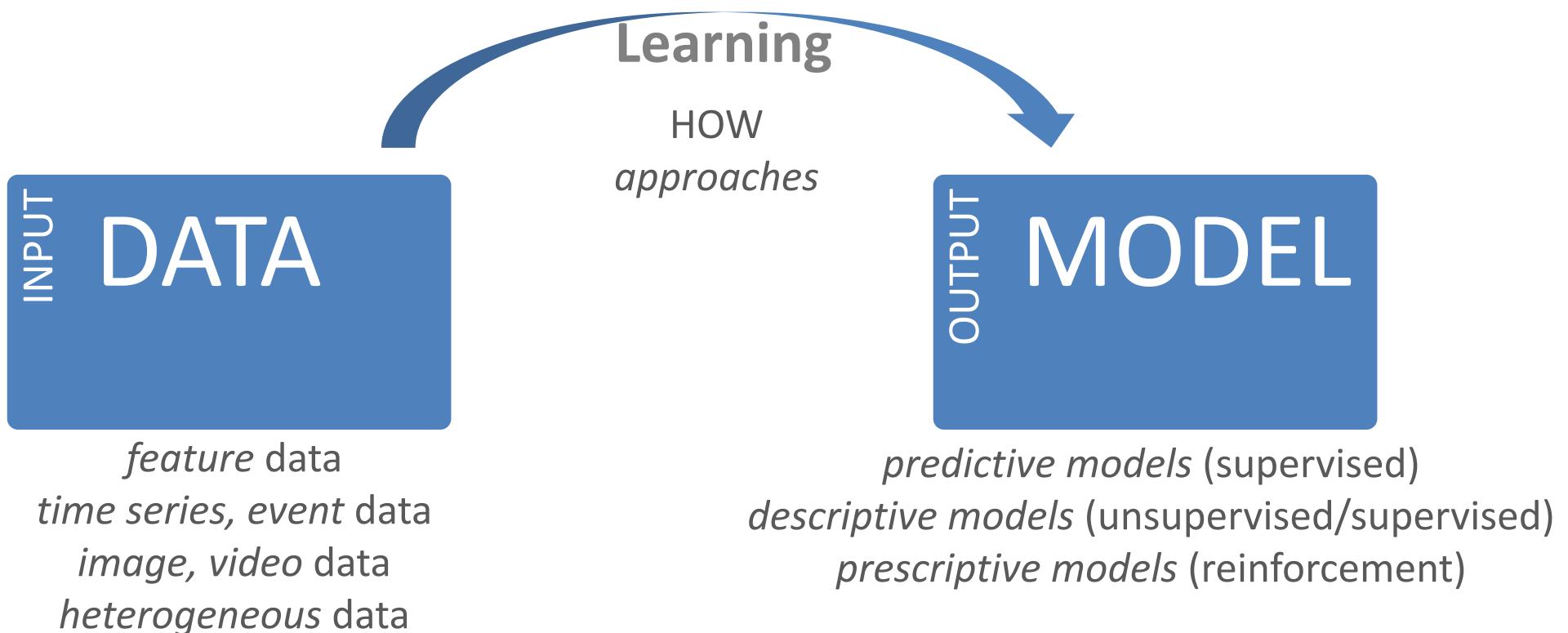
# When?

- Classic example of a task that requires machine learning:
  - Hard to say what makes a 2!



- What about clinical diagnostics? Product recommendations?

# Machine Learning



# Learning input-output functions

- **Supervised learning**

- with a teacher
  - learning from training data and desired outputs (labels, quantities, structures)

- **Unsupervised learning**

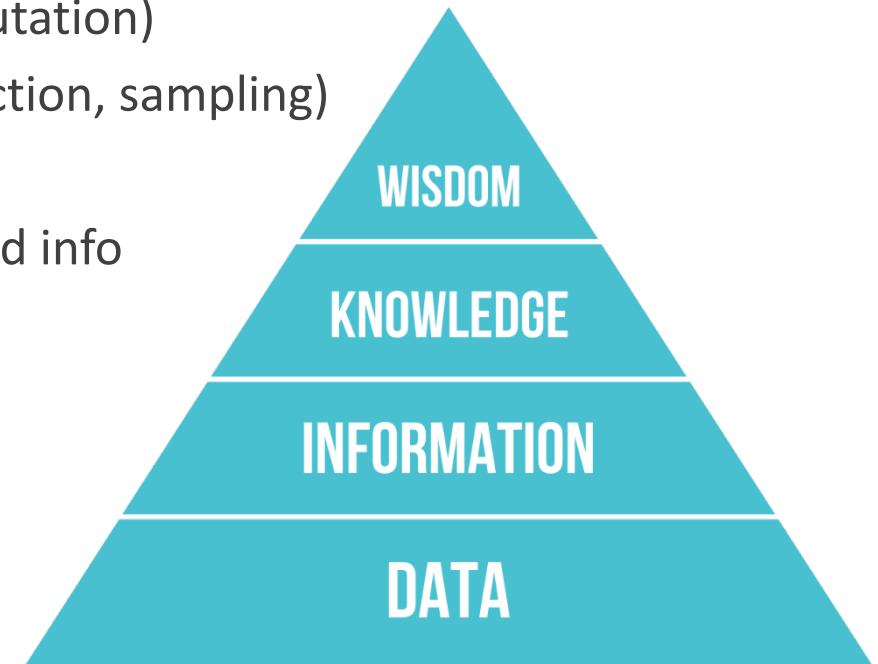
- without a teacher
  - learning from training data without desired outputs

- **Reinforcement learning**

- absence of a designated teacher to give positive and negative examples
  - learning rewards and penalties observed from sequence of actions within a given environment

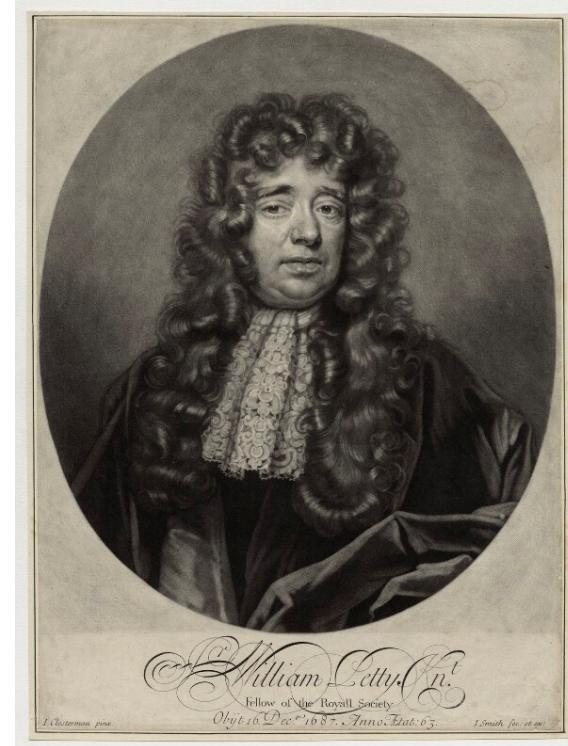
# Machine learning in practice

- The process of knowledge discovery is a composition of steps:
  - **data preprocessing**
    - data acquisition and integration
    - data cleaning (e.g. duplicate and outlier removal, missing imputation)
    - data transformations (e.g. normalization, dimensionality reduction, sampling)
  - **data mining** recurring to *machine learning*
  - **postprocessing** needs and knowledge retrieval from the extracted info (descriptive stance) or learned models (predictive stance)
    - interpret and validate results
    - consolidate and deploy discovered knowledge



# Data Science

- Data science
  - the rediscovery of “statistics” ...
    - descriptive statistics
    - inferential statistics
  - the rediscovery of “maths” ...
    - linear algebra
    - calculus

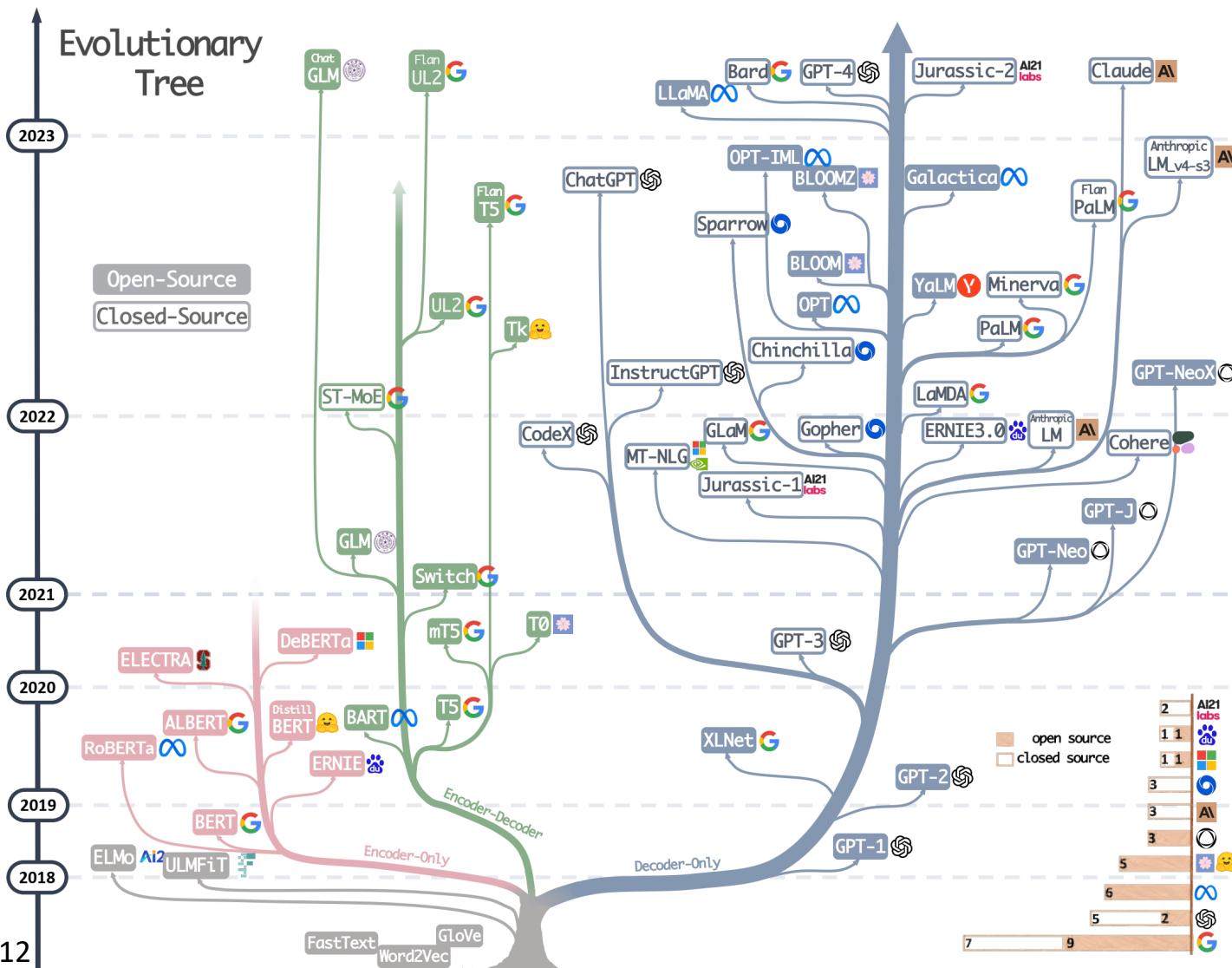


Sir William Petty, a 17th-century economist who used early statistical methods to analyse demographic data

# History of Machine Learning

- **1950s**
  - Samuel's checker player
  - Selfridge's Pandemonium
- **1960s**
  - Perceptron and its limitations
- **1970s**
  - Symbolic learning
  - Expert systems
  - Decision trees
- **1980s**
  - Resurgence of neural networks: backpropagation
  - Learning and planning
  - Explanation-based learning
  - Inductive logic programming
  - Utility problem, analogy
  - Cognitive architectures
  - PAC Learning Theory
- **1990s**
  - Data mining, text mining
  - Adaptive software agents
  - Reinforcement learning (RL)
  - Ensembles: bagging, boosting, stacking
  - Bayes network learning
- **2000s**
  - Support vector machines, kernel methods
  - Learning in robotics and vision
  - Graphical models
  - Relational learning
- **2010s**
  - Deep learning
  - Big data
  - Uncertainty
  - Multi-task learning
  - Large language models

# Deep Learning and Large Language Models



# Terminology



## Dataset:

- set of observations/instances/records,  $X = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$  (population)
- with values/features along a set of variables/attributes,  $Y = \{y_1, \dots, y_m\}$ 
  - input variables (explanatory)
  - optional output variables (targets)
- data size = number of observations,  $|X| = n$
- data dimensionality = number of variables,  $|Y| = m$

# Learning



**Learning** from a dataset: retrieving relevant **data relations**

- relations/patterns/abstractions  $\equiv$  distributions of interest on specific observations and attributes
  - *unexpectedly informative*
  - *unexpectedly discriminative* (different distribution between populations)
- learn classifiers, regressors, descriptors, forecasters, autoencoders from these relations

# Feature space

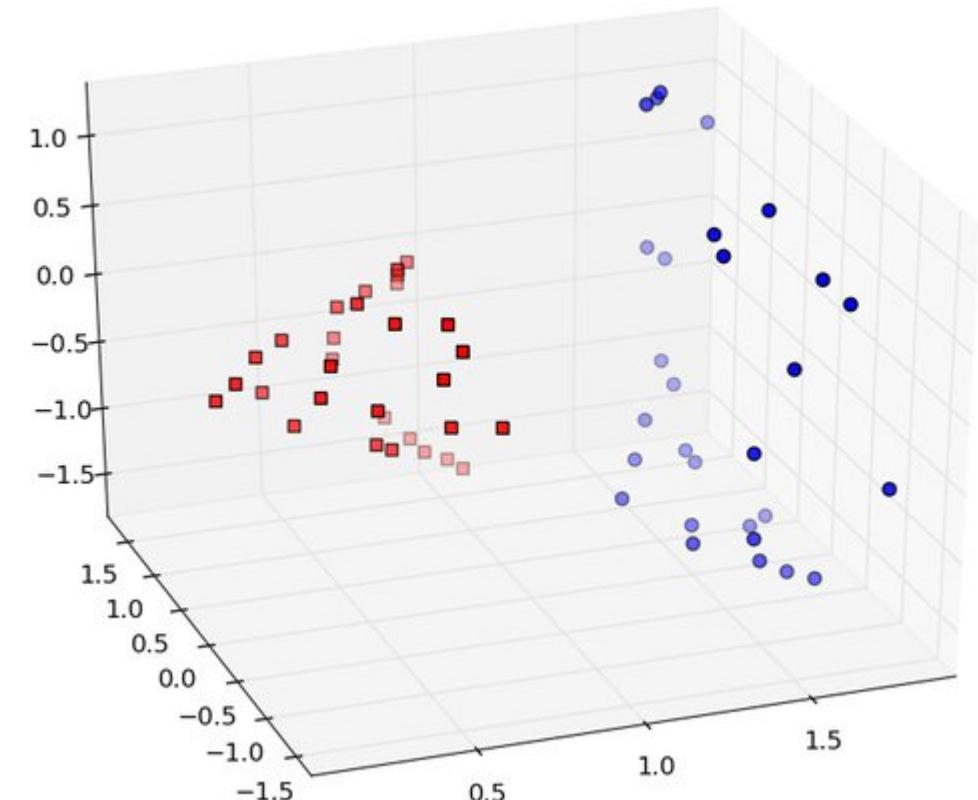
- When variables are numeric:
  - feature space  $\equiv$  vector space (e.g. Euclidean space)
  - observation  $\equiv$  data point

$$\mathbf{x} = \{x_1, \dots, x_m\} \in \mathbb{R}^m$$

$$\|\mathbf{a} - \mathbf{b}\| = \sqrt{\sum_{i=1}^m (a_i - b_i)^2}$$

NB: Encyclopedia of Distances (M. & E. Deza), Springer

<https://link.springer.com/book/10.1007/978-3-662-52844-0>

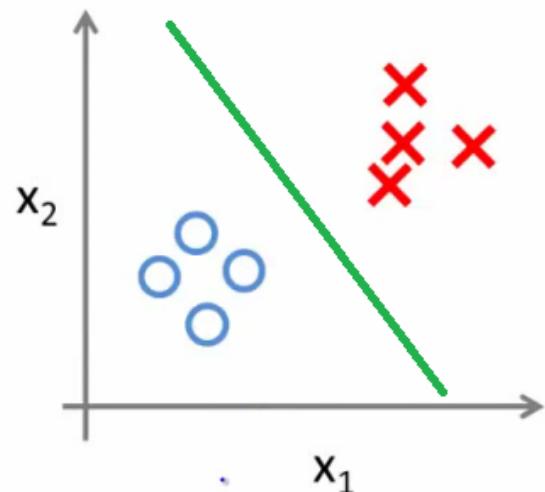


# Classification

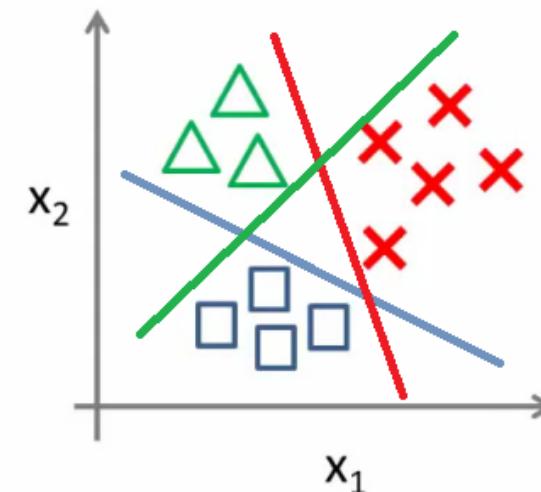
Given a set of labeled observations,  $\{(\mathbf{x}_1, z_1), \dots, (\mathbf{x}_n, z_n)\}$  where  $z_n \in \Sigma$ , a **classifier**  $M$  is a mapping function between input variables and a categoric variable:  $M : X \rightarrow Z$

- given a new unlabeled observation  $\mathbf{x}_{new}$ , use  $M$  to classify:  $\hat{z}_{new} = M(\mathbf{x}_{new})$

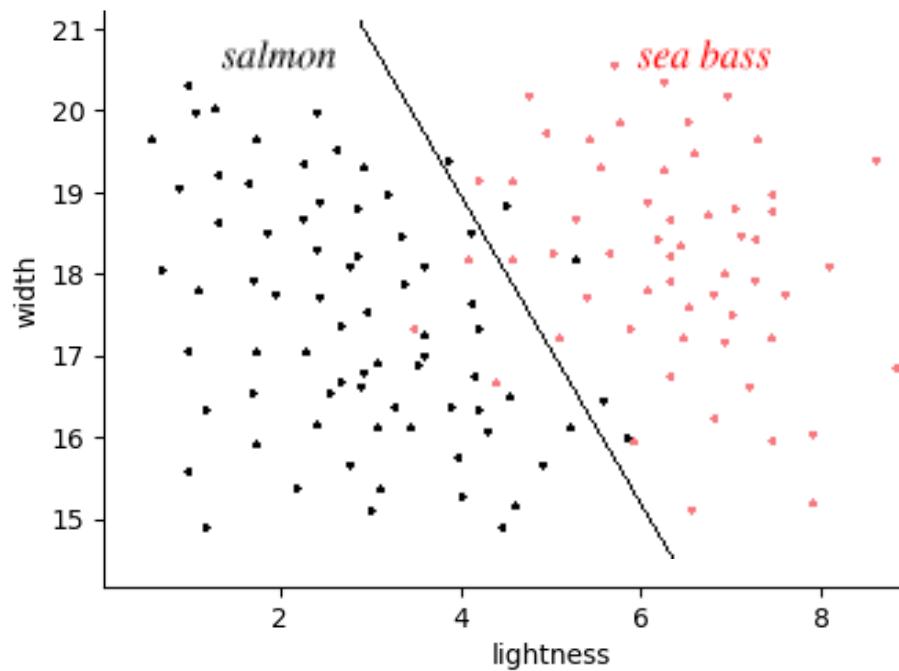
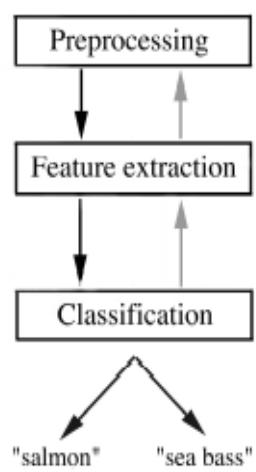
Binary classification:



Multi-class classification:

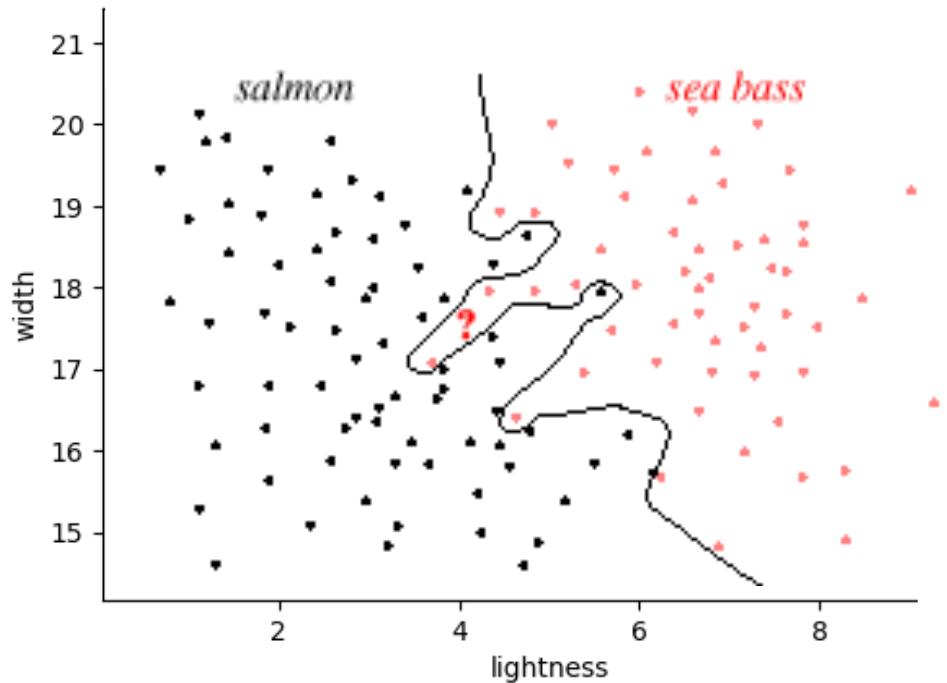


# Classification: *salmon*?



# Classification: salmon?

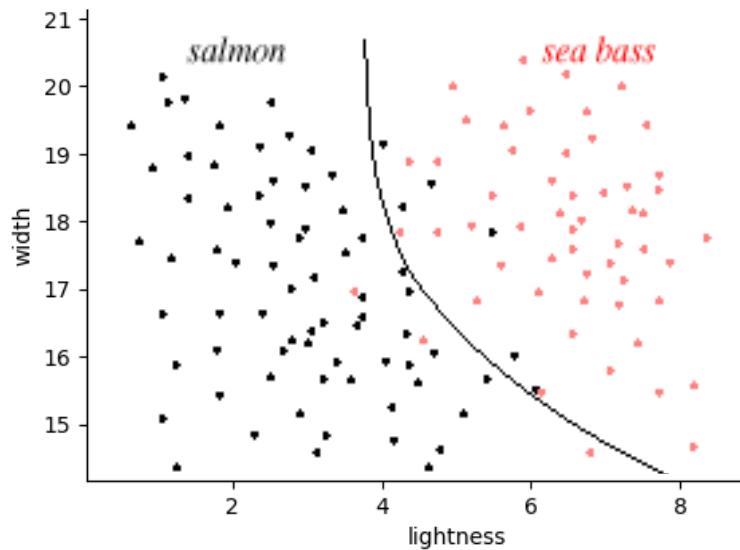
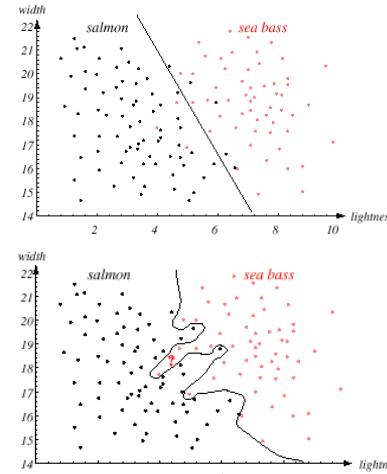
- we might add other variables that are not correlated with the ones we already have
  - caution should be taken not to reduce the performance by adding such “noisy features”
- the best decision boundary should be the one which provides an optimal performance



- However, our satisfaction is premature because the central aim of designing a classifier is to correctly classify novel inputs
  - issue of **generalization!**

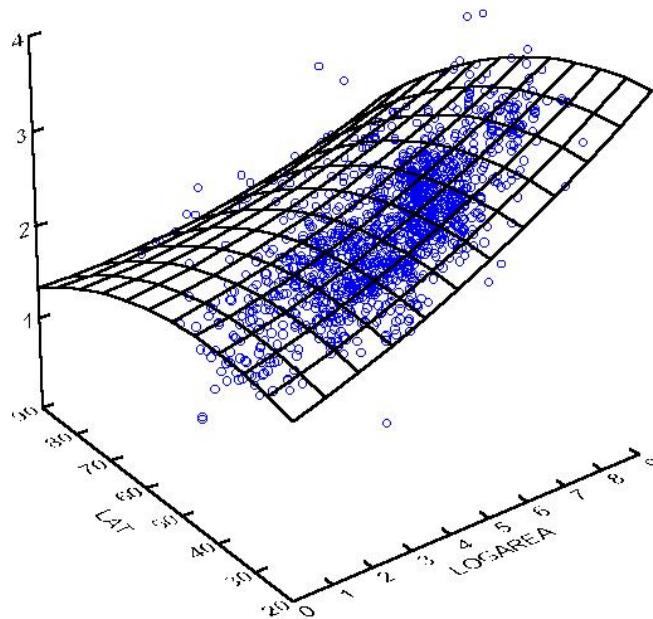
# Classification: salmon?

- Generalization ability linked with:
  - underfitting risks
  - overfitting risks
- Aim: find a balanced model capacity



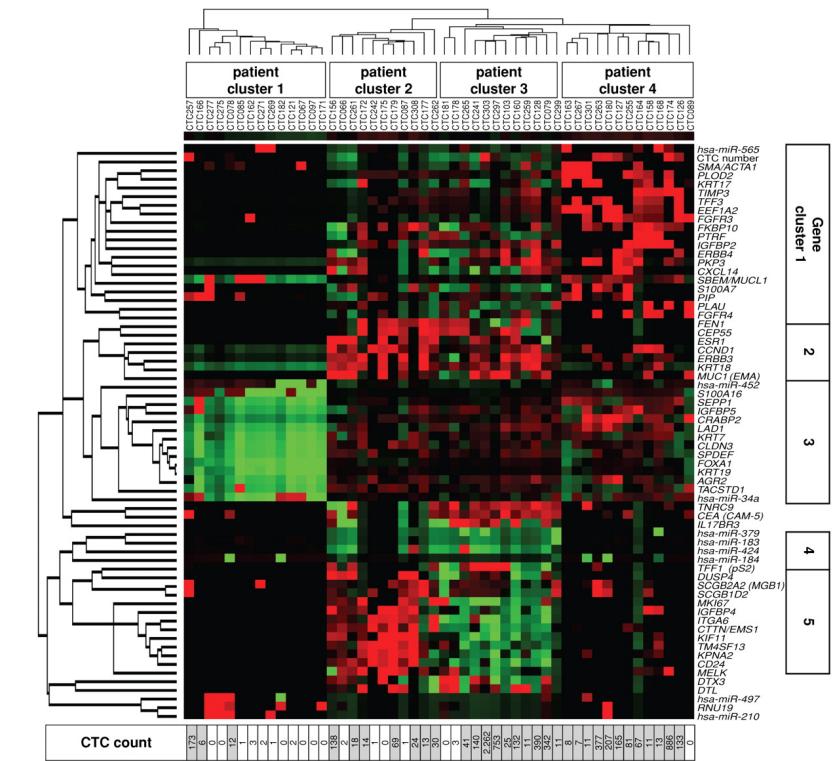
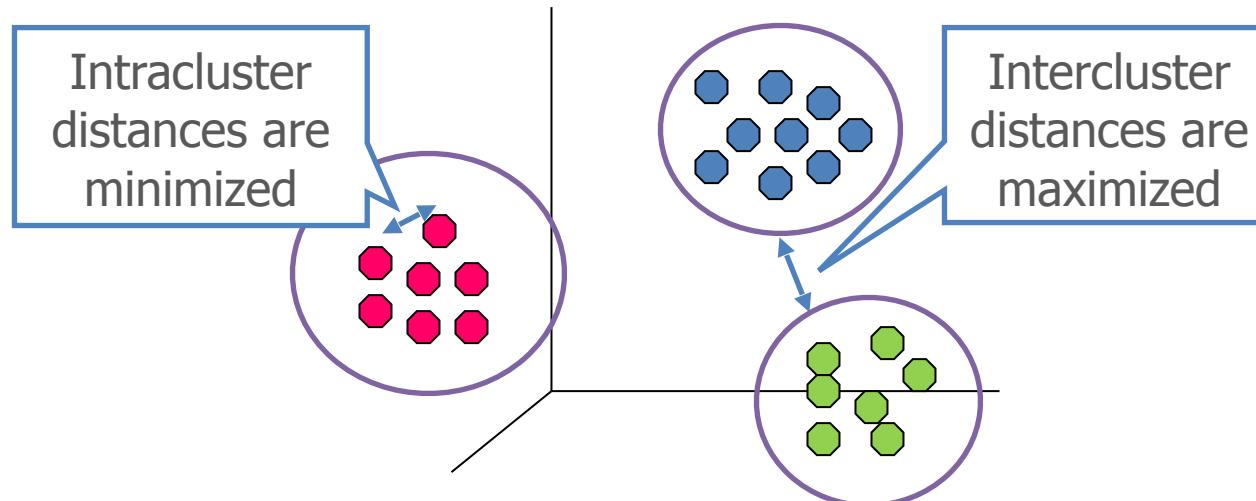
# Regression

- *Descriptive setting*: given a set of observations,  $\{(\mathbf{x}_1, z_1), \dots, (\mathbf{x}_n, z_n)\}$  where  $z_n \in \mathbb{R}$ , describe a relation between a set of (explanatory) variables and a target real-valued variable
- *Predictive setting*: given a set of observations with a real-valued outcome,  $\{(\mathbf{x}_1, z_1), \dots, (\mathbf{x}_n, z_n)\}$  where  $z_n \in \mathbb{R}$ , learn a mapping,  $M : X \rightarrow Z$ , to estimate the outcome of a new observation

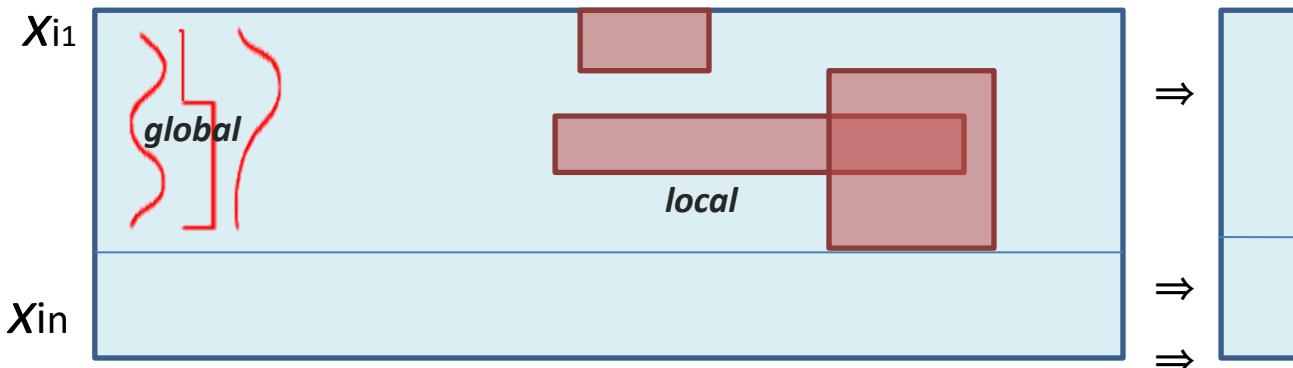


# Clustering

Given a set of data observations,  $X = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ , cluster analysis aims at grouping observations into clusters,  $C_i \subseteq X$  with  $i = 1..k$ , according to their (dis)similarity: observations in the same cluster are more similar than those in different clusters



# Pattern mining



$\{\text{symptomA, testBpositive}\} \Rightarrow \text{condition1} [\text{sup}=10\%, \text{conf}=80\%, \text{lift}=1.4, \text{sig}=1E-4]$

Given a dataset, find local associations (*aka* patterns) satisfying:

- statistical significance criteria (min number of observations to deviate from expectations)
- discriminative power (qualitative targets) or correlation (numeric targets) criteria

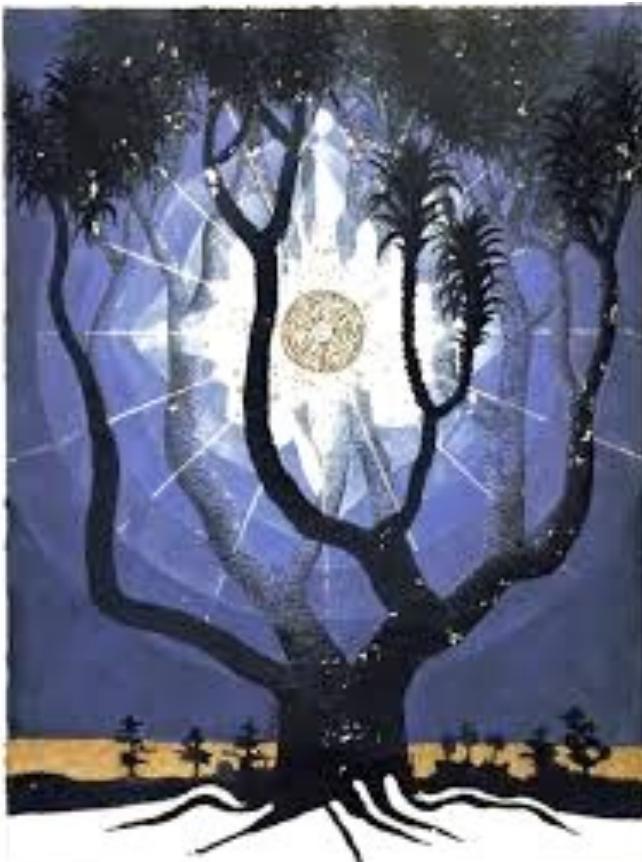
# Example: learning from biomedical data

- ***Descriptive modeling***: models of disease/treatment (e.g. health progression)
- ***Clustering***: group individuals in accordance with health profile
- ***Pattern mining and subspace clustering***: discover meaningful patterns and associations with impact on disease/treatment study and discrimination
- ***Classification***: diagnostics/prognostics, treatment recommendation
- ***Regression***: estimate risk, drug dosage or efficacy, quantifiable phenotypes

# Example: learning from biomedical data

- **observations** generally correspond to:
  - individuals
    - **input variables**: health-related features (multi-omics, clinical records, exposomics...)
    - **output variable**: outcome annotation
      - qualitative clinical condition (diagnostics, prognostics, therapies, traits)
      - quantifiable phenotypes (impairments, molecular levels, severity, survivability, drug dosage)
  - hospitals, undertaken procedures, care professionals, drugs...
- clinical trials (cohort studies) with enough, precise data observations, e.g. case-control populations
- ability to **generalize** from a population to new patients
  - prevent overfitting (including non-relevant relations in the learned models)
  - prevent underfitting (excluding relevant relations from learned models)

# Outline



- Machine learning
  - intelligence and learning
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# Univariate data analysis

- Random/aleatory variable

- function  $Y: \Omega \rightarrow E$  from a **sample space**  $\Omega$  to a **measurable space**  $E$
  - e.g. height variable is a function which maps a person from a population  $\Omega$  to her height in  $\mathbb{R}^+$  ( $E = \mathbb{R}^+$ )
    - the observed height is referred as a **measurement**
  - from now on, we will refer *random variable* simply as *variable*

- Univariate data

- single input variable
  - comprises univariate data statistics and, in the presence of an output variable, **bivariate data statistics**

- Multivariate data

- multiple (input) variables
  - **multivariate order** = number of (input) variables

# Variables

- **Categorical** (or qualitative) variables
  - values are categories
  - can either be **nominal**/symbolic or **ordinal** (e.g. low, average, high)
  - **binary** variables are variables with two categories (whether nominal or ordinal)
  - variable **cardinality** = number of categories
- **Numeric** (or quantitative) variables
  - values are quantities
  - can be either be **discrete** (e.g. integers) or **continuous** (e.g. real values)
- Exercise: classify the following variables – gender, age, height

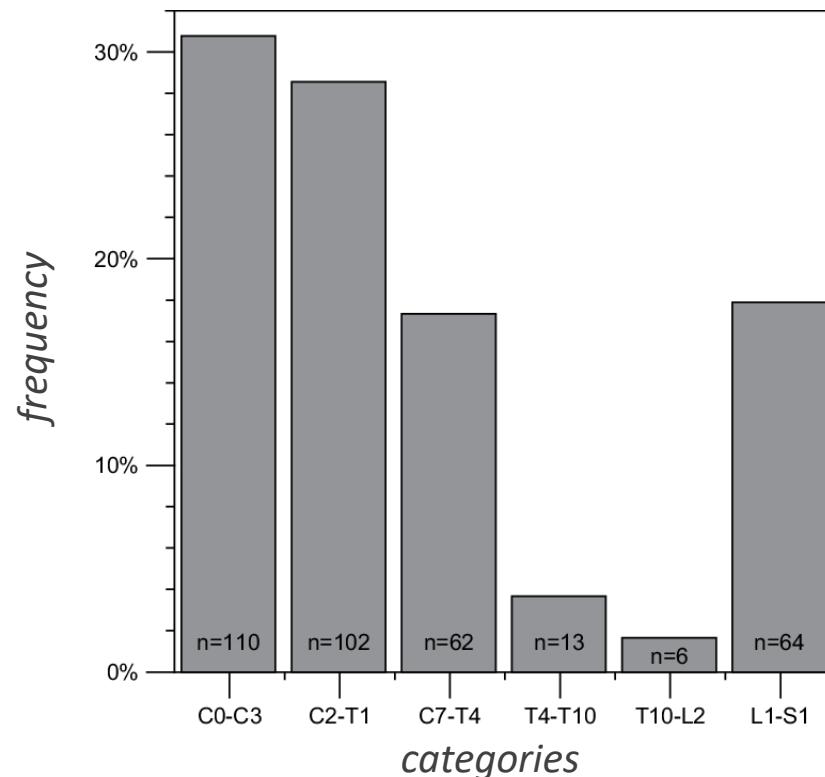
# Variables

- **[discretization]** numeric variables can be discretized into ordinal variables
  - e.g. age categories of 0-10, 11-20, 21-30, 31-40...
  - trade-off: loss of information versus utility for subsequent data analysis
- **[normalization]** numeric variables can be normalized
  - comparability between variables with different domains  $E$
- **[aggregation]** categorical variables with high cardinality can be aggregated
  - 100 colors can be aggregated into coarser categories in accordance with hue
- **[imputation]** missing values can occur
  - unobserved, error or noisy measurements
  - missing values can be imputed using variable expectations

# Data profiling

- Data profiling  $\equiv$  data exploration
  - essential step to know and learn from data

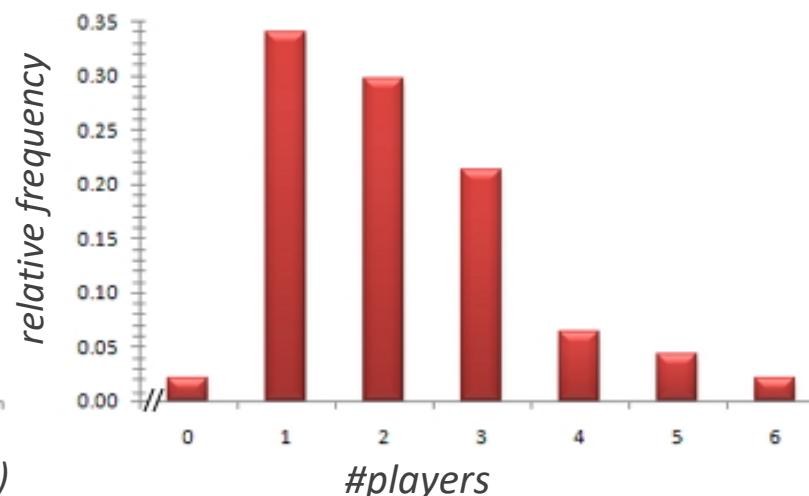
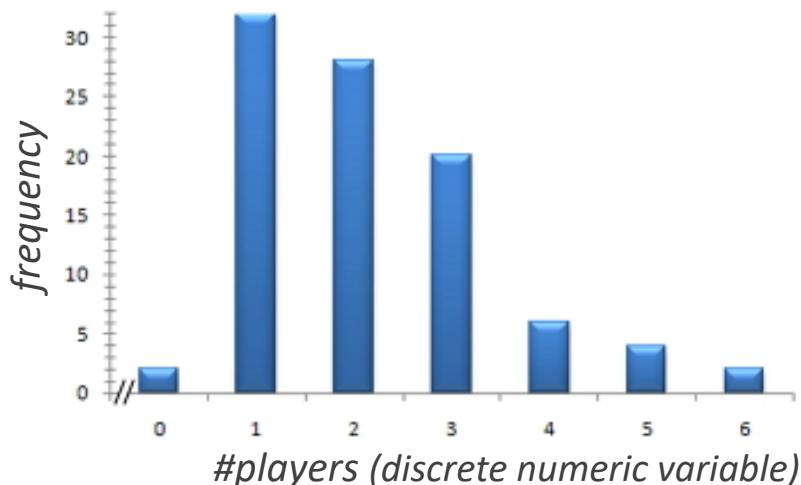
- Frequentist statistics
  - Categorical variables
    - summary statistics (e.g. mode)
    - category frequencies
    - category probabilities



# Data profiling

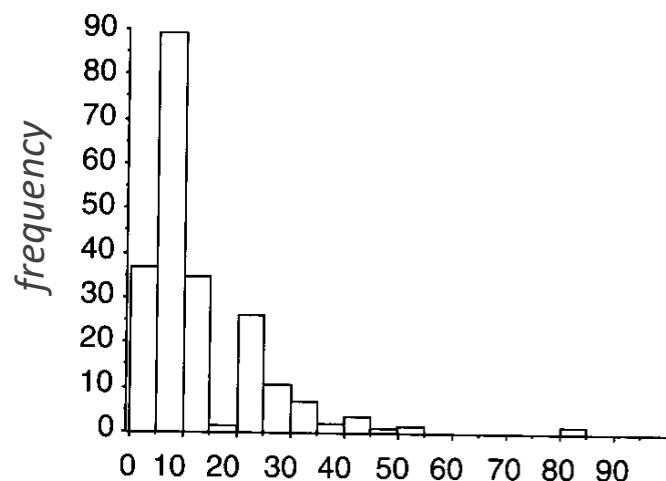
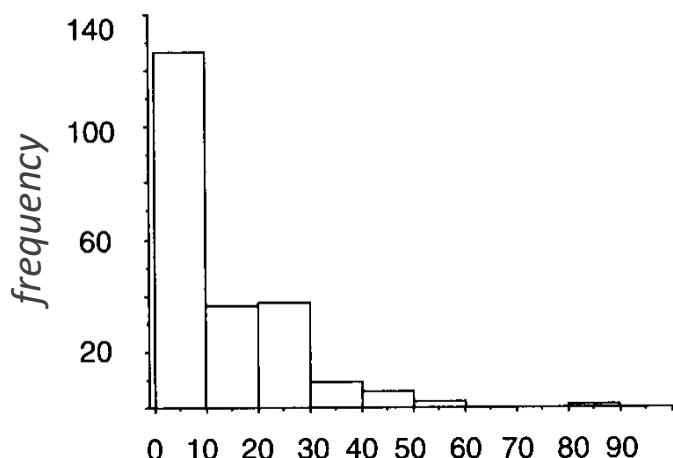
## ■ Frequentist statistics

- numeric variables
  - summary statistics (e.g., percentiles)
  - classic histograms (bin frequencies)
  - empirical probability distribution (bin probabilities)
  - density function for continuous variables
  - mass function for discrete variables, example:



# Data profiling: histograms

- How?
    - divide the range of values in a distribution into several bins of equal size
    - toss each value in the appropriate bin
  - The choice of bin size can strongly affect the frequency histogram
    - revealing details when we lower bin sizes, yet at times a result of overfitting
    - bin size also affect one's perception of the shape of distribution



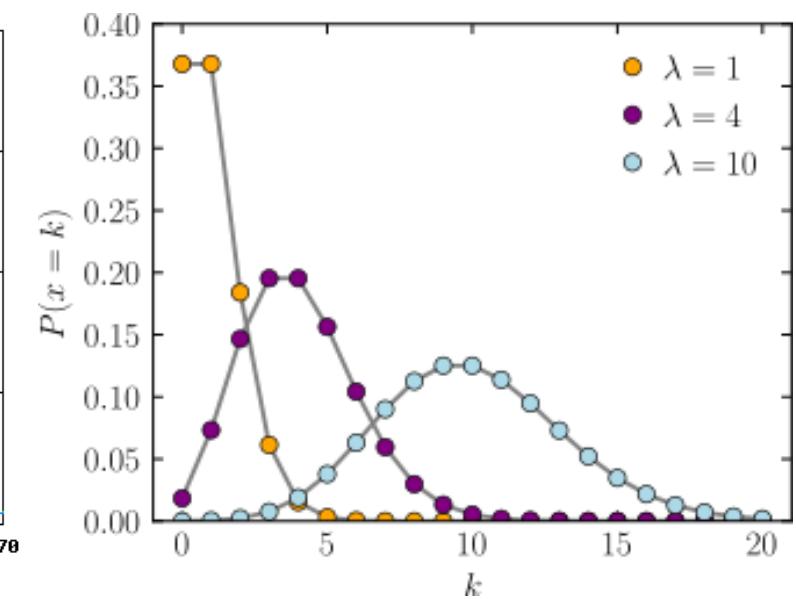
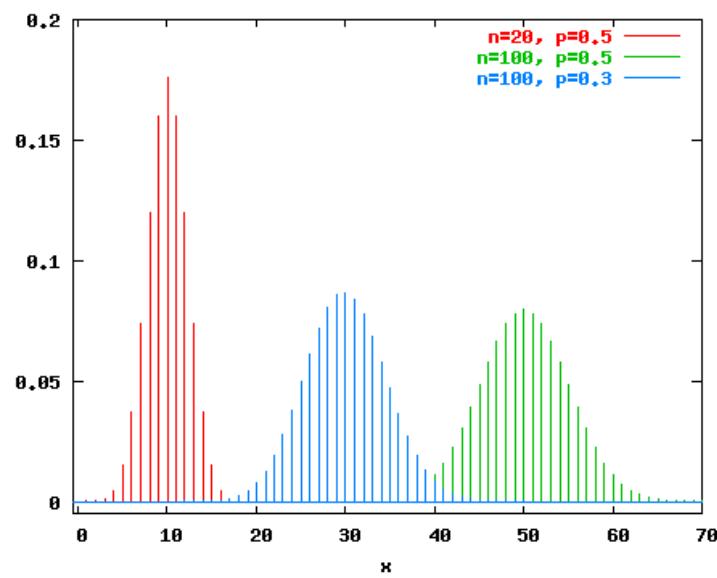
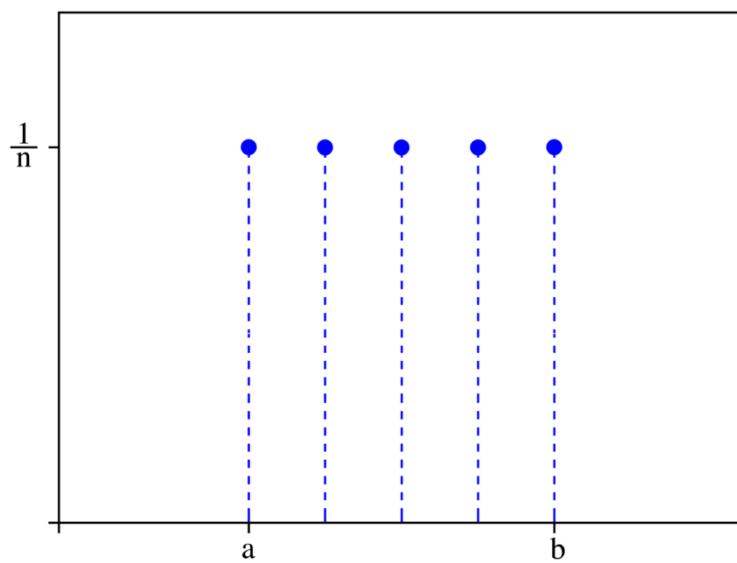
# Data profiling

- **Theoretical statistics**
  - summary statistics
    - mean and deviation statistics (Gaussian assumption)
  - fitting theoretical distributions
    - discrete numeric variables: fitted probability mass function
    - continuous numeric variables fitted probability density function
- **Empirical *versus* theoretical distributions**
  - empirical distribution are perfectly overfitted to observed data
    - this is problematic for low-to-moderate data sample size, otherwise preferable

# Data profiling: theoretical distributions

## ■ Discrete distributions

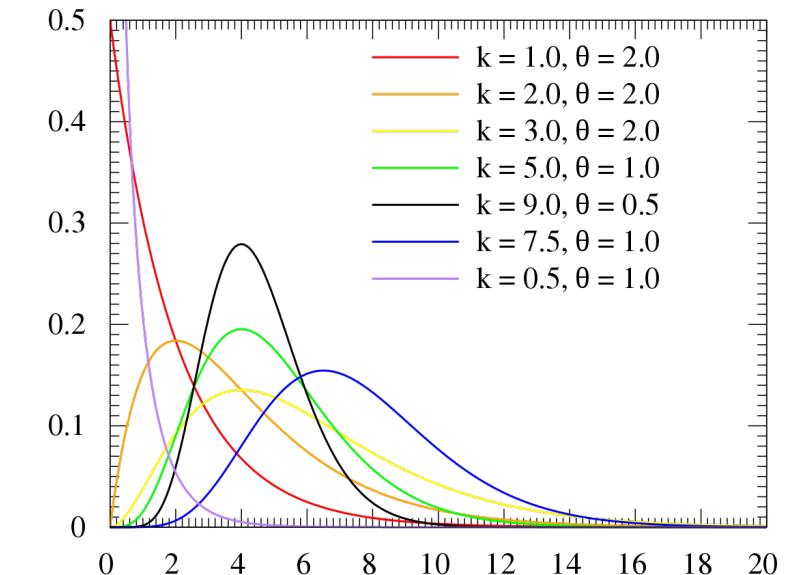
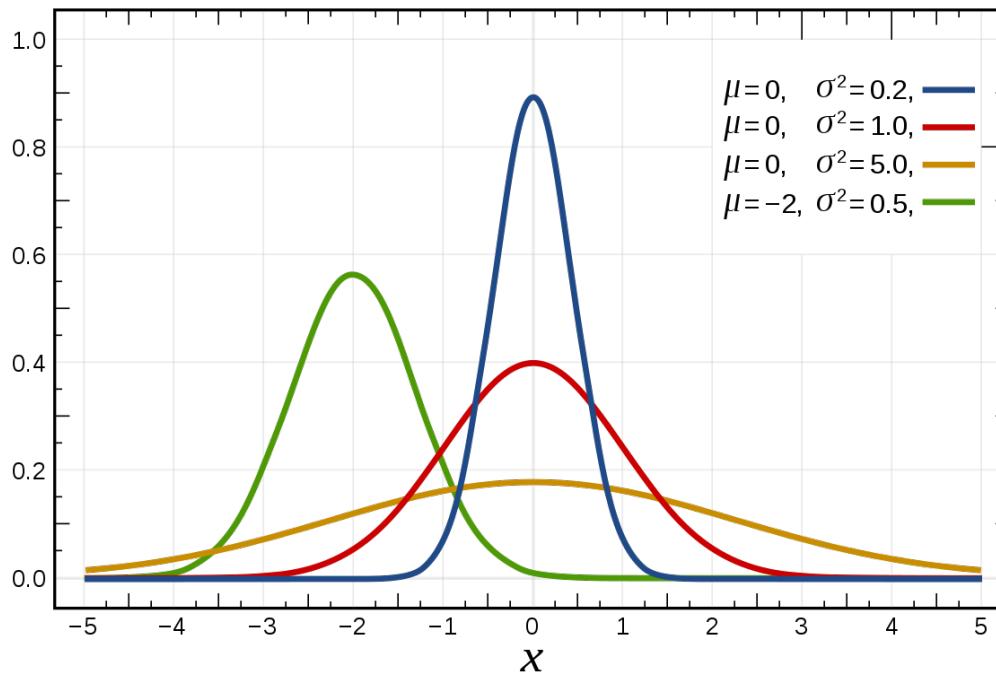
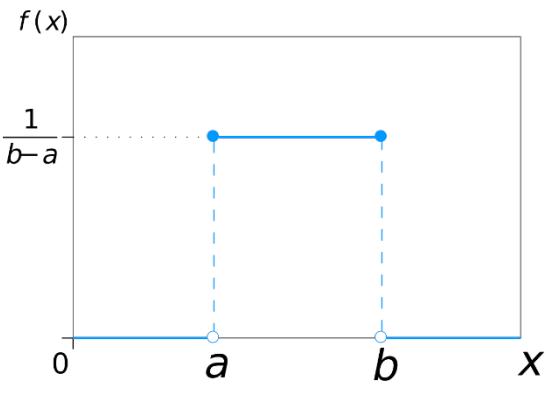
- uniform
- Binomial
- Poisson



# Data profiling: theoretical distributions

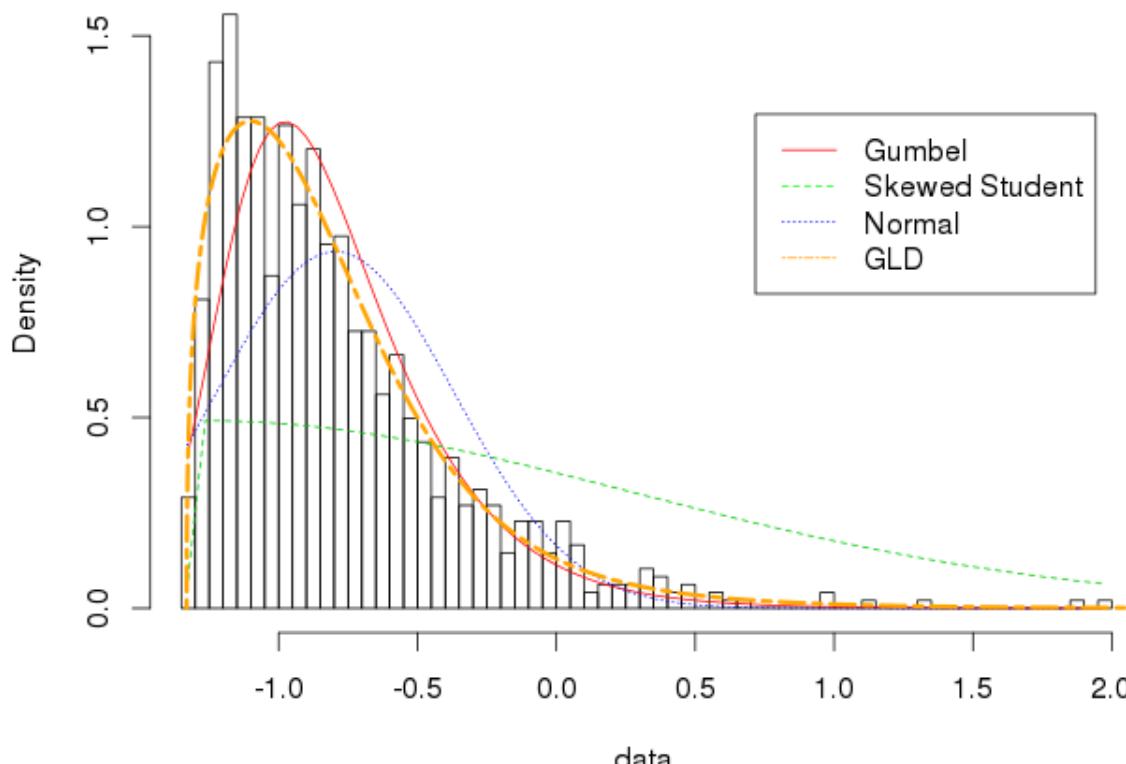
## ■ Continuous distributions

- uniform
- Gaussian
- Gamma



# Data profiling: fitting

- Learn parameters from sample to describe the variable
- Kolmogorov-Sminov statistical test to assess fitting between sample and theoretical distribution
  - <https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.kstest.html>

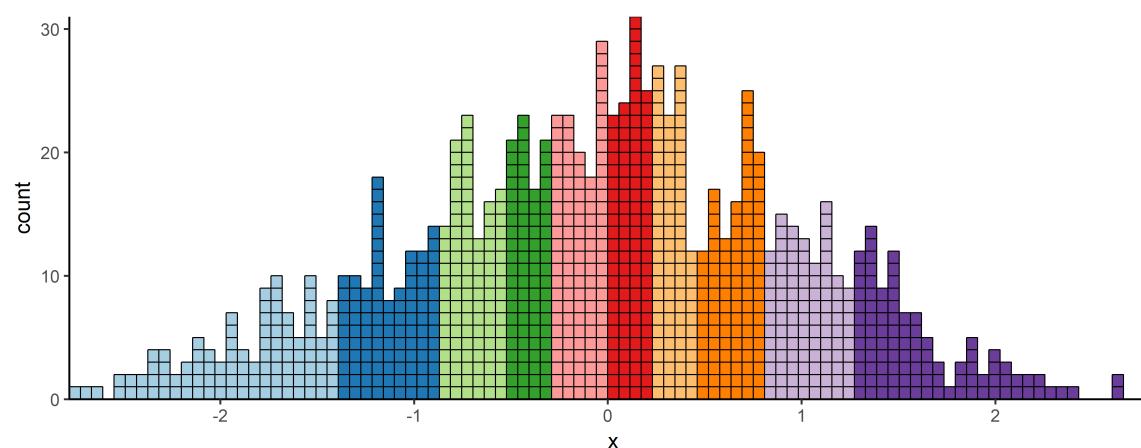


# Univariate summary statistics

- *sample size*: number of data observations,  $n$
- *mean*: arithmetic mean is the average value

$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$$

- *maximum, minimum, range* ( $\max - \min$ )
- *percentiles*
  - median, max and min correspond to the 50, 100 and 0 percentiles
  - 5, 10, 25 (first quantile), 75 (third quantile), 90, 95 are also informative



# Univariate summary statistics

**Center statistics** are relevant to understand expectations

- *harmonic mean*
- *median*
  - sorted values, the median is the value that splits the distribution in half
  - $\text{median}(1,1,1,2,3,4,5) = 2$
  - If  $n$  is even, the median can be found by interpolating them
- *mode* for categorical and discrete numeric values
  - $\text{mode}(1,2,2,3,4,4,4) = 4$
  - application in continuous variables: after rounding, bin sorting, discretization
- *trimmed mean*
  - lop off a fraction of the upper and lower ends of the distribution, and take the mean of the rest
  - Example with lop off two: 0,0,1,2,5,8,12,17,18,18,19,19,20,26,86,116
    - trimmed mean = 13.75
    - arithmetic mean = 22.75

# Univariate summary statistics

**Deviation statistics** are important to assess the variability of variable measurements

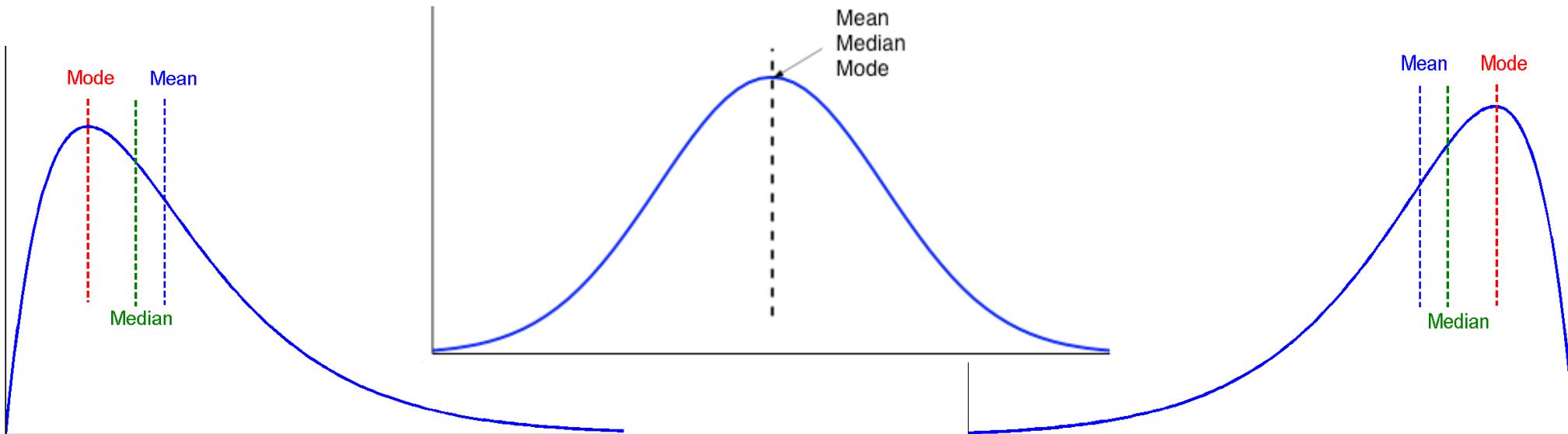
- *Standard deviation*: square root of the variance

$$\sigma_{population} = \sqrt{\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2}, \quad \sigma_{sample} = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2}$$

- **population-based** deviation
  - divided by  $n$
- **sample** deviation
  - divided by  $n - 1$
  - conservative estimate (higher variance) because as we are unable to observe the whole population
- *example*: 1, 2, 15 measurements
  - $\mu = 6, \sigma_{population} = 6$  (approx.),  $\sigma_{sample} = 7.3$  (approx.)

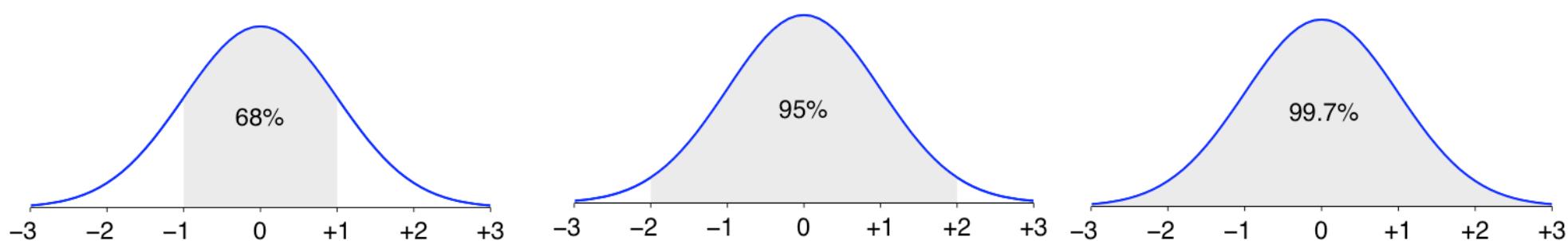
# Univariate data statistics: skew

- In a skewed distribution the bulk of the data are at one end of the distribution
  - If the bulk of the distribution is on the right (tail is on the left): **left skewed** or negatively skewed distribution
  - If the bulk of the distribution is on the left (tail is on the right): **right skewed** or positively skewed distribution
- **Symmetric** distributions are not skewed
- Percentile statistics are not distorted by outliers



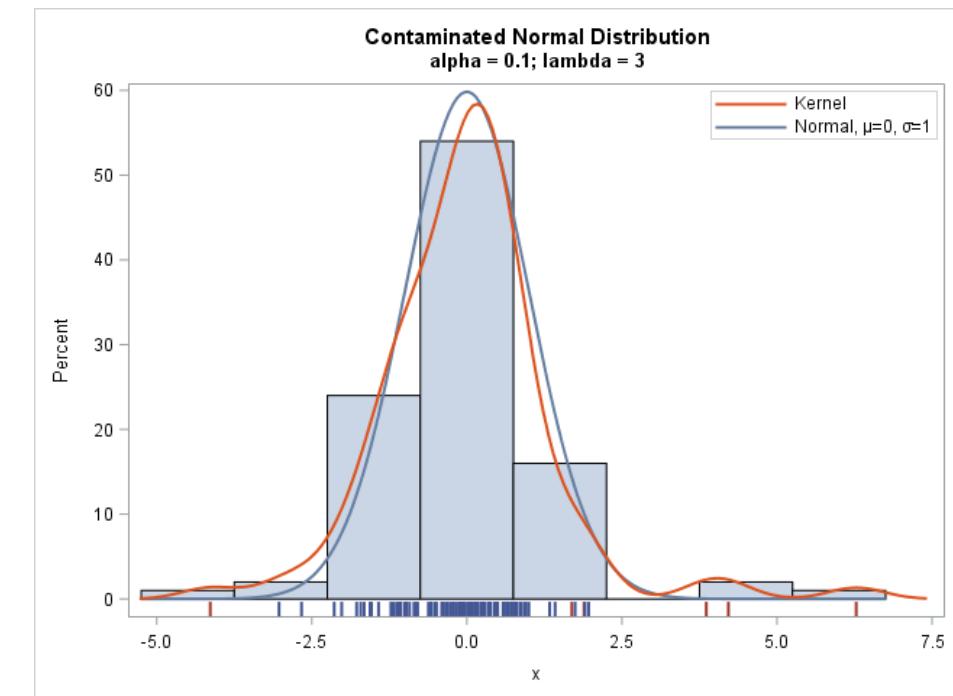
# Properties of Normal distribution

- Many real-world variables are well-approximated to a Gaussian curve
- How to check if one variable satisfies the Gaussian assumption?
  - use the introduce Kolmogorov-Sminov or, more suitably, Shapiro-Wilk test
  - remember the central limit theorem: 30 measurements are often necessary to check this assumption
- Interesting properties of the Normal curve:
  - from  $\mu-\sigma$  to  $\mu+\sigma$ : contains about 68% of the measurements ( $\mu$ : mean,  $\sigma$ : standard deviation)
  - from  $\mu-2\sigma$  to  $\mu+2\sigma$ : contains about 95% of it
  - from  $\mu-3\sigma$  to  $\mu+3\sigma$ : contains about 99.7% of it



# Outliers

- Outlier values = uncommon values
  - unexpected measurements against a variable distribution
- Mean and the variance are based on averages, hence sensitive to outliers
- Outliers can cause strong effects that can wreck our interpretation of data
  - for example, the presence of a single outlier can render some statistical comparisons insignificant
- Detecting and removing outlier values requires judgment and depend on one's purpose

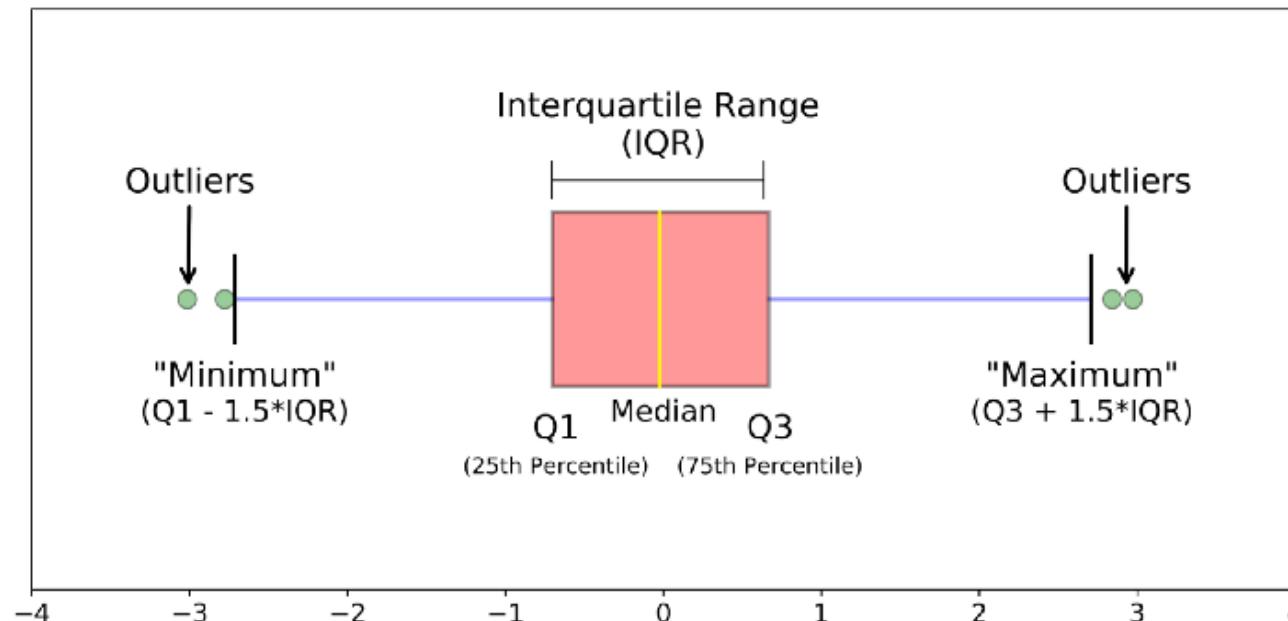


# Interquartile range (IQR)

- **Interquartile range** is used to measure value expectations
  - distribution can be divided into **quartiles**, each containing the same number of observations
  - the difference between the highest value in the third quartile and the lowest in the second quartile is the **interquartile range**
  - example:
    - $\text{quartiles}(1,1,2,3,3,5,5,5,5,6,6,100) = \{(1,1,2), (3,3,5), (5,5,5), (6,6,100)\}$
    - interquartile range  $5-3=2$
- IQR is empirically known to be robust against outliers
  - observations falling outside  $[Q1 - 1.5 \times IQR, Q3 + 1.5 \times IQR]$  are seen as outliers

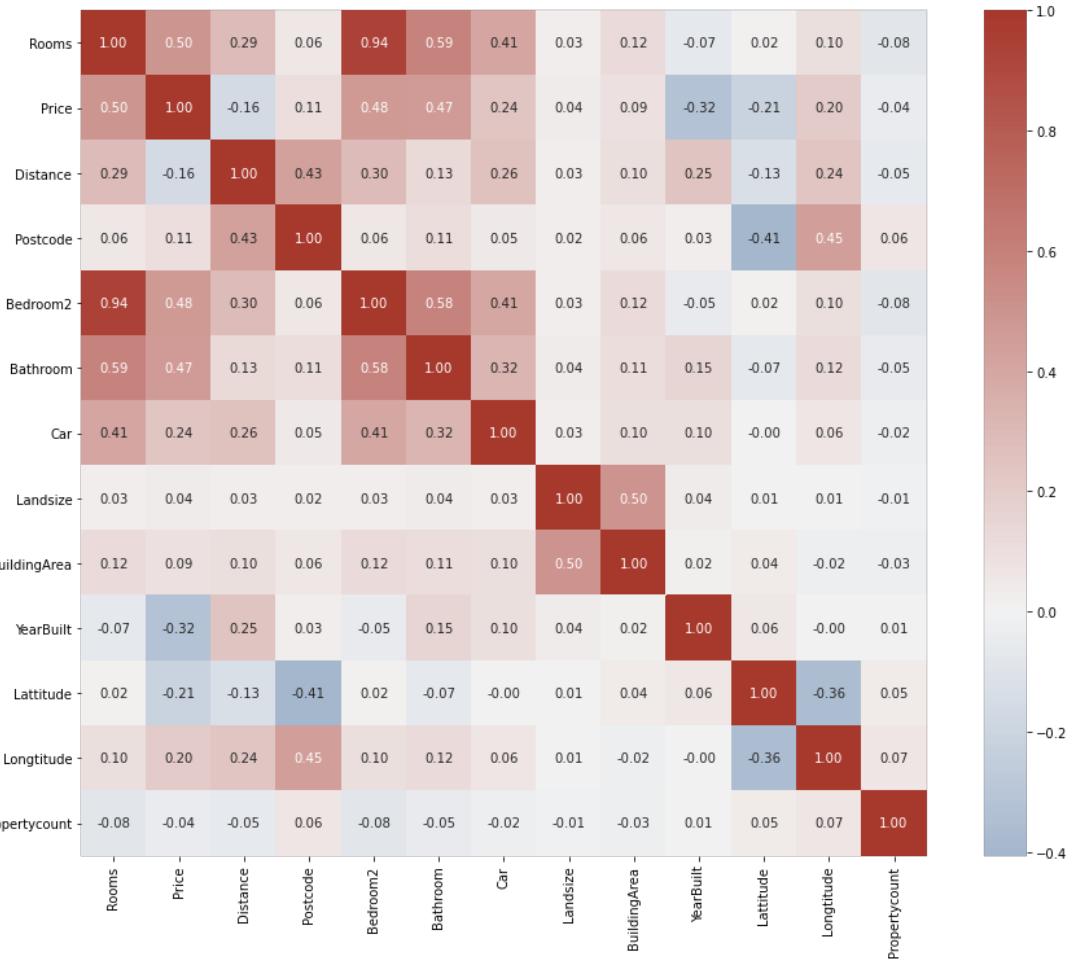
# Boxplot

- The distribution of variable can be visualized:
  - bar charts (categorical variables) and histograms (numeric variables)
  - theoretical probability distributions
  - boxplots: particularly useful to visually detect outlier values



# Bivariate data statistics

- Considering pairwise input variables:
  - check whether the two distributions are **correlated**
  - if highly correlated, variables may be **redundant**
    - select the one with the highest variability
- *Exercise:* select non-redundant variables on the provided right example



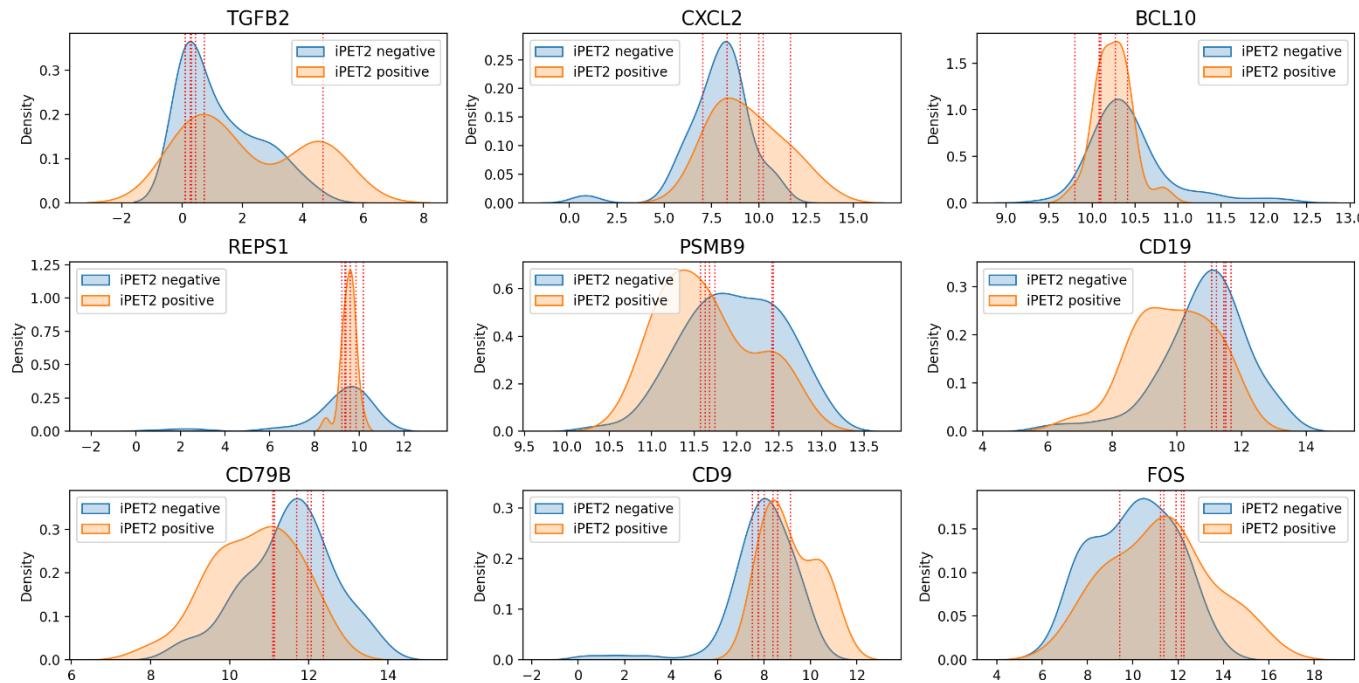
# Bivariate data statistics

- Considering one input and one output variable
  - when referring to class variables: we want to assess the ***discriminative power*** of the input variable
  - when referring to numeric output variables: we want to assess the ***correlation*** with the input variable
    - the higher the correlation, the higher the relevance of the input variable to characterize the targets
  - if both input-output variables are numeric
    - linear correlation given by **Pearson** correlation coefficient (PCC)
    - rank-based correlation given by **Spearman** tau prioritizes ranks instead of magnitude
  - if variables are either ordinal or numeric: **Spearman** tau is suggested
  - if one variable is nominal and other numeric: **analysis of variance** (ANOVA)
  - if both variables are nominal:  $\chi^2$

# Discriminative power

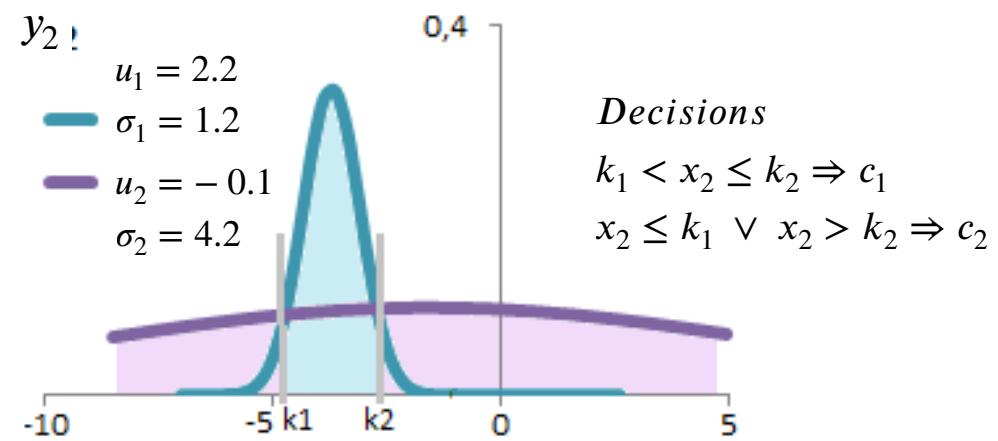
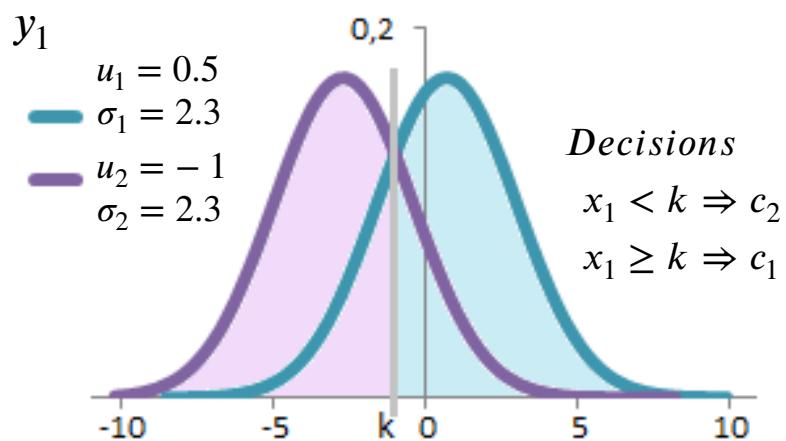
## ■ Class-conditional distributions

- the higher the dissimilarity between class-condition distributions: the higher the discriminative power
- *exercise*: consider a dataset composed by the following 9 numeric input variables and binary class
- are we in the presence of a simple or difficult classification task?



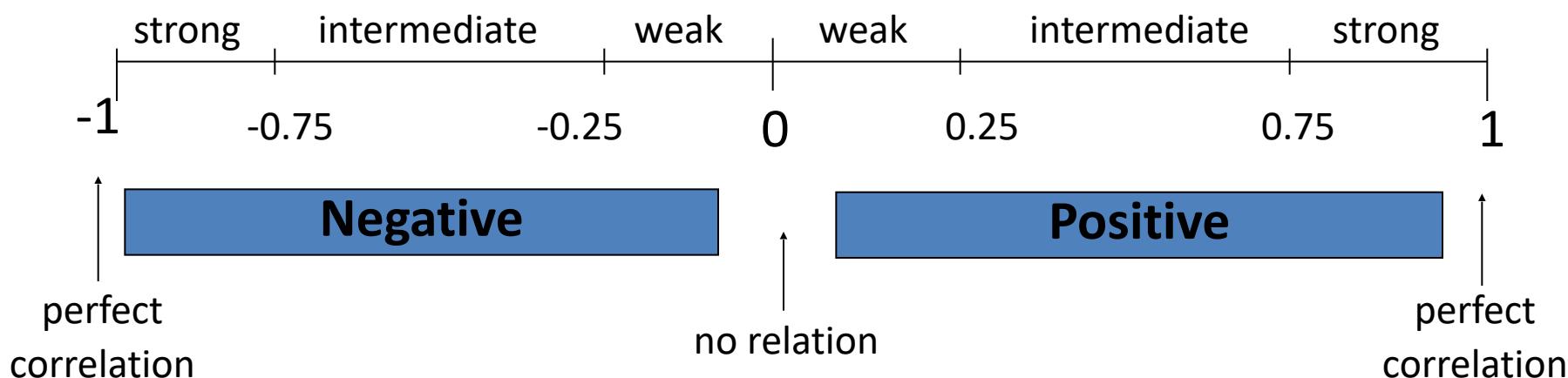
# Discriminative power

- Using class-conditional distributions:
  - **discriminative rules** can be inferred by identifying the class of higher probability along the input values
  - this classifier is termed **univariate discriminant**



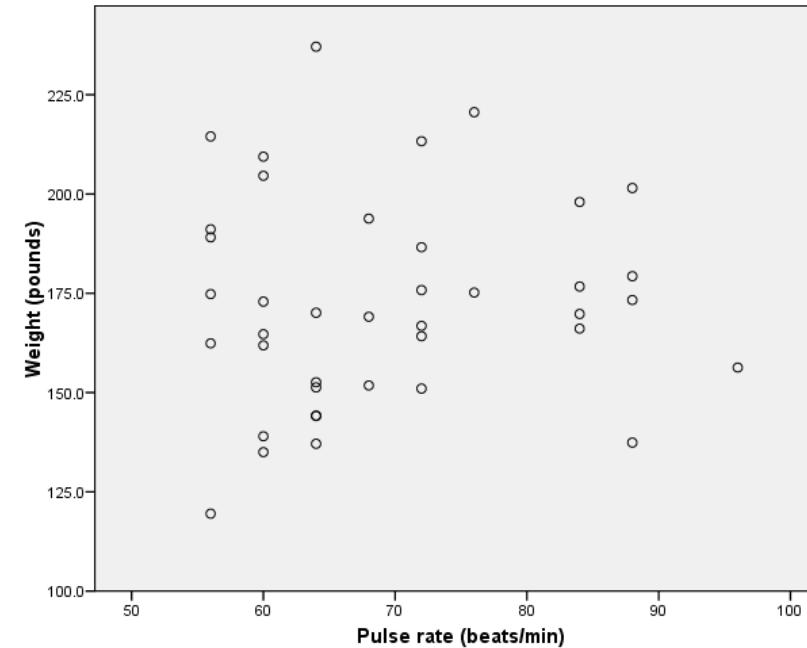
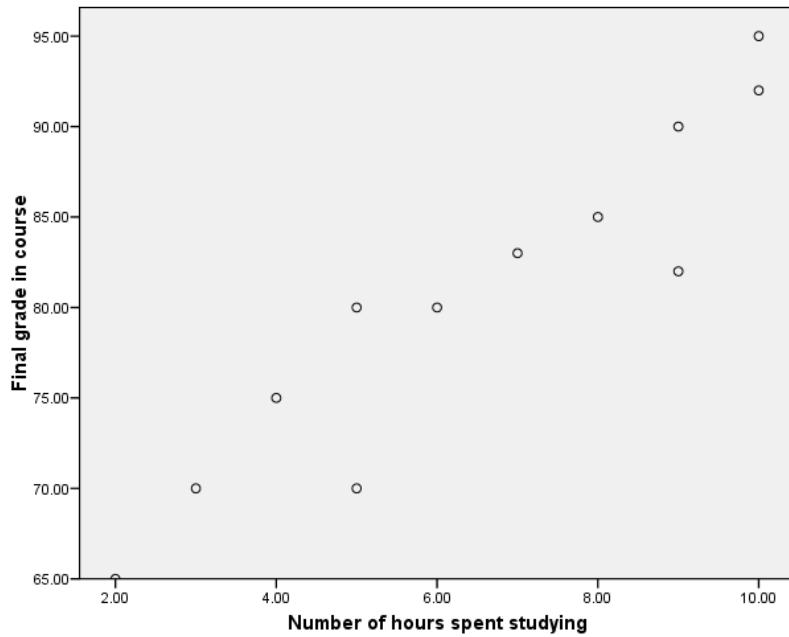
# Correlation...

- Relationship between two quantitative attributes
  - correlation: degree to which two attributes are related (in  $[-1,1]$ )
    - the *sign*: nature of association ( $> 0$  direct;  $< 0$  inverse)
    - the absolute *value* of  $r$ : strength of association
    - unable to infer causal relationships



# Correlation...

Scatter diagrams can be used to visually assess correlation

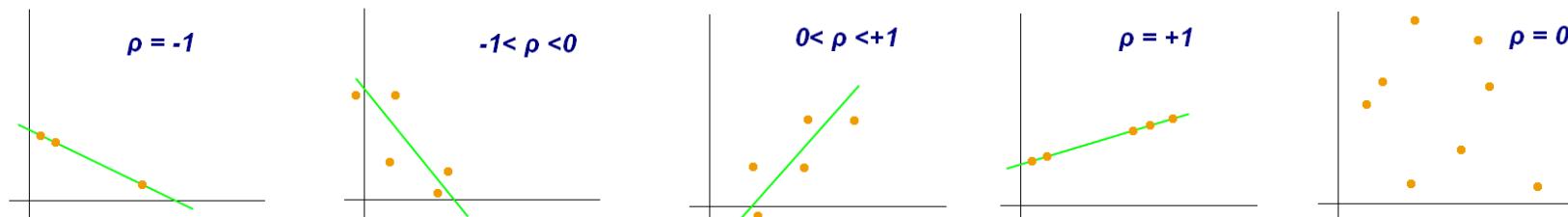
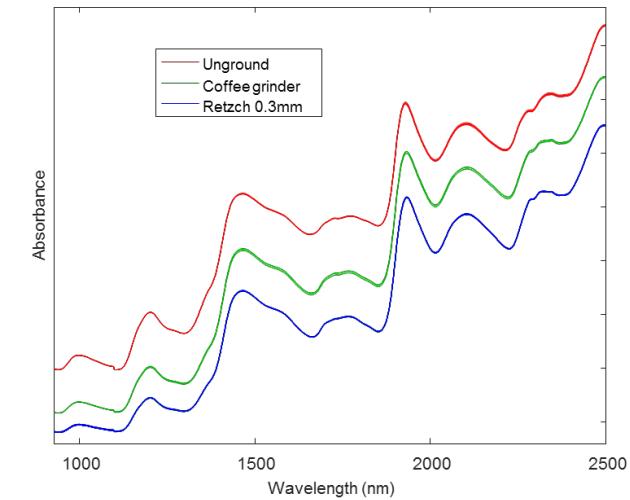


- each pair of values is treated as a pair of coordinates and plotted as points in the plane
- provides a first look at bivariate data to see clusters, outliers, etc.

# Pearson correlation

- Pearson correlation (or product moment correlation) coefficient
  - only suitable for numeric attributes
  - able to handle scales and shifts

$$r = \frac{cov(y_1, y_2)}{\sqrt{var(y_1)}\sqrt{var(y_2)}} = \frac{\sum y_1 y_2 - \frac{\sum y_1 \sum y_2}{n}}{\sqrt{\left(\sum y_1^2 - \frac{(\sum y_1)^2}{n}\right)\left(\sum y_2^2 - \frac{(\sum y_2)^2}{n}\right)}}$$



# Pearson correlation

Anxiety ()	Test score ()			
10	2	100	4	20
8	3	64	9	24
2	9	4	81	18
1	7	1	49	7
5	6	25	36	30
6	5	36	25	30
$\sum y_1 = 32$	$\sum y_2 = 32$	$\sum y_1^2 = 230$	$\sum y_2^2 = 204$	$\sum y_1 y_2 = 129$

$$r = \frac{(6)(129) - (32)(32)}{\sqrt{(6(230) - 32^2)(6(204) - 32^2)}} = -.94$$

indirect strong  
correlation

# Spearman rank

- Non-parametric coefficient
  - works with rankings instead of absolute values
- How?
  1. Rank the values of  $y_1$  and  $y_2$
  2. Apply the Pearson correlation

In the given example:

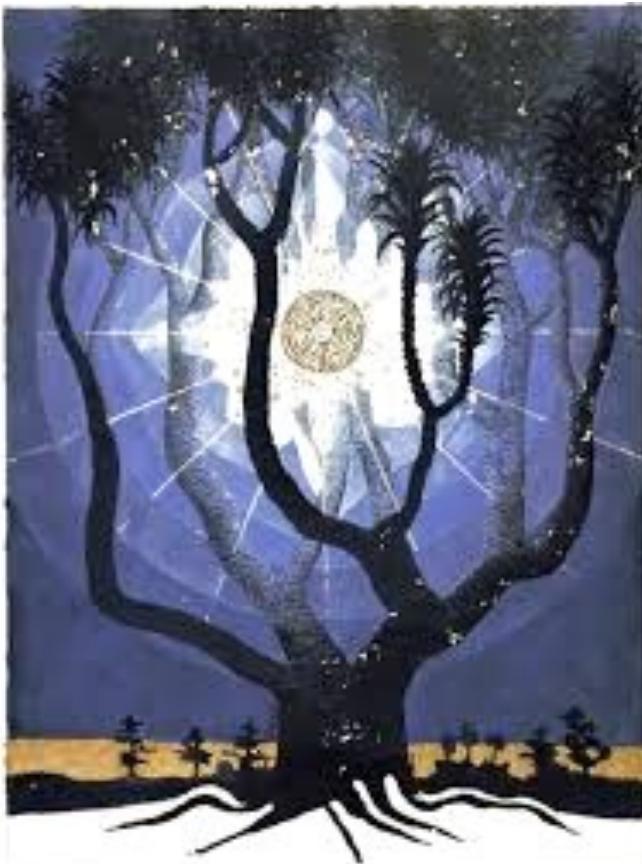
$$r_s = PCC((5 \ 6 \ 1.5 \ 3.5 \ 3.5 \ 7 \ 1.5), (3 \ 5.5 \ 7 \ 5.5 \ 4 \ 2 \ 1))$$

$$r_s = -0.17$$

education level ( $y_1$ )	income ( $y_2$ )	rank $y_1$	rank $y_2$
Preparatory	25	5	3
Primary	10	6	5.5
University	8	1.5	7
Secondary	10	3.5	5.5
Secondary	15	3.5	4
Illiterate	50	7	2
University	60	1.5	1

$r_s$  denotes the magnitude of association

# Outline



- **Machine learning**
  - intelligence and learning
  - data science and AI
  - symbolic learning
  - terminology
  - descriptive and predictive tasks
- **Univariate data analysis**
  - numeric and categoric variables
  - empirical and theoretical distributions
  - summary statistics
  - outlier removal
  - discriminant analysis
  - correlation

# Thank You



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