TÉCNICO LISBOA

DATA EXPLORATION

Cláudia Antunes

2018 / 19

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DATA SCIENCE

- "The art of discovering what we don't know from data"

  Carlos Somohano, founder of Data Science London

- "A systematic study of a generalizable extraction of knowledge from data"

  Vasant Dhar, Professor at Center for Data Science at NYU

- "The nontrivial extraction of implicit, previously unknown, and potentially useful **information** from **data**."

  William J. Frawley, *AI Magazine* in **1995**

BASIC CONCEPTS

Data sets are made up of records.

Records

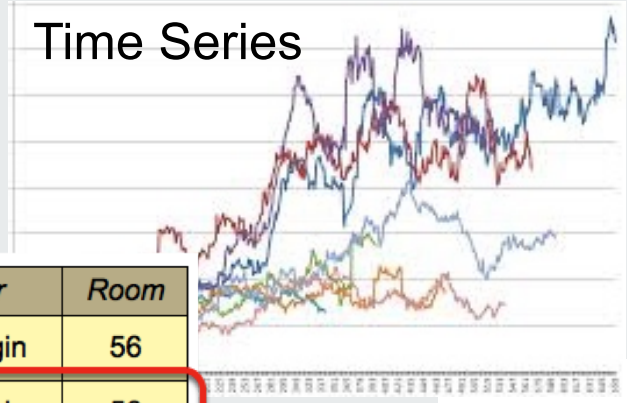
- also known as ***instances***, ***data objects*** or ***samples***
- the recorded facts that describe the state or behavior of some entity, in accordance with a set of attributes;

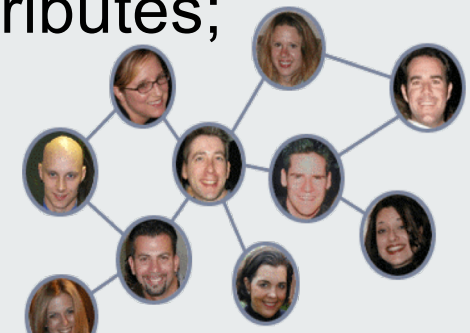
✦ Examples:

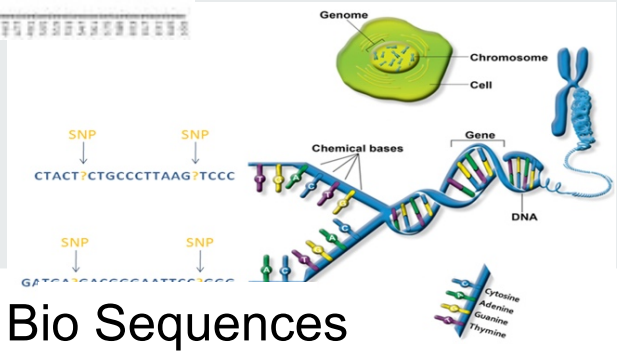
Tabular data

ID No.	Name	D.o.B.	Phone	Class	Tutor	Room
356	Jess	3 Mar 1995	7564356	5B	Mr Noggin	56
412	Hamad	12 Nov 1994	7465846	5B	Mr Noggin	56
459	Sita	9 Jan 1994	8565634	6Y	Ms Take	18
502	Hamad	3 Mar 1995	6554546	5B	Mr Noggin	56

One **Record**







Bio Sequences

BASIC CONCEPTS

Records are tuples of values, according to a set of attributes

Attribute

- also known as ***fields, dimensions***, ***variables*** *or* ***features***
- **Attribute Domains**: values that can be taken by the attribute
- **Attribute Range**: the values that are actually taken

✦ Examples

Tabular data

ID No.	*Name*	*D.o.B.*	*Phone*	*Class*	*Tutor*	*Room*
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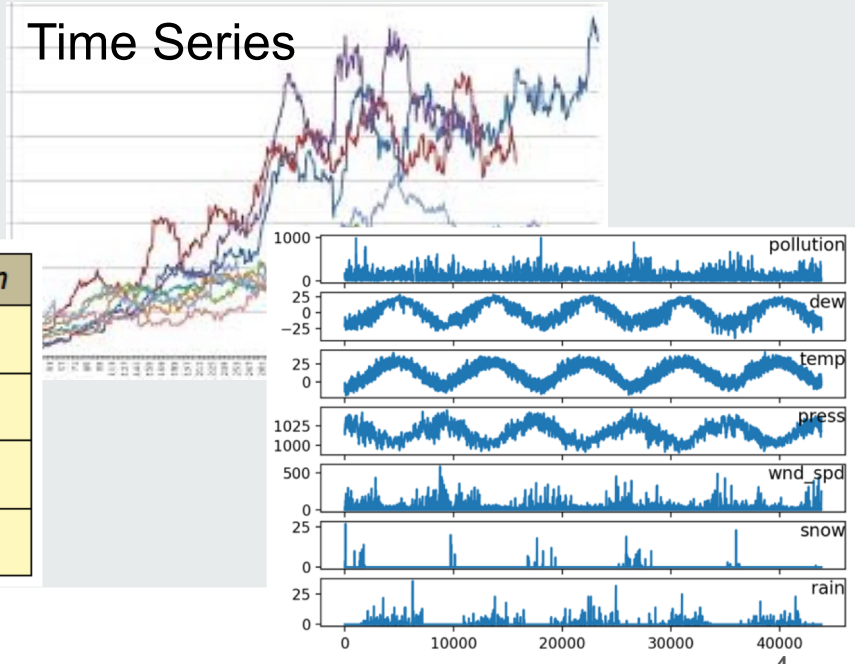
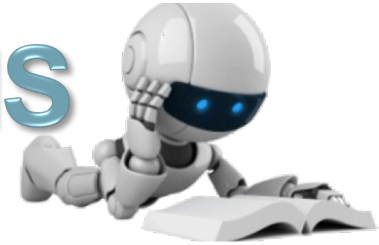


TABULAR DATA

- Data is usually represented as a ***n*x*d*** matrix, ***D***, with
  - ***n***, the number of records (lines) from x_1 to x_n
  - and ***d***, the number of attributes (columns) from A_1 to A_d

$$\mathbf{D} = \begin{array}{c|cccc} & A_1 & A_2 & \cdots & A_d \\ \hline \mathbf{x}_1 & x_{11} & x_{12} & \cdots & x_{1d} \\ \mathbf{x}_2 & x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_n & x_{n1} & x_{n2} & \cdots & x_{nd} \end{array}$$

ATTRIBUTE DOMAINS



Numeric

Real-valued

- Quantities

Interval-based

- Measured on a scale of equal-sized units
- Values have order
- No true zero-point

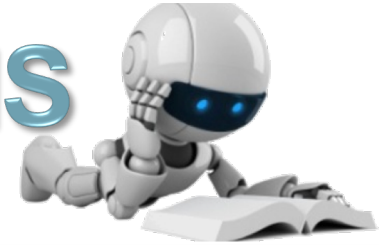
Ratio

- Inherent **zero-point**
- Known magnitude between values

Observations

- Real values can only be represented by a finite number of digits
- Typically represented as floating-point variables

ATTRIBUTE DOMAINS



Numeric

Real-valued
- Quantities

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- Measured on a scale of equal-sized units
- Values have order
- No true zero-point

Ratio
- Inherent **zero-point**
- Known magnitude between values

Symbolic

Binary
- With only 2 values

Symmetric x Asymmetric

Nominal
- Set of discrete values
- Categories, states, "names of things"

Ordinal
- Values have a meaningful order (ranking)
- Unknown magnitude between values

INFORMATION

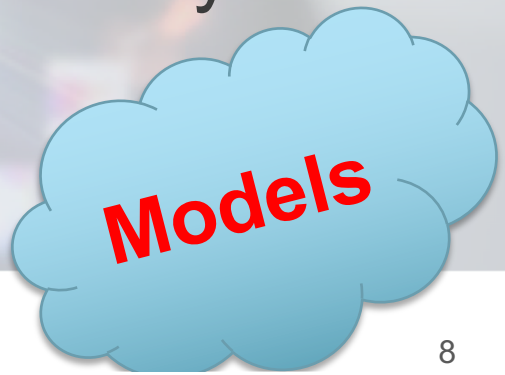
The **set of patterns** or expectations that underlie the data

Witten, 2000

From a mathematical point of view, the generation of information can be seen as **data compression**, since information can be seen as a **model** to represent several instances.

Addrians, 1996

As **the next step in the road of knowledge**, since it corresponds to an **abstraction** of the already known (recorded) data.



TABULAR DATA

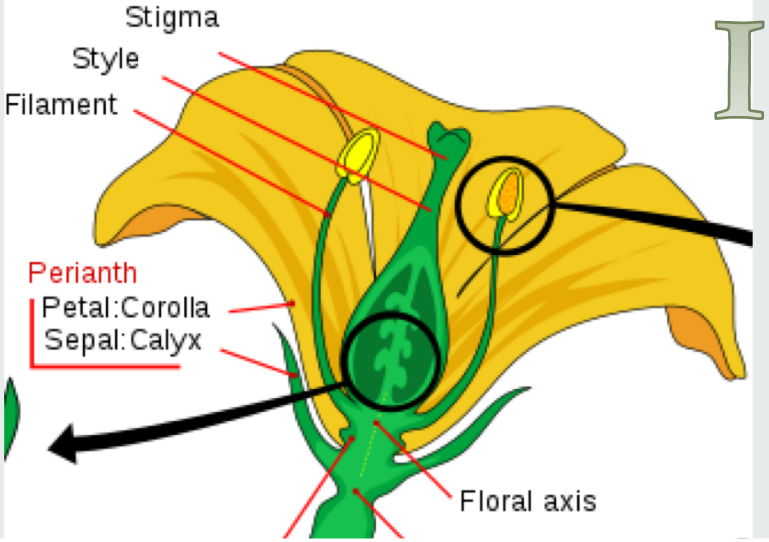
EXAMPLE

Versicolor

Verginica

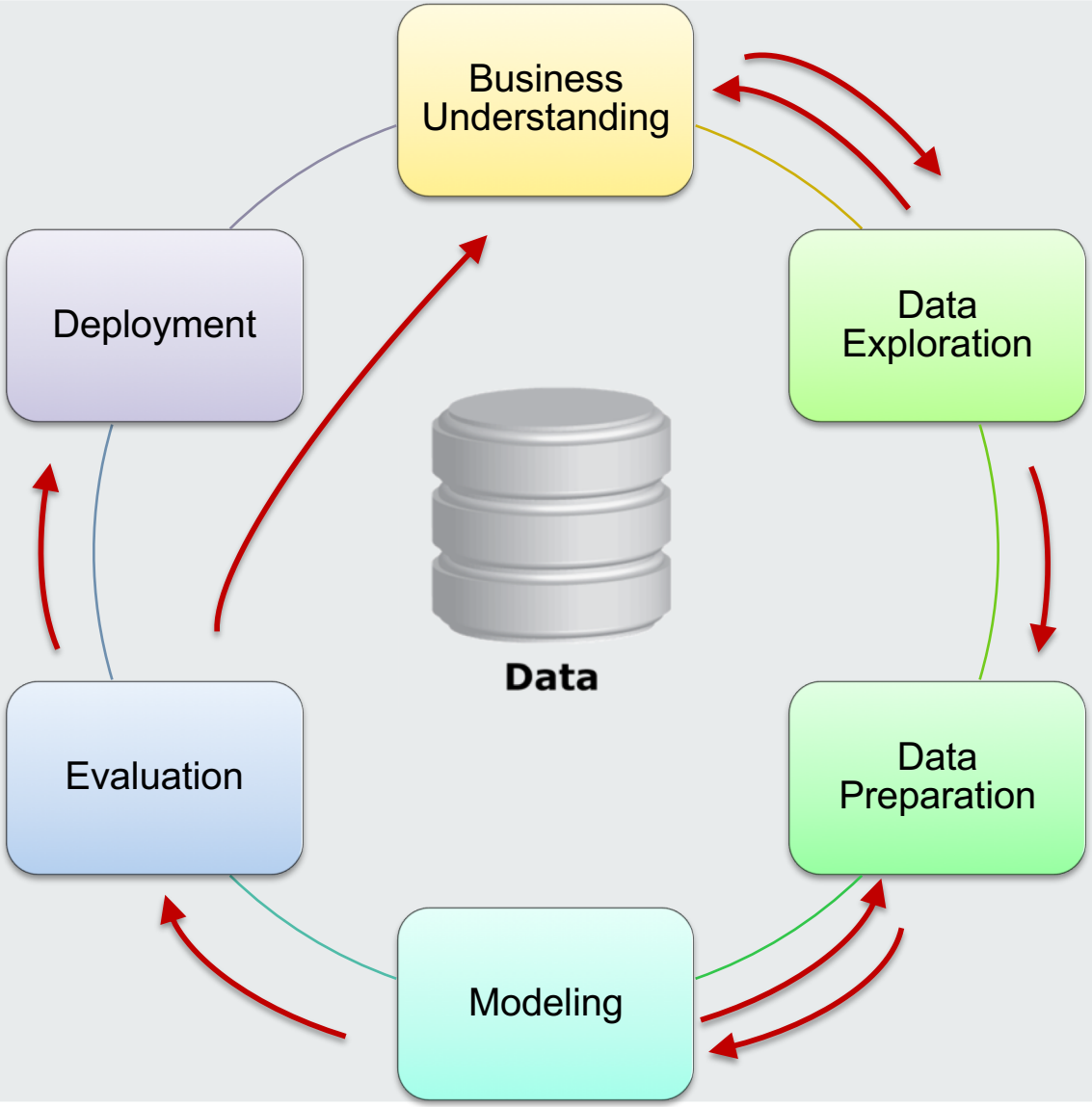
Setosa

Iris



	Sepal length	Sepal width	Petal length	Petal width	Class
$\mathbf{x}_1$	5.9	3.0	4.2	1.5	Iris-versicolor
$\mathbf{x}_2$	6.9	3.1	4.9	1.5	Iris-versicolor
$\mathbf{x}_3$	6.6	2.9	4.6	1.3	Iris-versicolor
$\mathbf{x}_4$	4.6	3.2	1.4	0.2	Iris-setosa
$\mathbf{x}_5$	6.0	2.2	4.0	1.0	Iris-versicolor
$\mathbf{x}_6$	4.7	3.2	1.3	0.2	Iris-setosa
$\mathbf{x}_7$	6.5	3.0	5.8	2.2	Iris-virginica
$\mathbf{x}_8$	5.8	2.7	5.1	1.9	Iris-virginica
⋮	⋮	⋮	⋮	⋮	⋮
$\mathbf{x}_{149}$	7.7	3.8	6.7	2.2	Iris-virginica
$\mathbf{x}_{150}$	5.1	3.4	1.5	0.2	Iris-setosa

DATA SCIENCE PROCESS



DATA EXPLORATION

- **Univariate analysis** focus at each attribute at a time

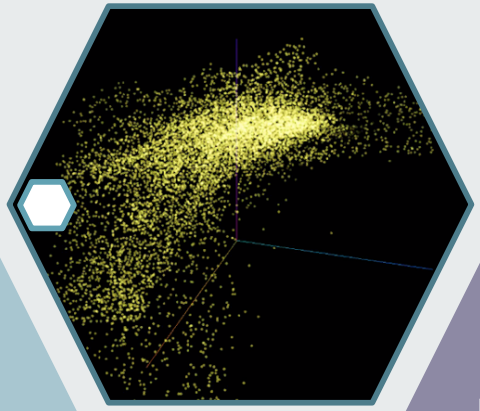
- **Multivariate analysis** focus at subsets of attributes at a time

$$\mathbf{D} = \begin{array}{c|c|c|c|c} & A_1 & A_2 & \cdots & A_d \\ \hline \mathbf{x}_1 & x_{11} & x_{12} & \cdots & x_{1d} \\ \mathbf{x}_2 & x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_n & x_{n1} & x_{n2} & \cdots & x_{nd} \end{array}$$

DATA EXPLORATION

Multivariate

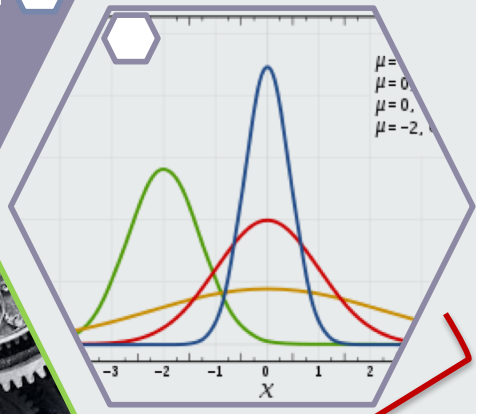
Curse of dimensionality

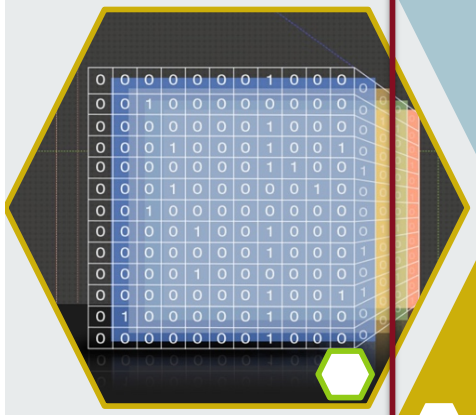


Dimension ality

Distribution

Centrality and dispersion





Granularity

Sparsity

Only presence counts

Patterns depend on the scale

Univariate

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DATA GRANULARITY

Analyzing each attribute individually

GRANULARITY

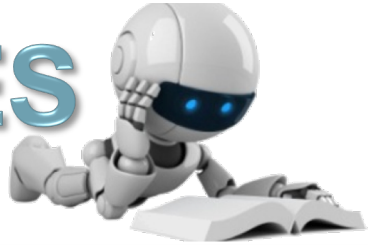
Granularity is the **data scale** or **level of detail**.

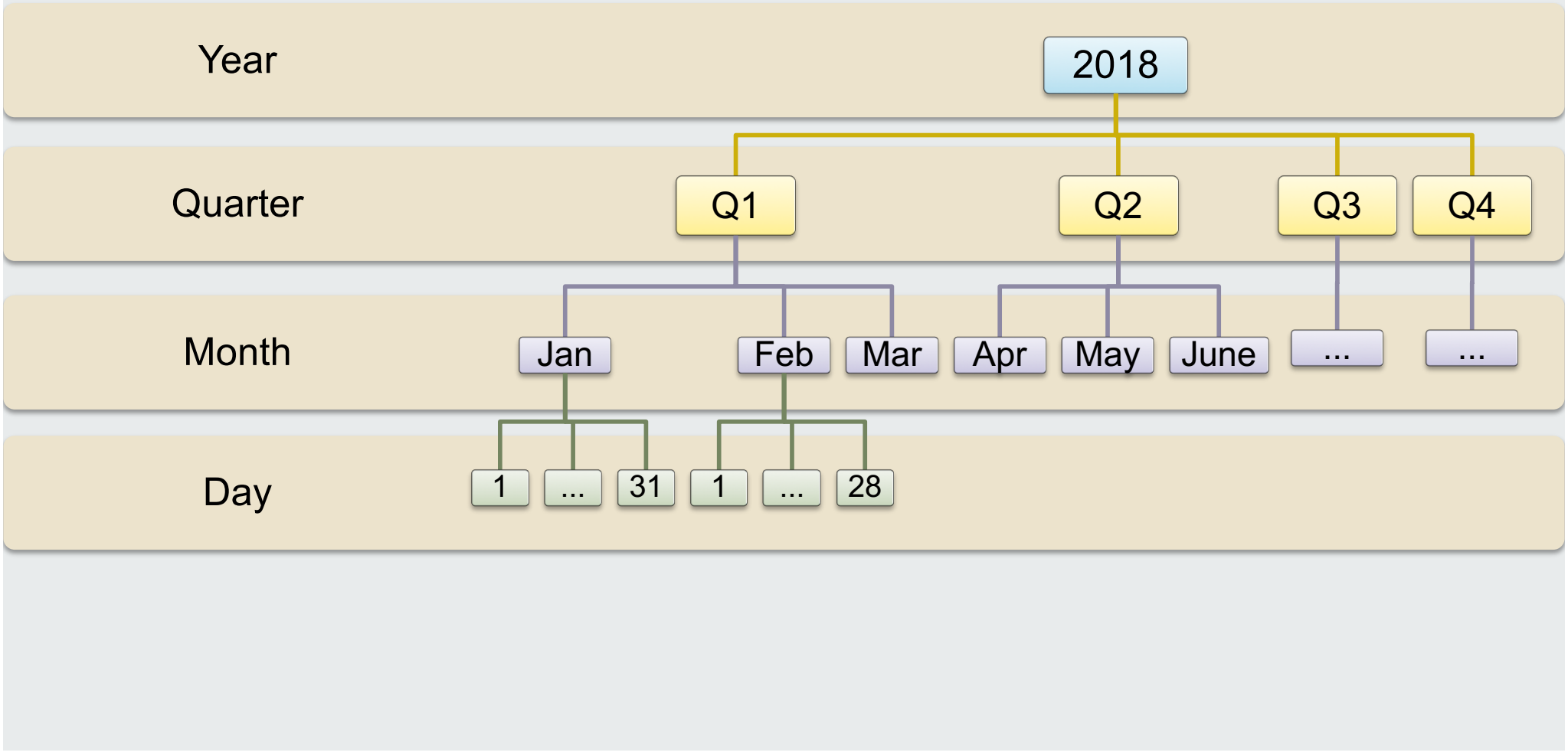
The finer the granularity,
the deeper the level of detail.

- Data at a finer granularity can be **aggregated** into a coarser one.

- Granularities are specified:
  - by **taxonomies** (concept hierarchies) for symbolic attributes
  - by **discretization** for numeric ones

TIME GRANULARITIES





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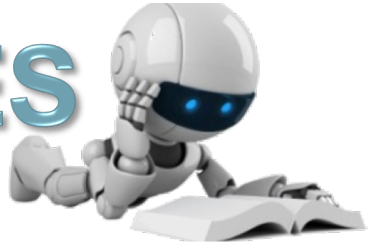
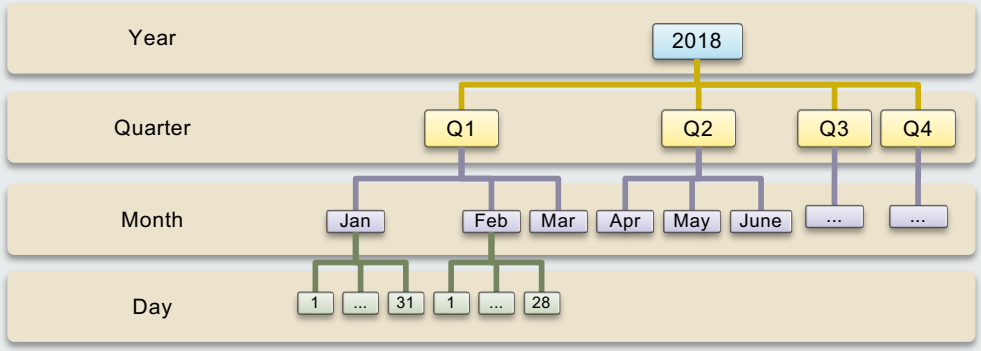
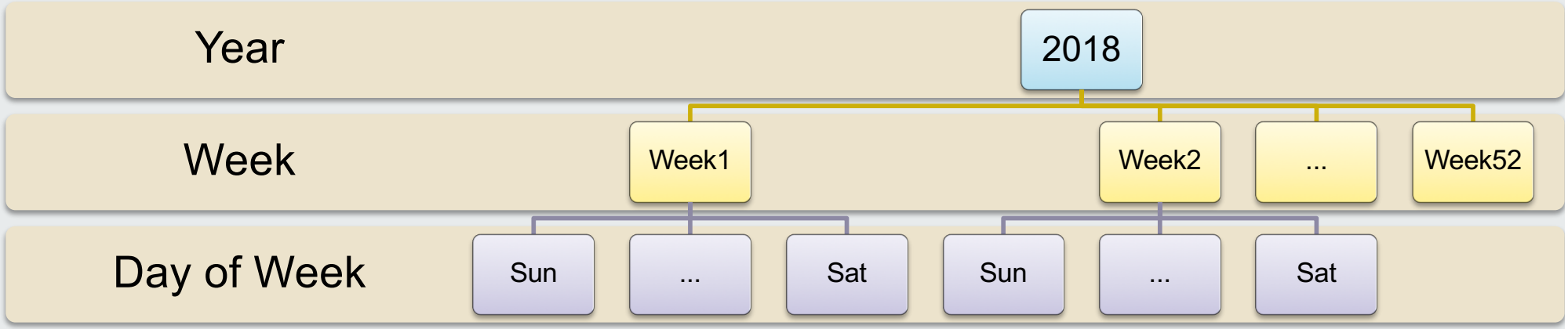
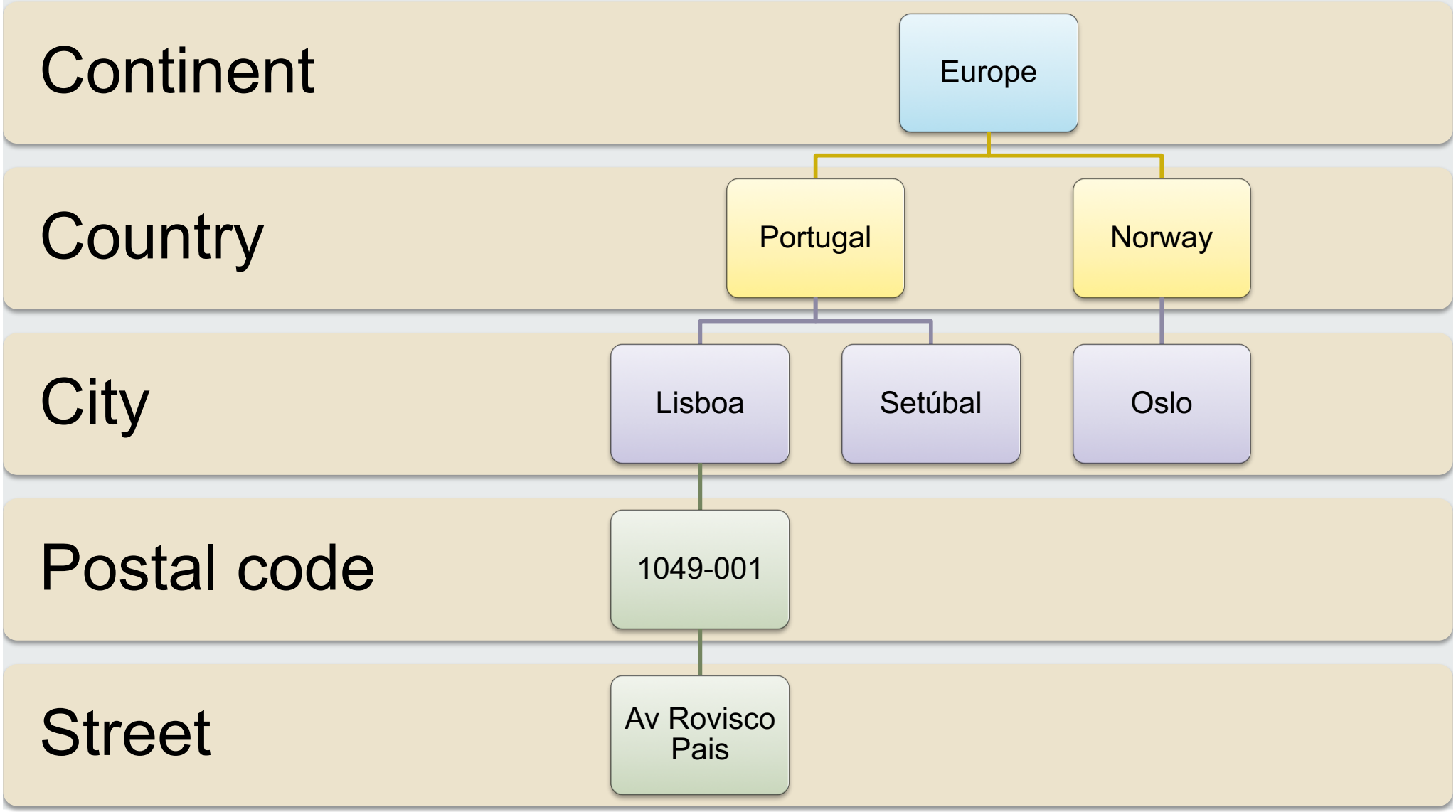






Local Granularities



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What about numerical data?

Discretization

Numeric Discretization

Transforms real-numbered into interval-based data

Equal-width

Partitions the range of A into k ***equal-width*** intervals.

Width corresponds to A's range divided by k

$$w = \frac{a_{max} - a_{min}}{k}$$

i^{th} interval boundary v_i is

$$v_i = a_{min} + iw, \forall i = 1, \dots, k-1$$

Equal-frequency

Divide the range of A into intervals containing approx. the same number of points, same **frequency**.

Each interval contains $1/k$ **of the probability mass**, and can be computed by the inverse cumulative distribution function $\hat{F}_A^{-1}$

i^{th} interval boundary v_i is

$$v_i = \hat{F}_A^{-1}\left(i/k\right), \forall i = 1, \dots, k-1$$

$$\hat{F}_A^{-1}(q) = \{a | P(A \leq a) \geq q\}, \quad for \ \ q \in [0,1]$$

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DATA DISTRIBUTION

Univariate analysis

Central Tendency

- **Mean** (algebraic measure) (sample vs. population):

  Note: *n* is sample size and *N* is population size.

  - Weighted arithmetic mean
  - Trimmed mean: chopping extreme values

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \mu = \frac{\sum x}{N}$$

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

- **Median**:
  - Middle value if odd number of values, or average of the middle two values otherwise
  - Estimated by interpolation (for *grouped data*):

$$median = L_1 + (\frac{n/2 - (\sum freq)l}{freq_{median}})width$$

- **Mode**
  - Value that occurs most frequently in the data
  - Unimodal, bimodal, trimodal
  - Empirical formula:

$$mean - mode = 3 \times (mean - median)$$

age	*frequency*
1–5	200
6–15	450
16–20	300
21–50	1500
51–80	700
81–110	44

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- **Median**:
  - Middle value if
    middle tw
  - Estimated

$$med$$

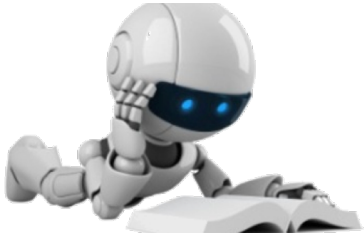
- **Mode**
  - Value that occur
  - Unimodal, bimoda
  - Empirical formula:

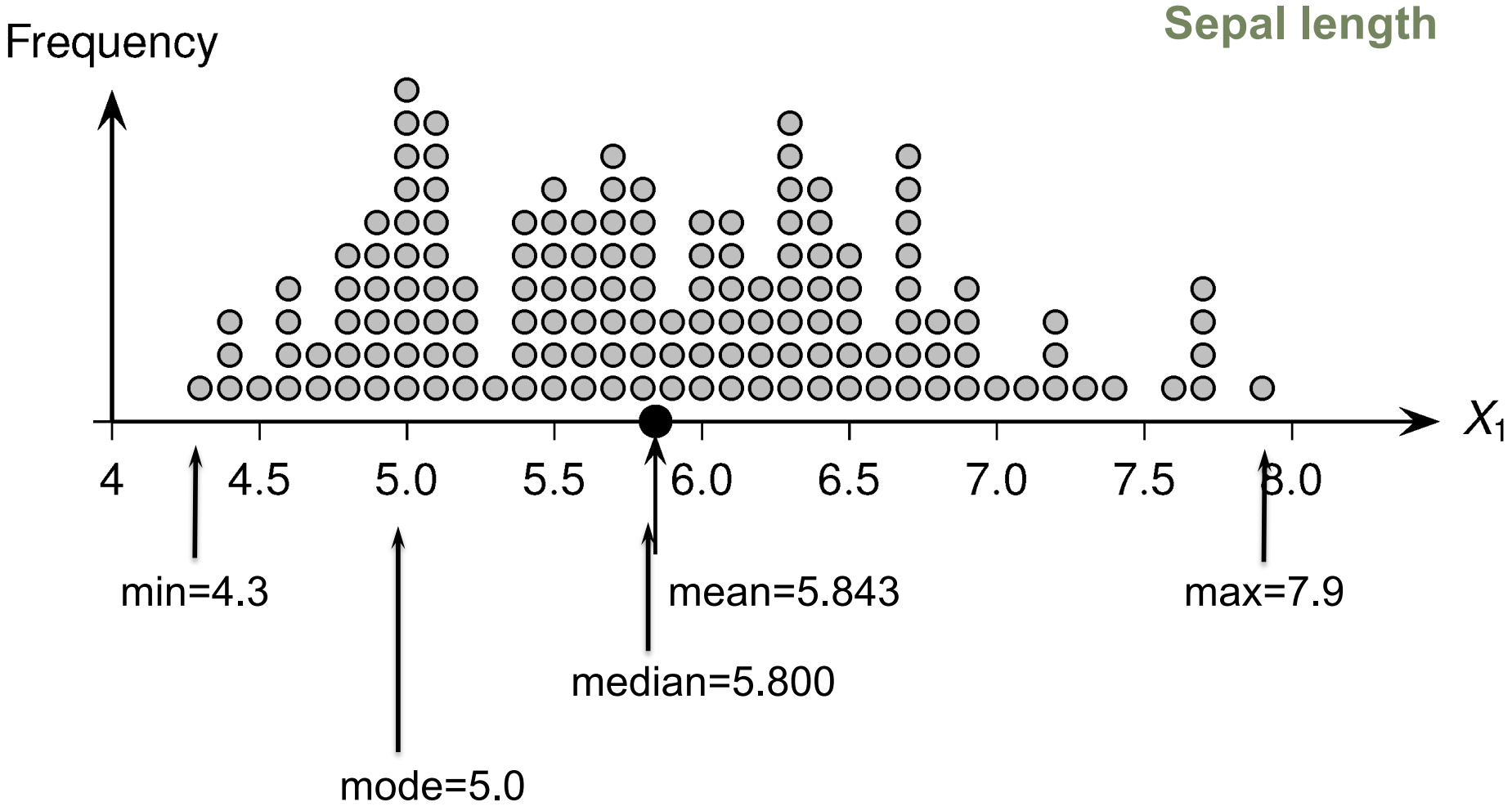
$$mean - mode = 3 \times (mean - median)$$

The median is robuster, because its value is not distorted by outliers

age	*frequency*
1–5	200
6–15	450
16–20	300
21–50	1500
51–80	700
81–110	44

IRIS EXAMPLE





Measuring Dispersion

Variance and standard deviation

- (*sample: s, population: σ*)
- **Standard deviation** σ is the square root of variance σ^2

$$\sigma^2 = \frac{1}{N}\sum_{i=1}^{n}(x_i - \mu)^2 = \frac{1}{N}\sum_{i=1}^{n}x_i^{\,2} - \mu^2$$

$$s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2 = \frac{1}{n-1}[\sum_{i=1}^{n}x_i^{\,2} - \frac{1}{n}(\sum_{i=1}^{n}x_i)^2]$$

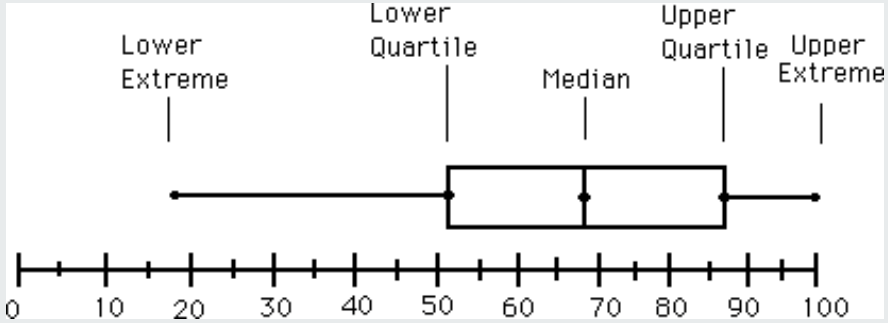
Quartiles

- **Quartiles**: Q_1 (25th percentile), Q_3 (75th percentile)
- **Inter-quartile range**: **$IQR = Q_3 - Q_1$**

BOXPLOT ANALYSIS

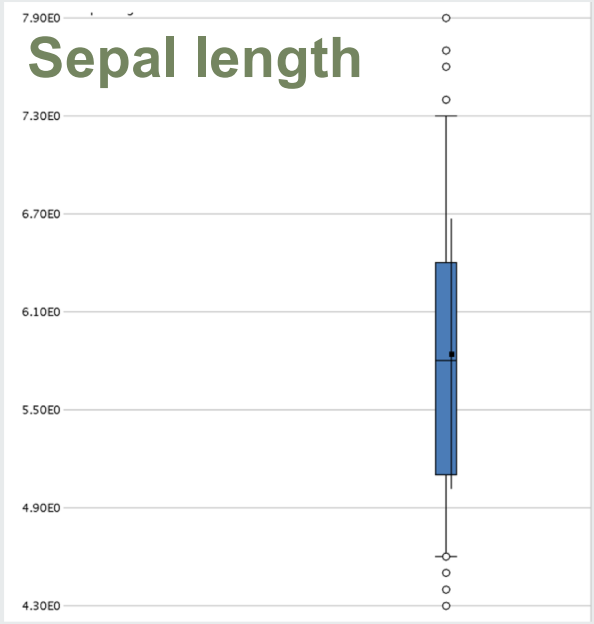
Five-number summary of a distribution

- Min, Q1, Median, Q3, Max

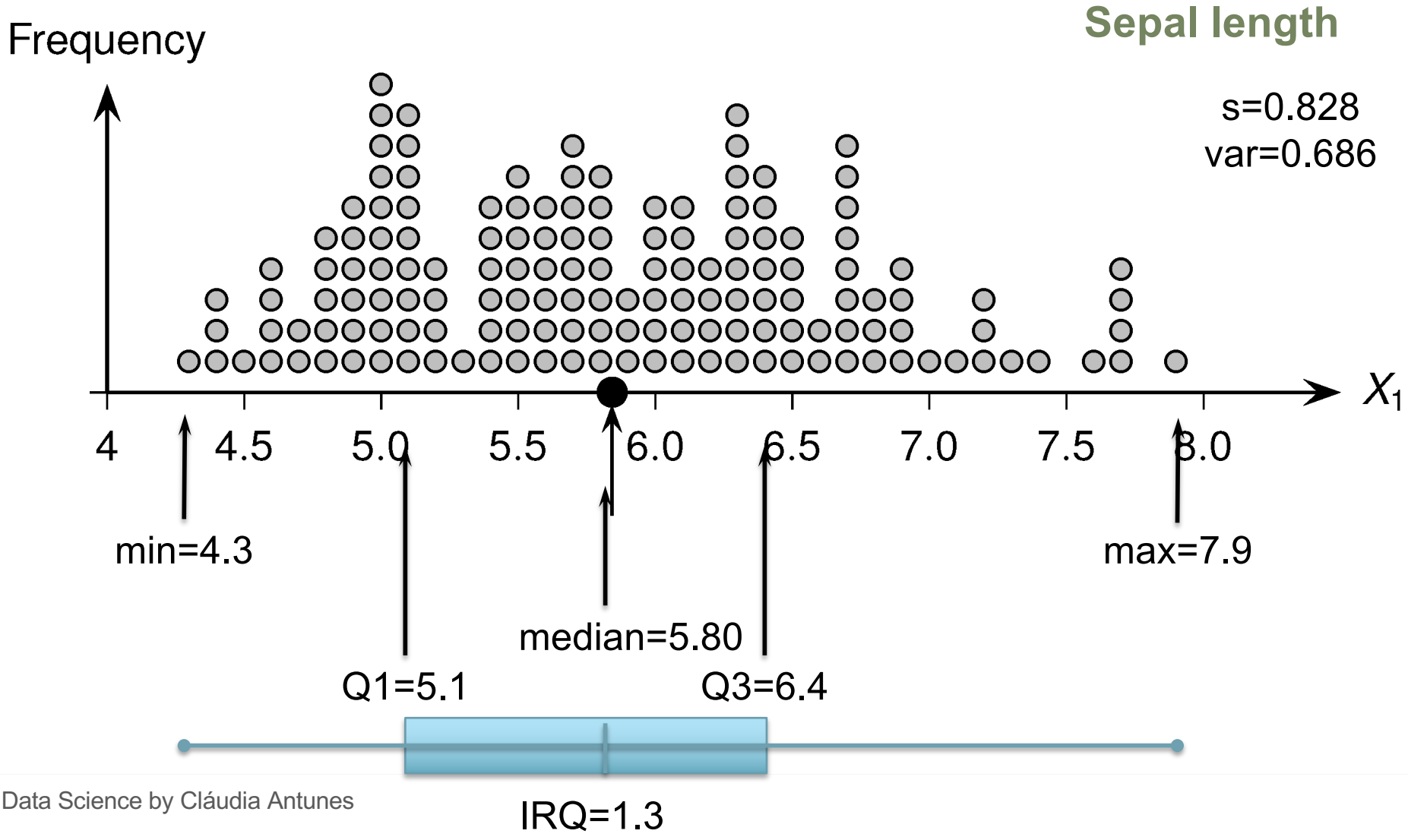


Boxplot

- Data is represented with a box
- The ends of the box are at **Q1** and **Q3**
- The **median** is marked by a line within the box
- Whiskers: two lines outside the box extended to **Min** and **Max**



IRIS EXAMPLE



OUTLIERS

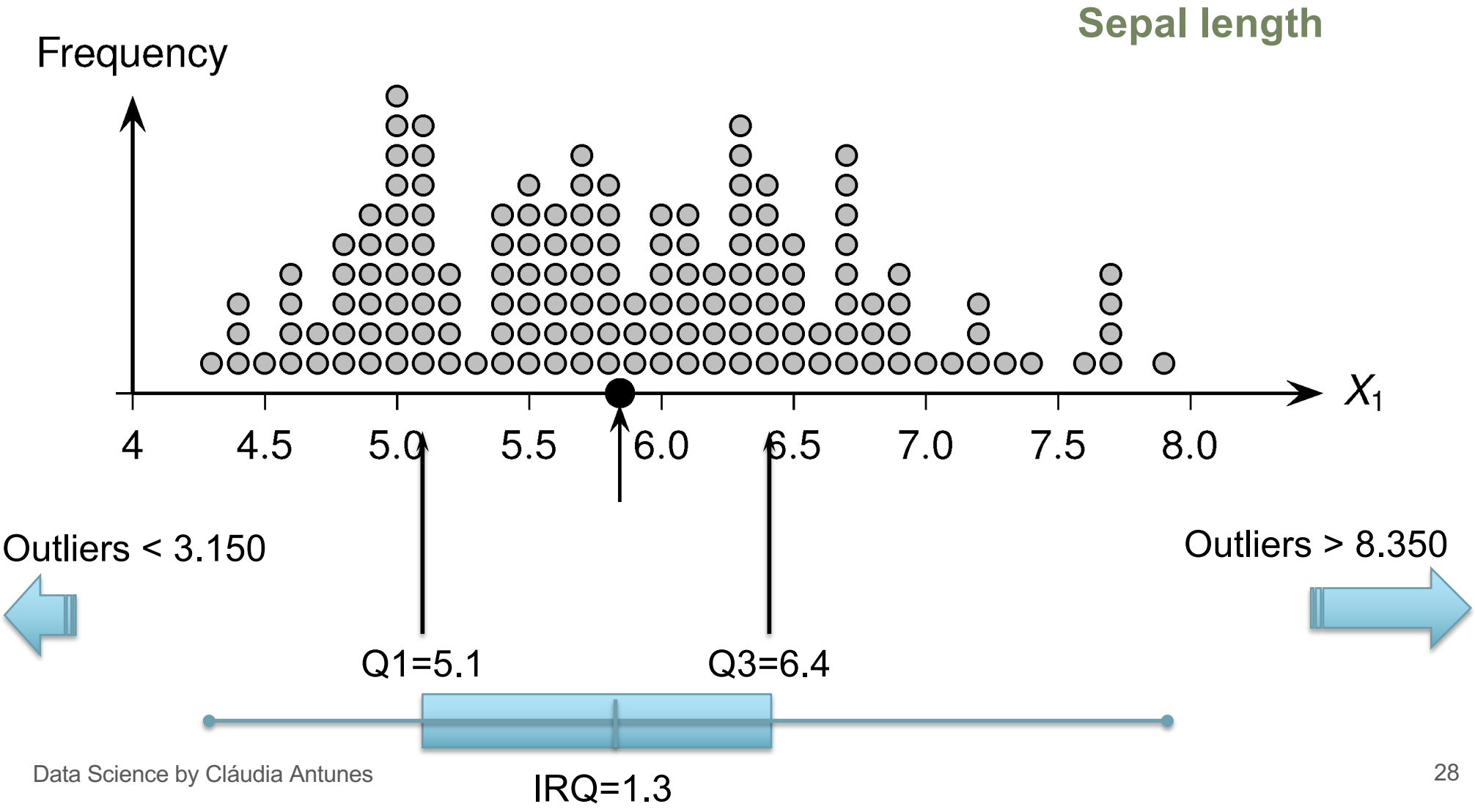
Outliers

- values that are very large or small and very uncommon;
- points beyond a specified threshold

If is a value lower than **Q1 - 1.5 x IQR**

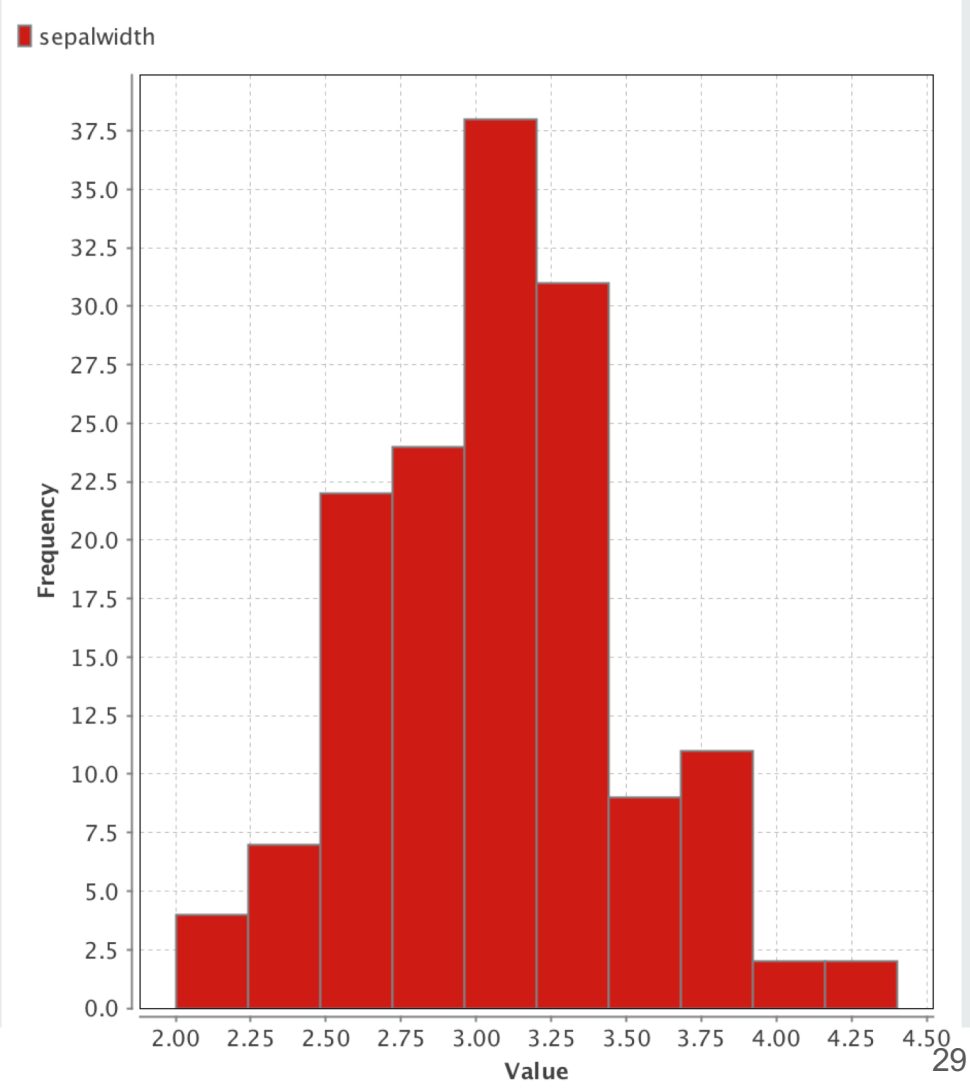
If is a value higher than **Q3 + 1.5 x IQR**

IRIS EXAMPLE



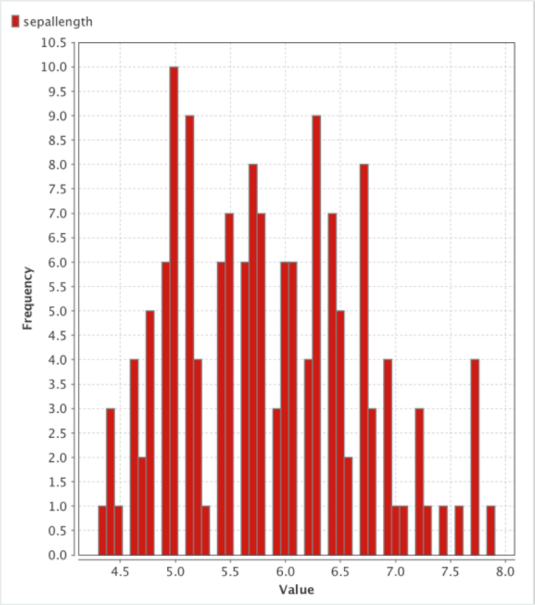
DISTRIBUTION

- A common visualization is the **frequency histogram**
  - It plots the relative frequencies of values in the distribution
- To construct a histogram
  - Divide the range between the **highest** and **lowest** values into **equal size bins**
  - Toss each value in the appropriate bin
  - Each bar in the histogram represents the number of values in the corresponding bin

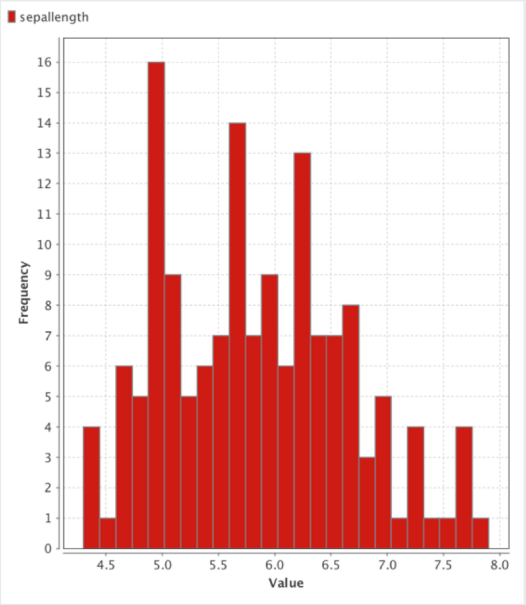


HISTOGRAMS

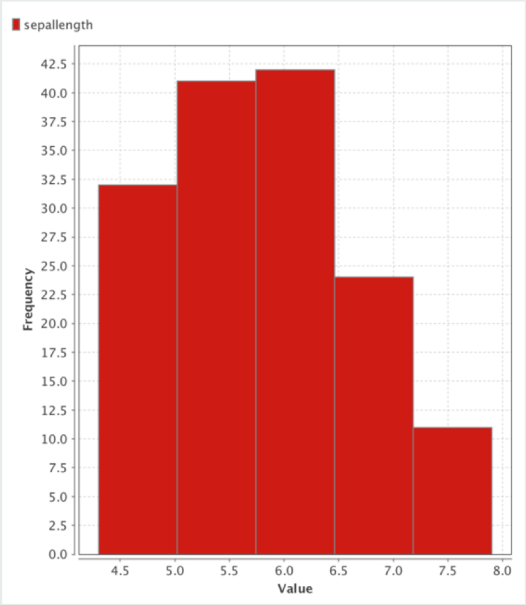
- The choice of bin size affects:
  - The details we see in the frequency histogram
    - Changing the bin size to a lower number illuminates things that were previously not seen
  - The one‘s perception of the shape of distribution



50 bins

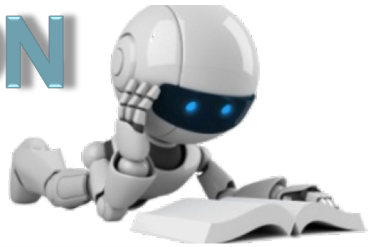


25 bins

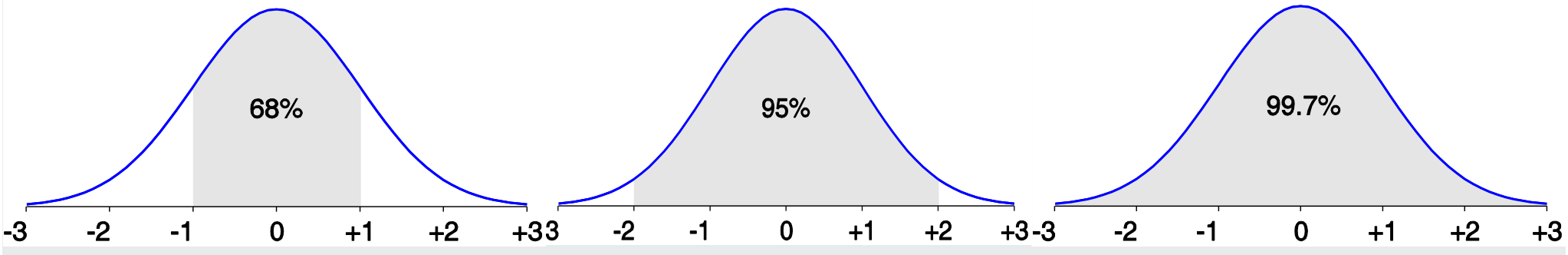


5 bins

Normal Distribution Properties

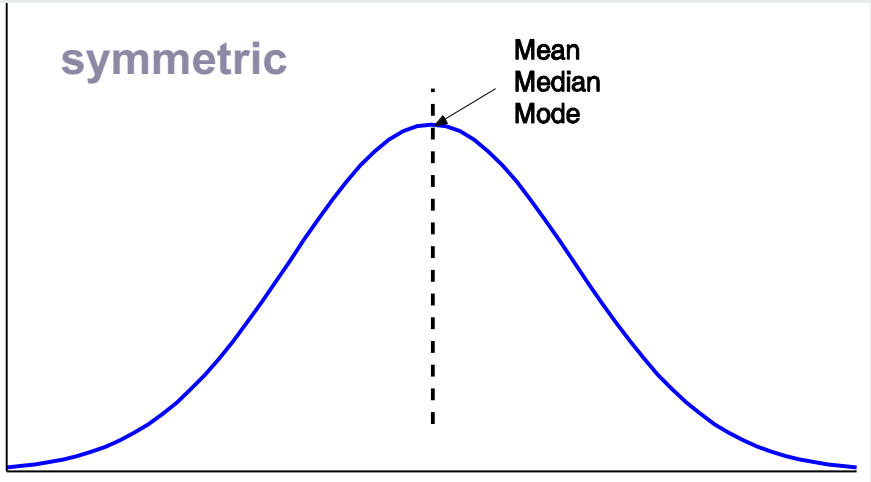


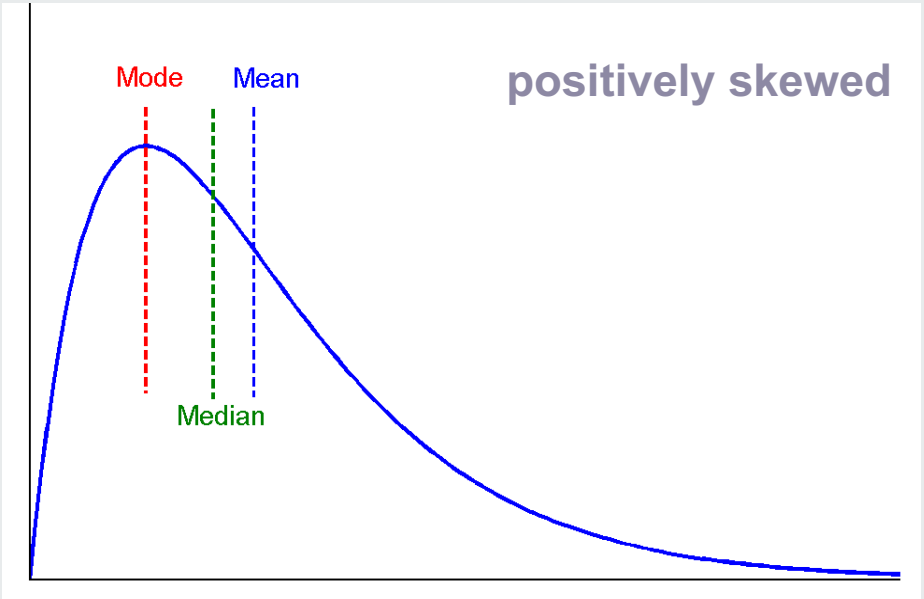
- The normal curve $N\sim(\mu, \sigma^2)$
  - **$[\mu-\sigma, \mu+\sigma]$** contains about 68% of the records
  - **$[\mu-2\sigma, \mu+2\sigma]$** contains about 95%
  - **$[\mu-3\sigma, \mu+3\sigma]$** contains about **99.7%**

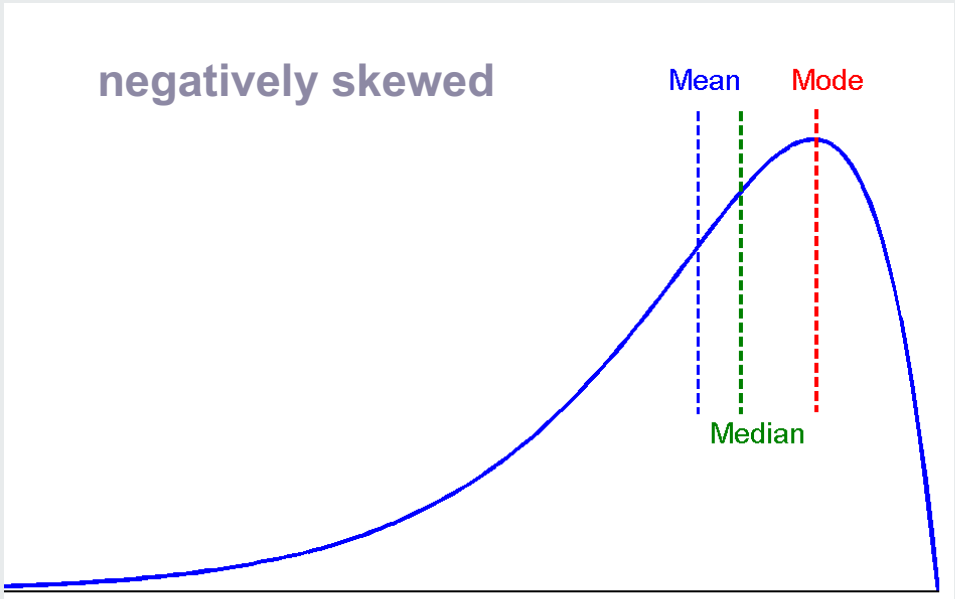


SYMMETRIC X SKEWED

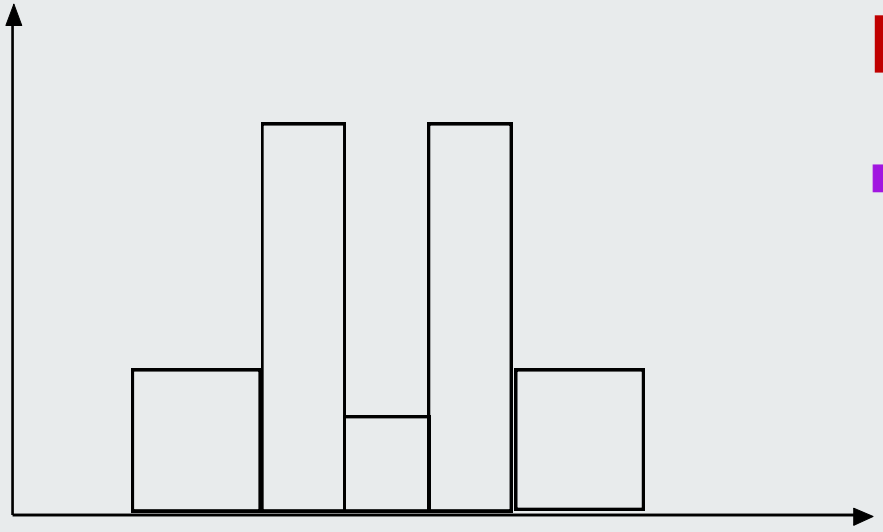
- Median, mean and mode of symmetric, positively and negatively skewed data

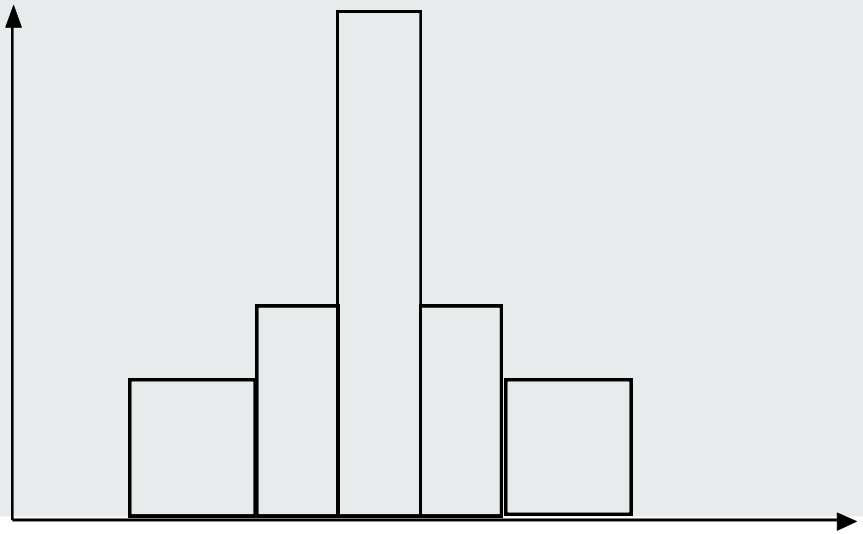






HISTOGRAMS X BOXPLOTS





BE CAREFUL:

- The two histograms shown in the left may have the same boxplot representation
  - The same values for: min, Q1, median, Q3, max
- But they have rather different data distributions

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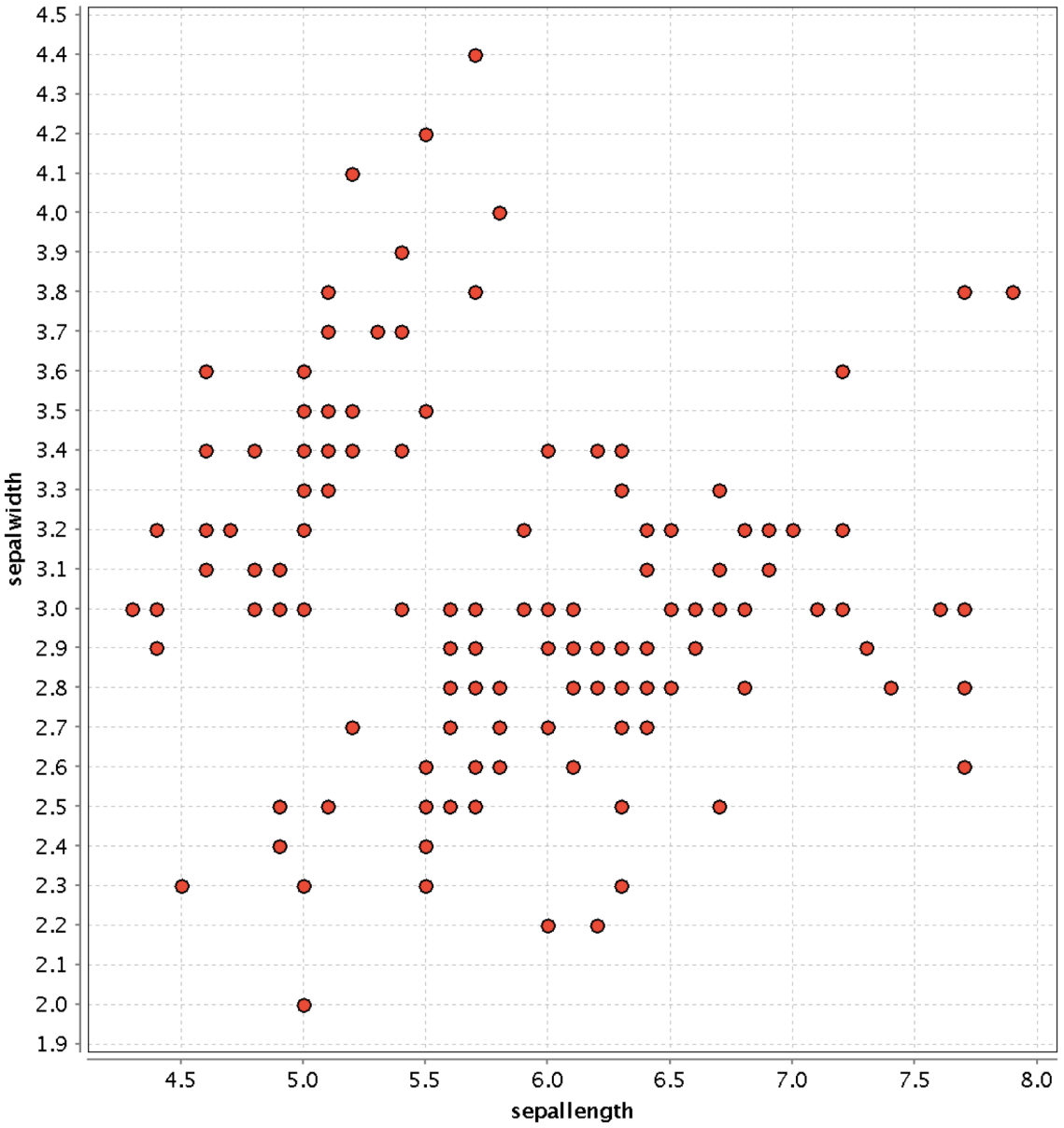
DATA SPARSITY

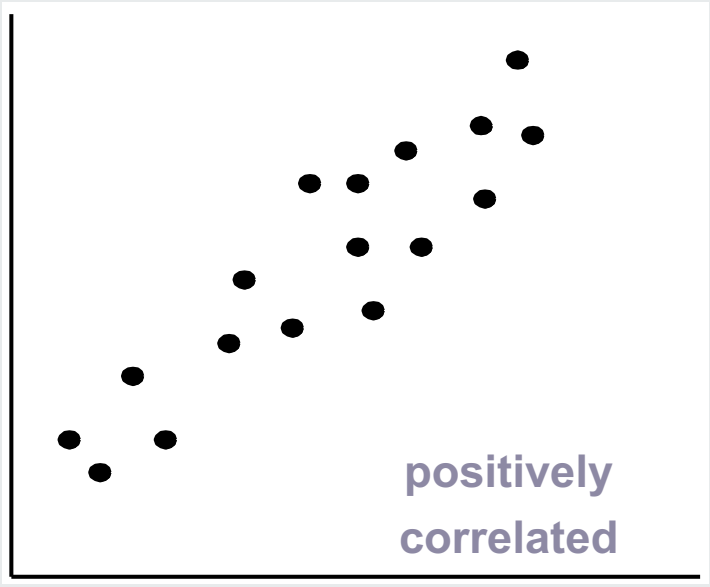
Multivariate analysis

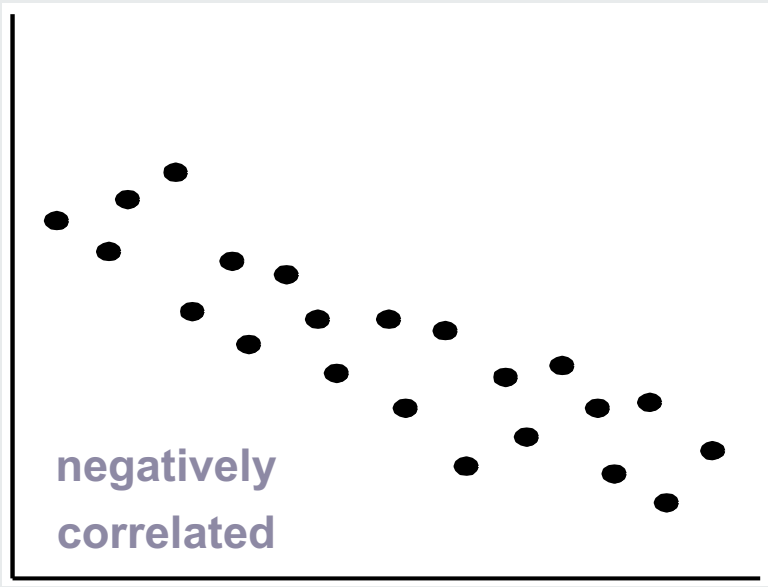
SCATTER PLOT

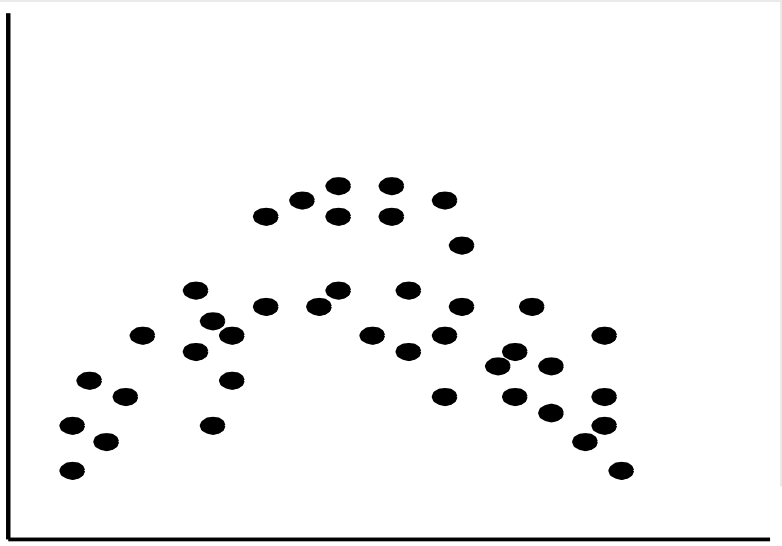
- Provides a first look at bivariate data to see clusters of points, outliers, etc
- Each pair of values is treated as a pair of coordinates and plotted as points in the plane



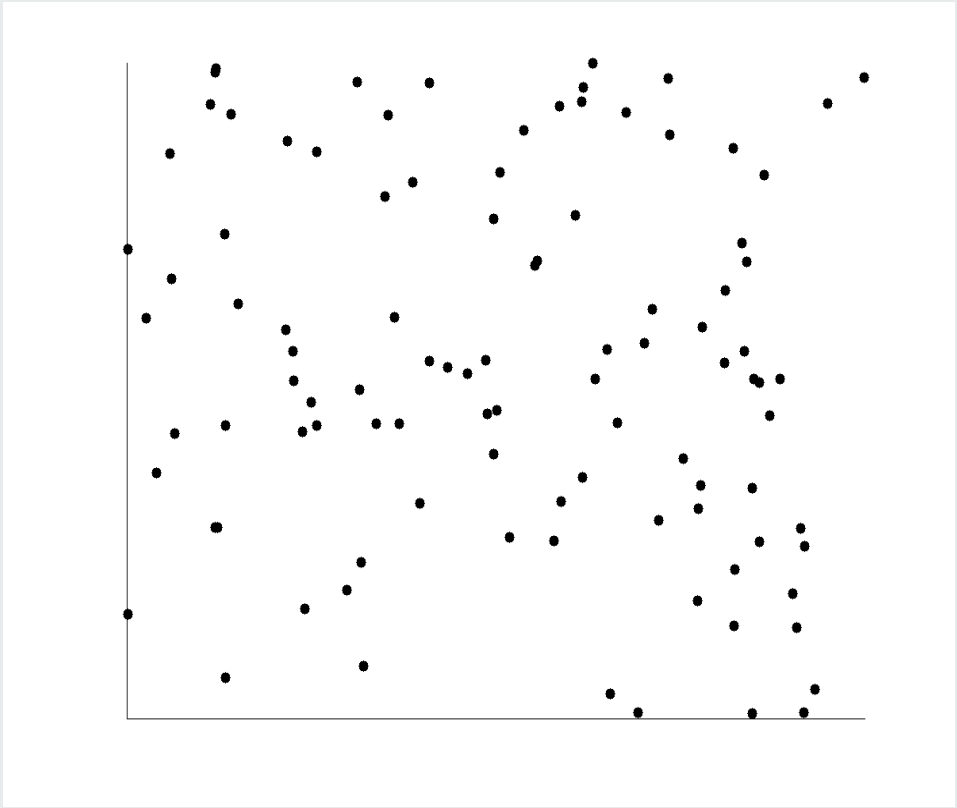
Positively and Negatively Correlated Data

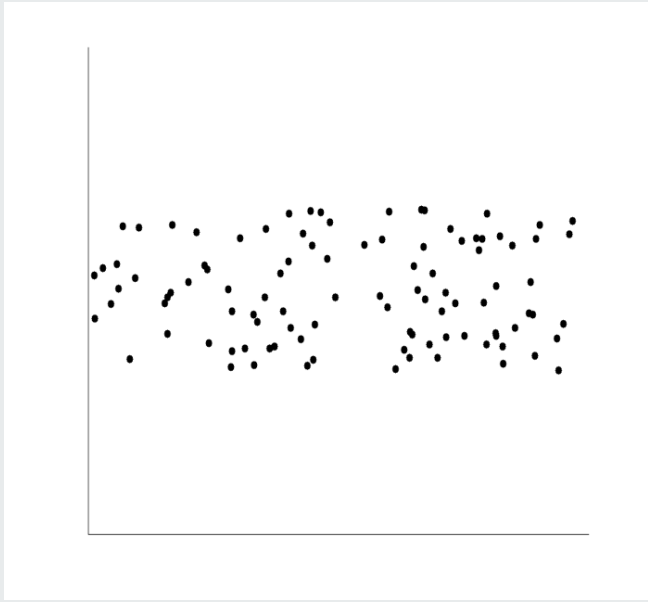


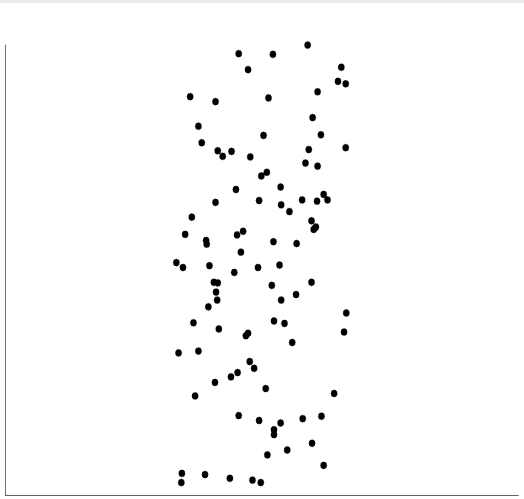


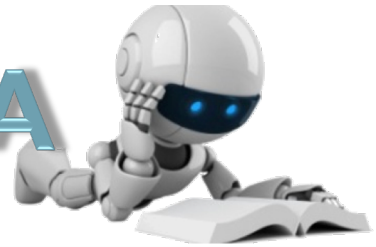


Uncorrelated Data









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DIMENSIONALITY

DIMENSIONALITY

- Usually, it corresponds to **the number of attributes** describing the data (***extrinsic dimensionality***)

$$dim(D)=d$$

- However, it can be lower, say k, when some of the attributes are not linearly independent

$$k<<d$$

Data Reduction

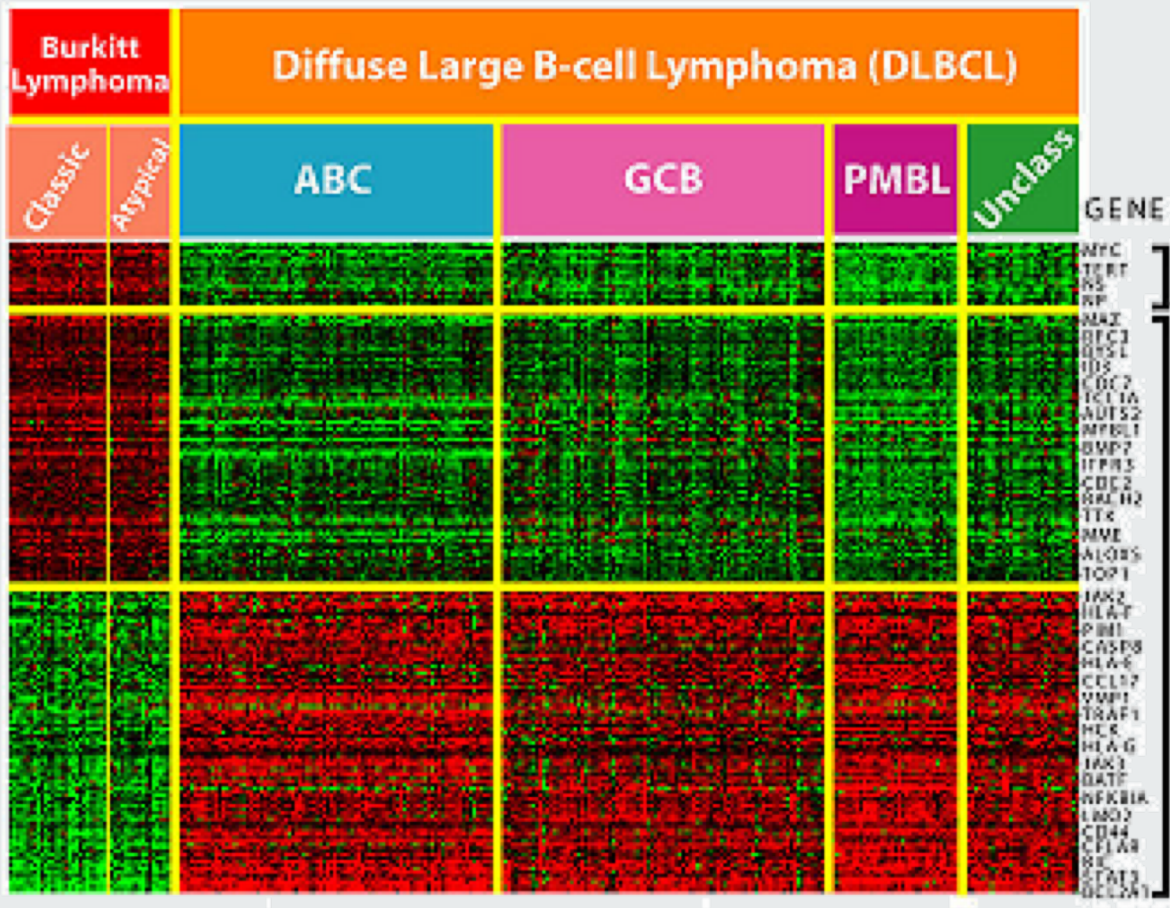
k is called the ***intrinsic dimensionality*** of the data.

Issues

High Dimensionality

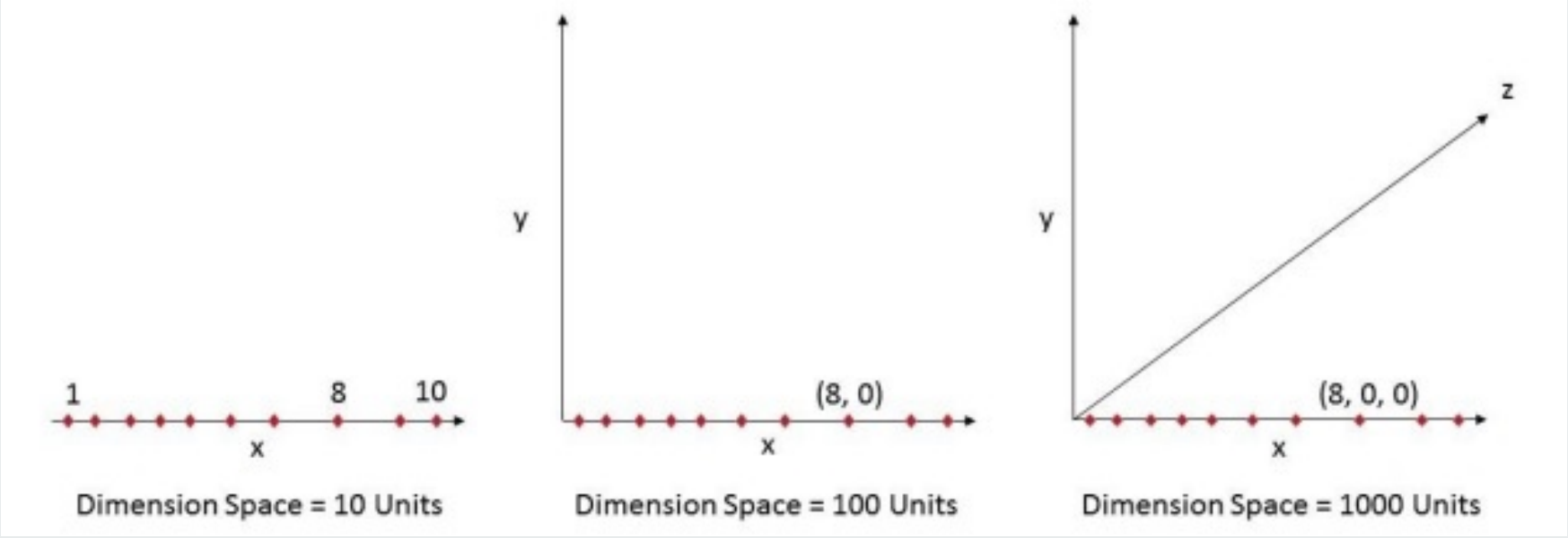
Sometimes, dimensionality d is much larger than the number of records n

$$n << d$$



Issues

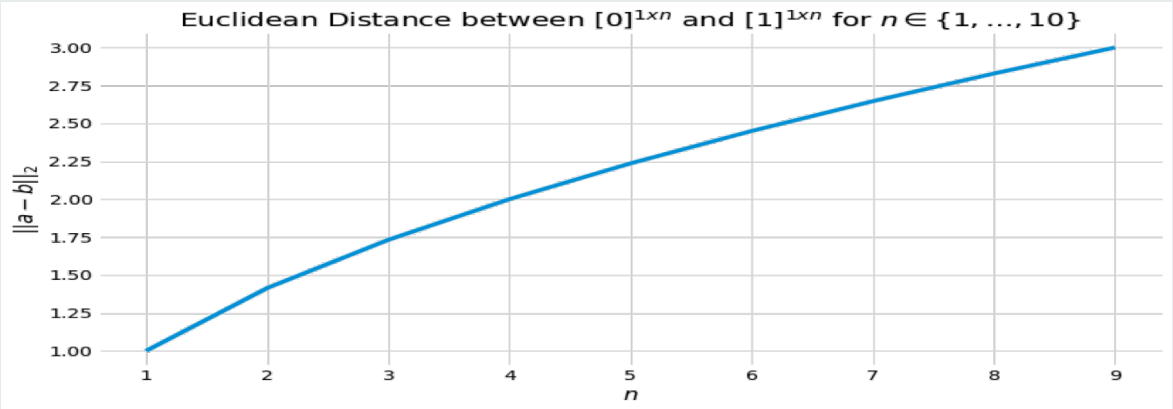
- Points in high-dimensional space are **highly sparse**



$$|1-0| = 1$$
$$\|(1,1)-(0,0)\| = \sqrt{2}$$
$$\|(1,1,1)-(0,0,0)\| = \sqrt{3}$$

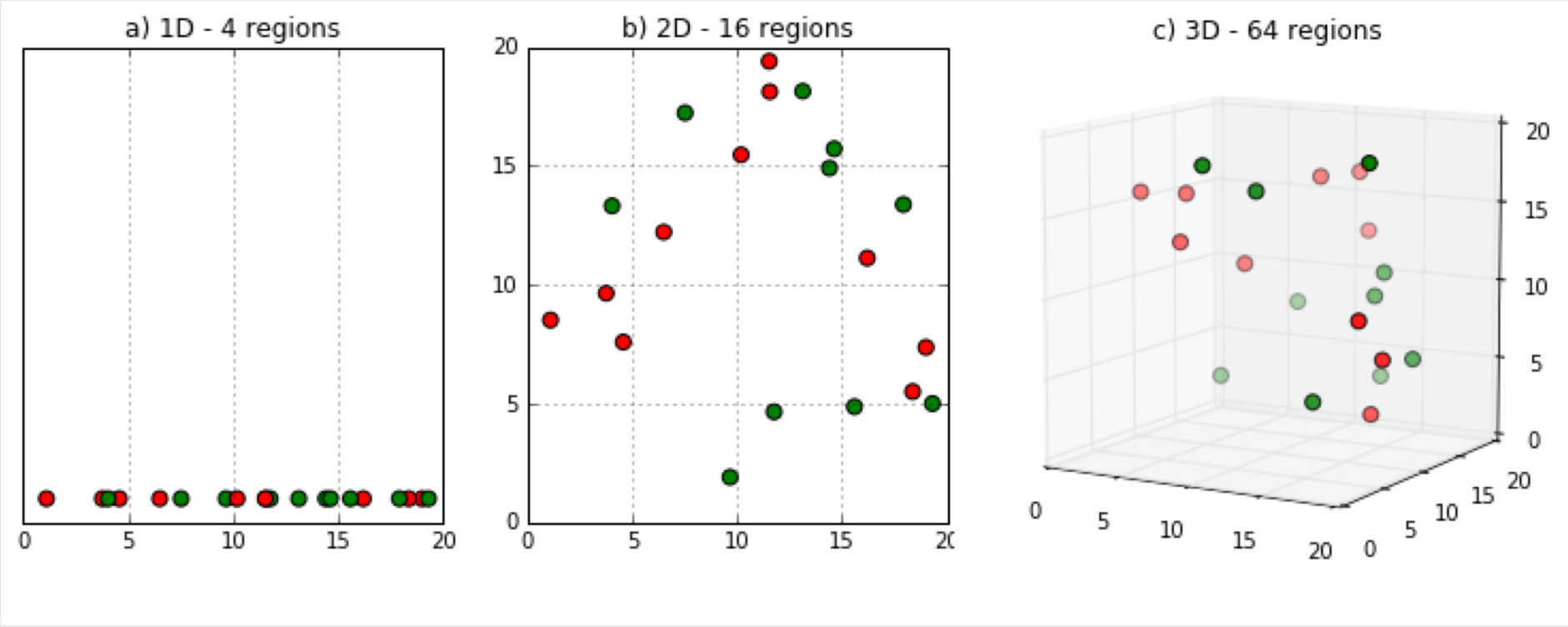
...

$$\|[\![1]\!]^{1\times 10} - [\![1]\!]^{1\times 10}\| = 3$$



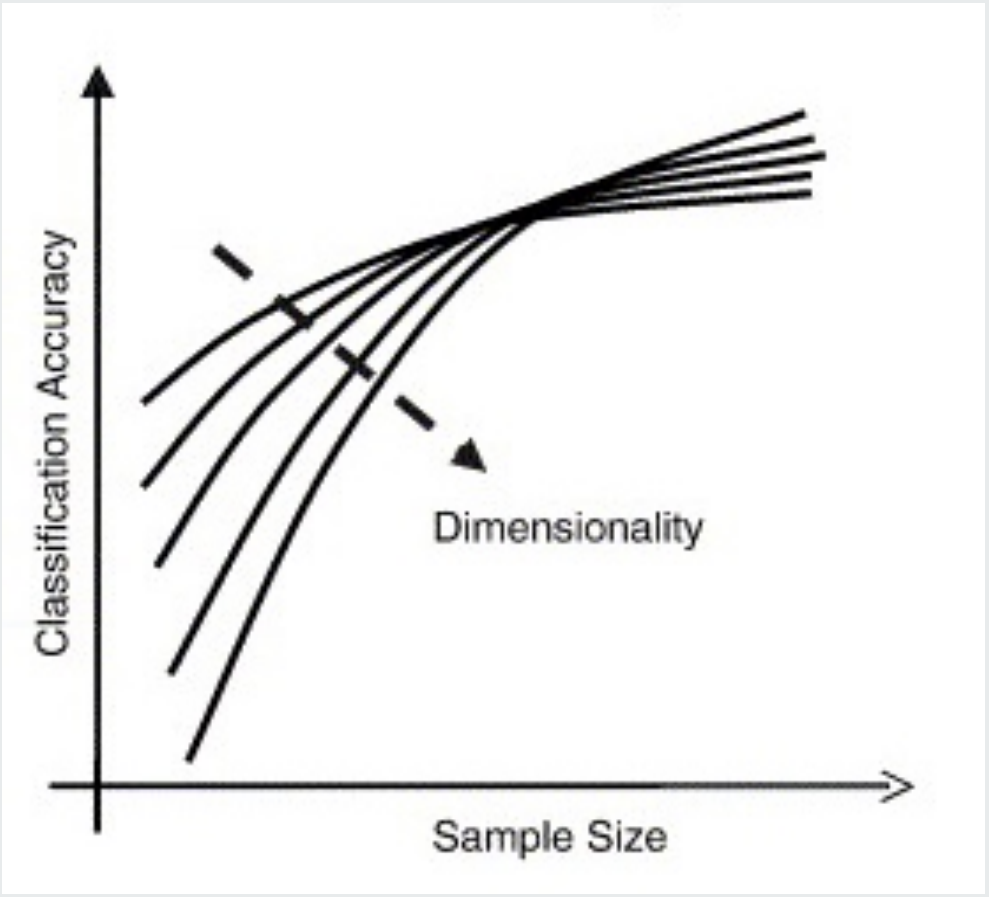
ISSUES

- *"As the number of attributes (dimensions) grows, the amount of data to constitute a sample grows exponentially."*



CURSE OF DIMENSIONALITY

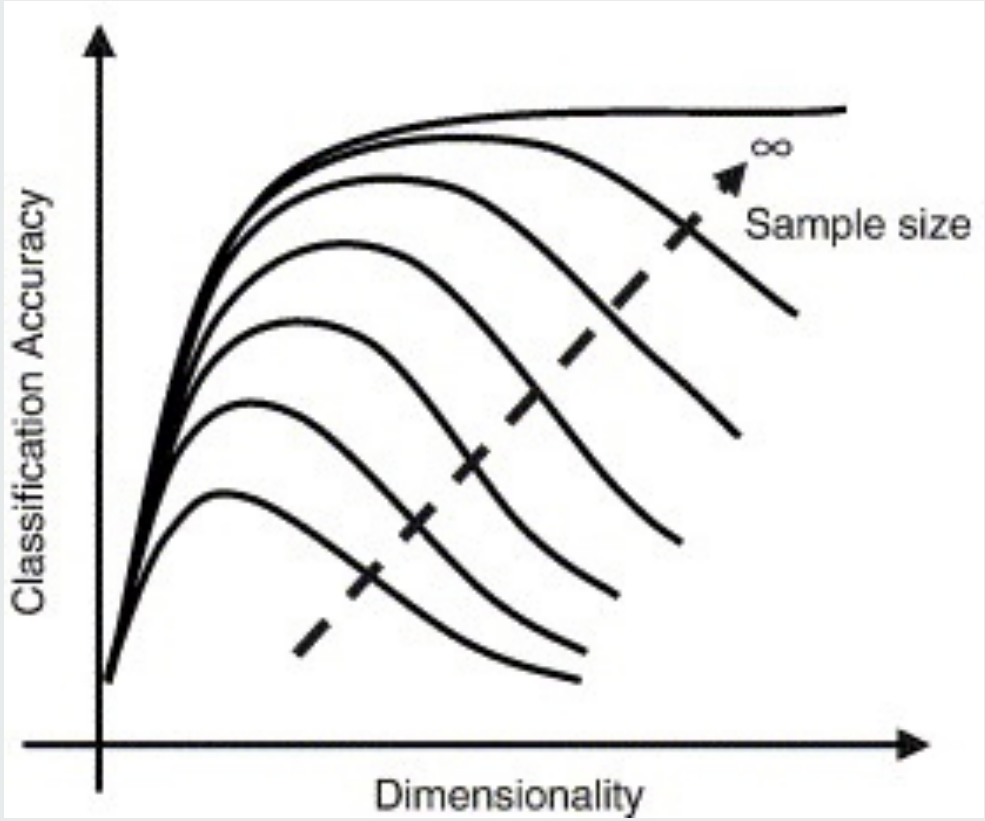
✦ *"As **the number of attributes (dimensions) grows**, the amount of data we need to generalize accurately **grows exponentially**."*



Larger the dimensionality ➔ larger the sample

HUGHES PHENOMENON

- Given a fixed number of records, **the predictive power** of a model **increases** with **the increase of the number of dimensions** until it reaches a maximum value, but then **it starts decreasing**



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