Managing Big Data

Preliminaries: About Algorithms and Data

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Asymptotic analysis of algorithms

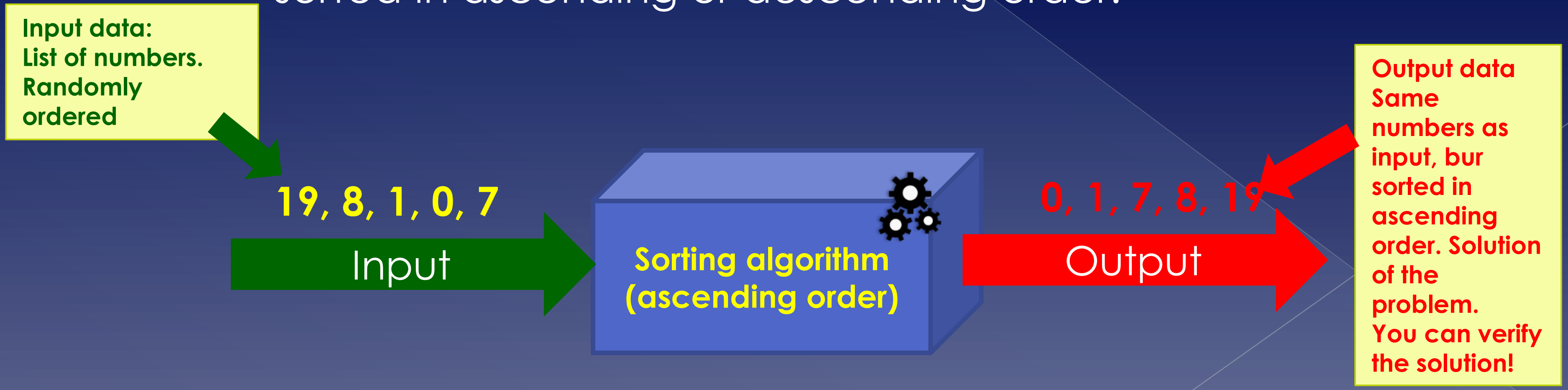
- Computers are machines that through programs can solve many problems including
  - Sorting (ascending/descending) of numbers, strings, dates etc.
  - Finding the roots of polynomials like $x^7+3x^4+2=0$ e.g. by applying the Newton-Raphson method
  - Solving system of linear equations e.g. by using the Gauss-Jordan elimination
  - Calculate functions such as Sine, Cosine, Logarithms etc using e.g. Taylor and McLaurin Series
  - ...and many more (but not all ☹)

Asymptotic analysis of algorithms

- Steps to solve a problem using computers
  - **Write** the appropriate program
    - E.g. To find the roots of some polynomial, write a program that implements the Newton-Raphson method
  - **Give** the program the appropriate input i.e. required data
  - **Execute** the program on the computer with the data provided
  - After some time, **the program will emit (on screen/disk) the solution** to the problem (output)
    - E.g. in case of finding the roots of a polynomials, it will show the roots. You can verify the solution, i.e. roots
  - **You can always verify the solution**

Asymptotic analysis of algorithms

- In our context «Program = Algorithm»
  - What's an algorithm? = a well defined order of commands and operations (steps) that when executed by machines called computers and given the appropriate input can solve a particular problem on it's output.
    - «**Solve a problem**»: the algorithm on it's output will produce data which are the solution to the problem (as it has been defined).
    - Example: Algorithm which sorts numbers: it's a set of commands/operations that when given as input a random list of numbers will produce as output the same numbers sorted in ascending or descending order.


Input data:
List of numbers.
Randomly ordered
19, 8, 1, 0, 7
Input
Sorting algorithm (ascending order)
0, 1, 7, 8, 19
Output
Output data Same numbers as input, bur sorted in ascending order. Solution of the problem.
You can verify the solution!

Asymptotic analysis of algorithms

- There **exist algorithms** that solve many, many problems:
  - Calculate the average of a set of numbers
  - Calculate sine, cosine, logarithm of a number
  - Find min, max, median, stdev etc from a set of numbers
  - Find the roots of a polynomial
  - Find solution(s) of a system of linear equations
  - Find a particular character in a string
  - Find webpages that contain the word "economics"
  - …and many, many more
- Problems for which there exist an algorithm that solve them (correctly) are called **"Decidable"** ☺

Asymptotic analysis of algorithms

- But not all! Unfortunately there are some problems for which there **exist NO algorithm** that can solve them. E.g.
  - "**Halting problem**": whether or not an algorithm with some input will terminate or not (i.e. crash). Such algorithm (currently) does not exists.
  - "**Matrix mortality problem**": Given a finite set of nxn matrices, is there a way of multiplying them (with or without repetition) that will result in the zero matrix? Such algorithm (currently) does not exist.
- Problems for which there are no algorithms that can solve them are called **"Undecidable"** ☹

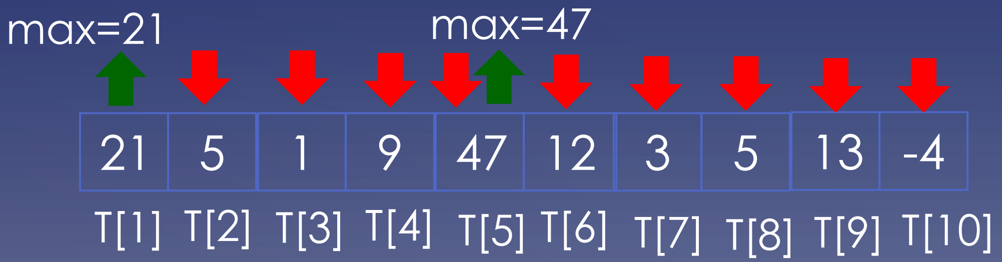
Asymptotic analysis of algorithms

- Example of algorithm?

Simple algorithm that finds the greatest number in an array of numbers.
Input: **Array with 10 random numbers**
Output: **The greatest number (max) contained in the input numbers**

Order of execution

```
Step 1:  Read 10 numbers from user (keyboard) and insert these numbers in an array T such
         that T[1] contains the first number given and T[10] the last number given
Step 2:  Assume that the greatest number is the number in the first position of the array
         i.e. T[1]. Store this number in a variable called max: max=T[1].
Step 3:  For each position of array T, starting from 2 up until position 10 of the array T
         do the following:
Step 4:      Compare number in current array position with max. If current position of
             array has number greater than max then:
Step 5:          Store in variable max the number in current position of array
Step 6:  Output on screen the variable max. This will be the greatest number in array T.
```



🟥	= Compare with max
🟩	= Replace max. Found new max

Asymptotic analysis of algorithms

- Same algorithm in a real programming language (Python)

Simple algorithm that finds the greatest number in an array of numbers.
Input: **Array with 10 random numbers**
Output: **The greatest number (max) contained in the input numbers**

Order of execution

```
#Array T will hold the numbers
T=[]                                                          Step 1
#Ask for 10 numbers from user.
for i in range (0, 10):                                       Step 2
    number = int (input("Give me the number: ") )             Step 3
    T.append(number)                                          Step 4

#Ok. Got 10 numbers. Do your thing now.
#Set as max the first number. In python, array indices start at 0, not 1!
currMax = T[0]                                                Step 5
i=1                                                           Step 6
while (i < len(T)):                                           Step 7
       #Is current position T[i] greater than currMax?
       if ( T[i] >= currMax ):                                Step 8
            #Yes, it is! Found a new max value
            currMax = T[i]                                    Step 9
       #advance to next element in array
       i = i + 1                                              Step 10

print("The result is: ", currMax)                             Step 11
```

Asymptotic analysis of algorithms

- An algorithm can be represented in many ways (form does not matter)
  - Pseudocode (first example)
  - Programming language (second example)
- ...as long as
  - Specifies concrete steps
  - Takes well defined input
  - Each step can be executed by the machine (computer)
  - Solves (correctly) the problem at the output

Asymptotic analysis of algorithms

- For a given problem there might be two or more different algorithms that solve the problem
  - Different? They execute different set of steps
- For example we can come up with two different algorithms for finding the greatest number in a list
  - Earlier example

Asymptotic analysis of algorithms

Two different algorithms solving the "find greatest number" problem

First algorithm (see previously)

Step 1: Set as max the first element of the list

Step 2: Compare other elements with current max

Step 3: If current max is smaller than current element, set current element as max

Step 4: If all elements of list have been compared, output max. This will be the greatest number. Output it and terminate.

Second algorithm

Step 1: Compare first element with all other elements of table to see if this is greater than all other elements

Step 2: If it is, then output first element as greatest and terminate.

Step 3: If first element is not the greatest, compare second element to all other elements to see if this is greater than all other elements

Step 4: If it is, then output second element as greatest and terminate.

…

Step 19: Display last element of list as the largest number (no need to compare).

Both algorithms solve the problem (correctly)!

Asymptotic analysis of algorithms

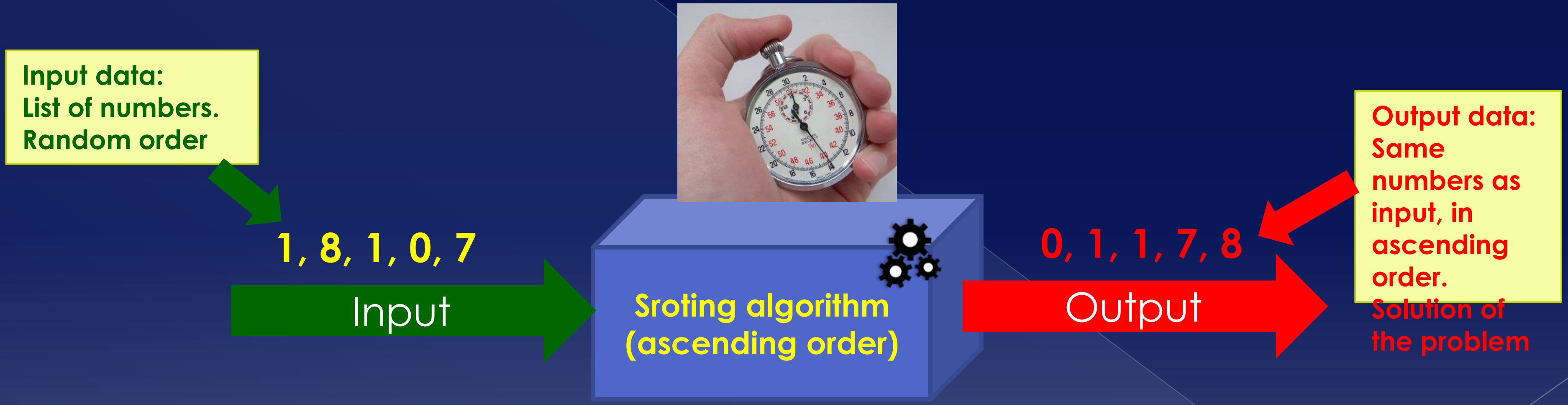
- Many different algorithms that solve the same problem
  - E.g. Sorting algorithms (numbers, strings, dates etc):
    - **BubbleSort**
    - **QuickSort**
    - **HeapSort**
    - **MergeSort**

Asymptotic analysis of algorithms

- Since there might be different algorithms that solve the same problem, **which algorithm is better?**
  - **What does "better" mean?** Here it means "**faster**" i.e. which algorithm solves a given problem in the shortest time (= Execution time of algorithm)
    - Many different interpretations of "better": in terms of execution time, space used etc.
  - Of course we are interested in solving the problem quickly
    - An algorithm A solving a problem in less time than algorithm B, is faster and hence in our context is better.
- To answer such questions, we need to answer another important and related question:
  - ***How to measure the execution time of algorithms? What is the best metric to assess the time needed by an algorithm to solve a problem?***
    - One approach: use real time (measured in min, sec, msec, ns etc) . Measuring the real time elapsed: when the algorithm starts executing until it produces the solution of the problem on the output and terminates

Asymptotic analysis of algorithms

- Is time (measured in min, sec, msec etc) a good metric for assessing the execution speed of algorithms?



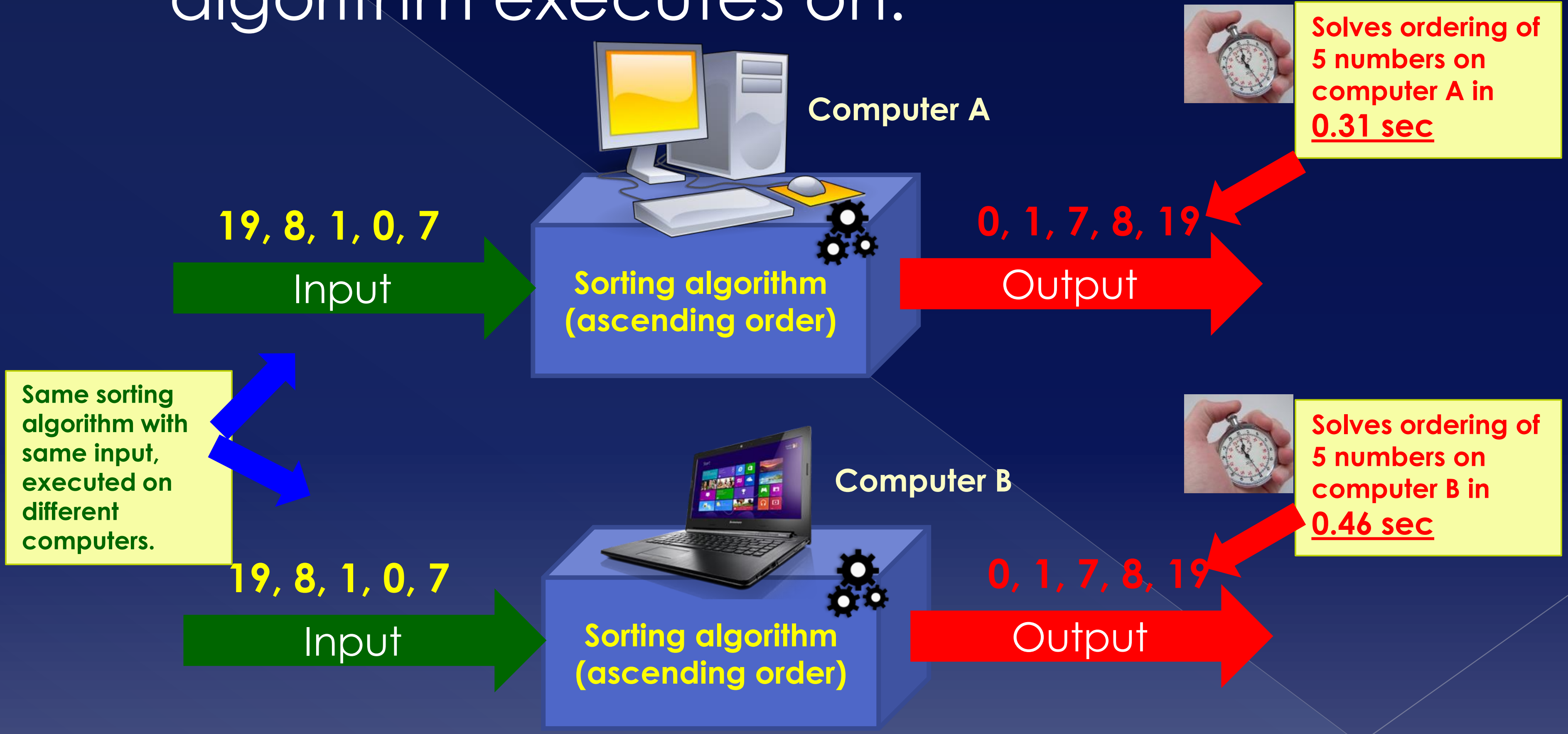
- It's one (valid) approach. Used today in many practical situations.

Asymptotic analysis of algorithms

- But, using the (real) time as a metric to assess running time of algorithms, **is not the best idea**. This, for two reasons:
  - Measured that way, running time depends on the computer/machine the algorithm runs on
  - Time does not tell us how the running time of an algorithm is affected, when the size of input data changes
- Using time as the metric, makes it difficult to **compare algorithms in a systematic way**.

Asymptotic analysis of algorithms

- 1) Time depends on computer the algorithm executes on.



Solves ordering of 5 numbers on computer A in <u>0.31 sec</u>

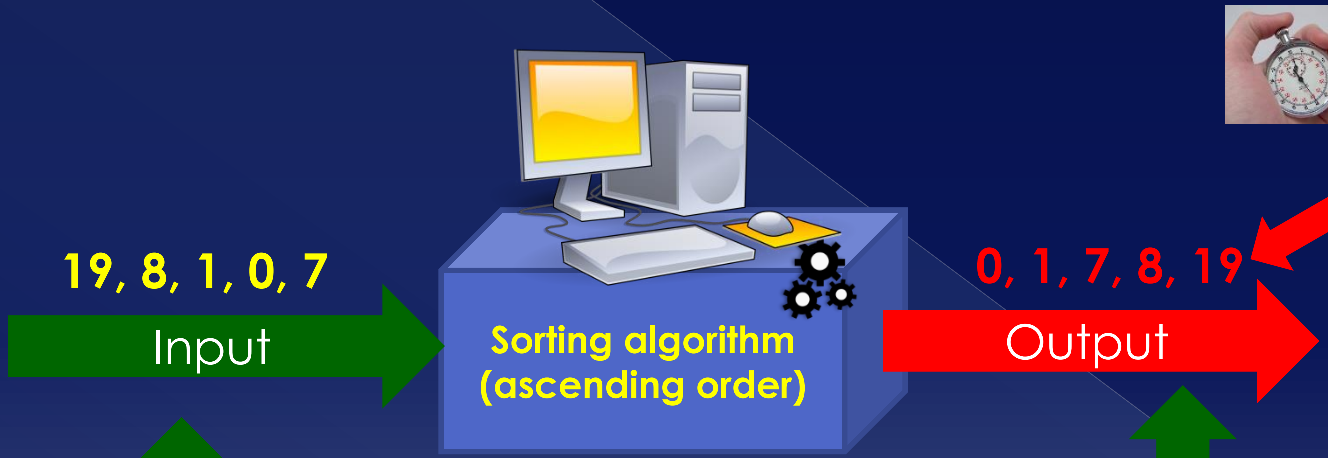
Solves ordering of 5 numbers on computer B in <u>0.46 sec</u>

Same sorting algorithm with same input, executed on different computers.

<u>What is the execution time of the algorithm (same in both situations)? The average? What if the same algorithm executes on another computer and sorts these 5 numbers in say 0.08 secs?</u>

Asymptotic analysis of algorithms

- 2) Time dos not tell us what happens, when input data changes e.g. is increased in size.



Solves ordering of 5 numbers on computer A in <u>0.3 sec</u>

If we double the input numbers that need to be sorted by the same algorithm e.g. 19,8,1,0,7,-1, 13, 7, 1, -91 ...

Then

...will the execution time also double? Will it increase by a factor of 4 or 8 ? The only thing we can say is that that particular algorithm, executed on that particular computer, sorts 5 numbers in 0.3 sec. Nothing more ☹

Asymptotic analysis of algorithms

- Time is not an appropriate metric for assessing the speed of algorithms
  - Can't compare different algorithms that solve the same problems
  - In practice though, time is used under very specific circumstances and as an indication of the efficiency of an algorithm
- Use a different metric: **count the number of steps** an algorithm performs/executes until it finds the solution.
  - This is today the established way to assess the running time of algorithms!
  - Don't forget: an algorithm is a finite number of steps that execute and solve a problem
  - The idea is that an **algorithm A** who solves a problem is faster than **algorithm B** who solves the same problem, **when A executed fewer number of steps (commands/operations)**.

Asymptotic analysis of algorithms

- How to express the number of steps executed?
  - As a function T of a variable called the "problem size" : T(n) .
  - **Problem size =** An **aspect of the input data, that definitely will affect the number of steps** or how many times the steps will be executed, until the algorithm finds the solution to the problem
    - Example: In the context of a sorting algorithm, sorting 10 numbers (input data) will require each step of the algorithm to be executed more times than say the sorting of 8 number by the same algorithm (more comparisons). Hence, **Problem size for sorting algorithms = Count of numbers to be sorted (more numbers => more steps)**
    - Example: in the context of an algorithm which finds the greatest from a list of numbers, the count of numbers given as input will affect the times each step will be executed and hence its running time. Hence, **Problem size for finding max = Count of numbers in the input list (more numbers => more comparisons)**
    - Example: in an algorithm that searches if character "a" is contained in a string (say "John" or "Nabuzennezor"), how many times each step is executed depends on the length of the input string (bigger strings will result in more execution of steps). Hence, **Problem size for fining char in string = the length of the input string (more chars in string => more comparisons)**

Asymptotic analysis of algorithms

- Examples of running times expressed as a function T of the problem size, denoted as n:
  - Number of operations of algorithm, T: **$T(n) = 2n$, $n > 0$**
    - This means that when given an input of size n, then algorithm will do **2n operations** until it outputs the solution.
  - Number of operations of algorithm, T: **$T(n) = n^2 + 3$**
    - If given input of size n, algorithm will make **n^2+3 operations** until it solves the problem.
- From now on: Number of operations of algorithm = running time of algorithm
  - We say: running time of algorithm **$T(n) = 2n$, $T(n) = n^3+n+4$, $T(n) = 2^n$** , etc.

Asymptotic analysis of algorithms

- Example of computing running time, T(n)

Simple algorithm to find the biggest from a list of 10 numbers. 10 numbers provided by user.
Input: **10 random numbers.**
output: **the greatest number in input set.**

```
/* generalization: assume that we ask for n numbers*/
T=[]
for i in range (0, 10):
    number = int (input("Give me the number: ") )
    T.append(number)

#Assume first number as greatest
currMax = T[0]
i=1
while (i < len(T)):
       #current number at T[i] greater than current maximum?
       if ( T[i] >= currMax ):
            #Yup! Found a bigger number
            currMax = T[i]
       i = i + 1

print("The result is: ", currMax)
```

Step 1 Executed 1 time
Step 2 Executed n+1 times
Step 3 Executed n times
Step 4 Executed n times

Step 5 Executed 1 time
Step 6 Executed 1 time
Step 7 Executed n+1 times

Step 8 Executed n times

Step 9 Executed n times
Step 10 Executed n times

Step 11 Executed 1 time

+

Running time: T(n)=7n+6

Asymptotic analysis of algorithms

- Calculating running time $T(n)$ also referred to as calculating exact time
- This form of representing $T(n)$ tells us useful things like
  - Which algorithm is faster
    - E.g. If algorithm A with running time **$T(n)=n+3$** and algorithm B with running time **$T(n)=2^n$** solve the same problem, then algorithm A is faster.
  - How running time changes when input changes
    - E.g. If **$T(n) = 2n$** then if input doubles, then number of operations will double, because:
      - **$T(2n) = 4n = 2(2n) = 2T(n)$**

Asymptotic analysis of algorithms

- Expressing running time of algorithm in the form of T(n) usually captures the **worst case of the running time** of the algorithm
  - "**Worst case**": an input for which the algorithm will do its **maximum number of operations**
    - E.g. when sorting ascending order, worst case is input in descending order
  - "**Best case**": an input for which the algorithm will do its minimum number of operations to solve the problem
    - E.g. giving an already sorted list of number as input to an sorting algorithm
  - "**Average case**": a "typical", "average" input (which is encountered in the real world most of the time)

Asymptotic analysis of algorithms

Simple algorithm to find the biggest from a list of 10 numbers. 10 numbers provided by user.
<u>Input:</u> **10 random numbers.**
<u>output:</u> **the greatest number in input set.**

```
/* generalization: assume that we ask for n numbers*/
T=[]
for i in range (0, 10):
    number = int (input("Give me the number: ") )
    T.append(number)

#Assume first number as greatest
currMax = T[0]
i=1
while (i < len(T)):
        #current number at T[i] greater than current maximum?
        if ( T[i] >= currMax ):
            #Yup! Found a bigger number
            currMax = T[i]
        i = i + 1

print("The result is: ", currMax)
```

Step 1 Executed 1 time
Step 2 Executed n+1 times
Step 3 Executed n times
Step 4 Executed n times

Step 5 Executed 1 time
Step 6 Executed 1 time
Step 7 Executed n+1 times

Step 8 Executed n times

p 9 Executed n times
p 10 Executed n times

p 11 Executed time

This line will never be executed, if greatest number is at the beginning. You can "save" (these) n operations!

Asymptotic analysis of algorithms

- Running time of algorithm also referred to as **time complexity**
  - There is also space complexity (guess what this measures…)
- What is asymptotic analysis of algorithms?
  - It's when we are interested **what happens when n->∞ i.e. problem size "goes to infinity"**
  - Does it matter?
    - Yes, very much!

Asymptotic analysis of algorithms

- Why does it matter?
  - Assume algorithm A has time complexity **$T(n) = 2^n$** and algorithm B has time complexity **$T(n) = n^{20} + 4$** . Assume that both solve the same problem.
    - Which algorithm is faster?
      - ***Practically***, i.e. for some $n < n_0$, faster is A (i.e. for n=1,2,3,4,..)
      - ***Theoretically***, **when $n > 143$ and $n \to \infty$, things change: B will always be faster since then $2^n > n^{20} + 4$. Hence B is asymptotically faster.**
        - Solve **$2^n > n^{20} + 4 \Rightarrow n > 143$**
        - Useless note to show how big this is: Our sun has ~2^{80} hydrogen atoms. (so 2^{143} is really, really, really huuuuge).

Asymptotic analysis of algorithms

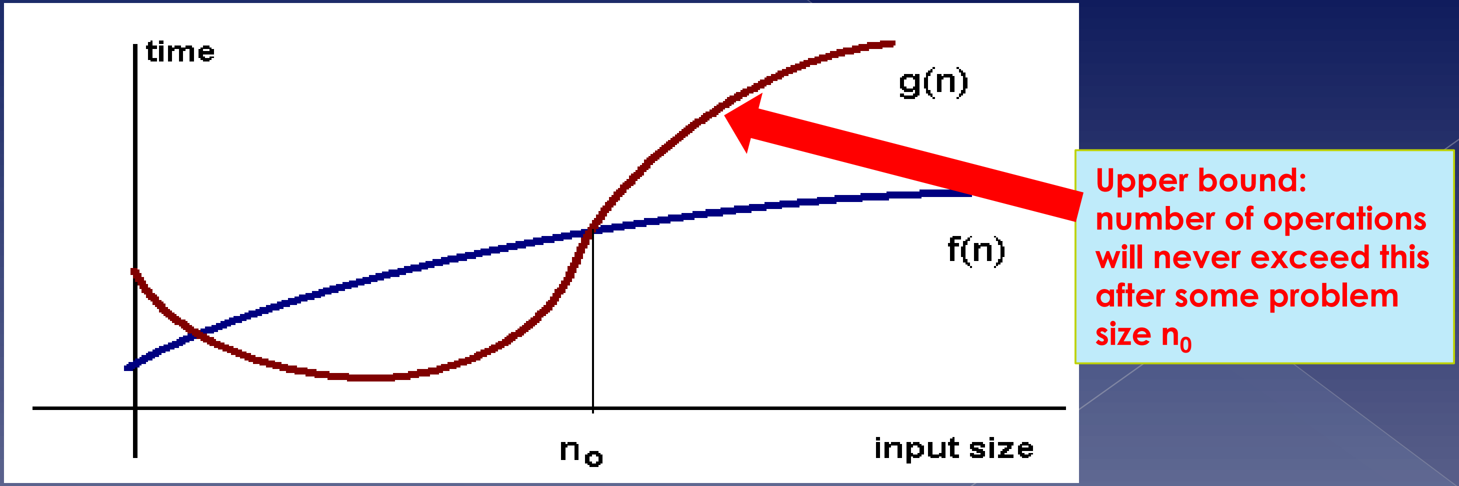
- Explanation?
  - 2^n grows faster than $n^{20}+4$.
  - In general the biggest term in running time determines the magnitude
    - i.e. if **$T(n) = 3n^2 + 45n + 2$**, then factor **$3n^2$** would be the most important **when $n \to \infty$**, since **$3n^2$** $>>$ **$45n$** and **$3n^2$** $>>$ **2**
    - **$3n^2$** grows faster than **$45n$** and (of course constant) **2**

Asymptotic analysis of algorithms

- Take this as a starting point **to define formalisms** that characterize the asymptotic running time of algorithms (or the theoretical running time:
  - **O( ), Θ( ),** Ω( ), ω( )
- Definition of these formalisms?

Asymptotic analysis of algorithms

- Definition **O () (Big-O notation)**
  - Let there be an algorithm with running time **T(n)**. We say that **T(n) = O(g(n))** if there exist a constant c and a n_0 such that **T(n) <= cg(n) for every n > n_0**
    - This means that saying **f(n) = O(g(n))** tells us that **g(n)** is an upper bound of the number of steps an algorithms executes to solve a problem of size n.



Upper bound: number of operations will never exceed this after some problem size n_0

Asymptotic analysis of algorithms

- Examples of Big-O notation
  - **$T(n) = 2n+3 \Rightarrow T(n) = O(n)$. We say that algorithm with running time $T(n)$ has time complexity $O(n)$.**
    - Why? We can find constant **c** and a **n_0 such that $2n+3 \leq cn$**, for each **$n > n_0$** (e.g. for each $c \geq 5$ and $n_0 = 1$)
    - Since time complexity is O(n) we say that running time is linear O(**n**)
  - $T(n) = \lg(n) + 5 \Rightarrow T(n) = O(\lg(n))$
    - Logarithmic time (note: lg is base-2 logarithm)
  - **$T(n) = n^2+n+7 \Rightarrow T(n) = O(n^2)$**
    - Polyonimic time algorithm
  - **$T(n) = 2^n + 3 \Rightarrow T(n) = O(2^n)$**
    - Exponential time algorithm

Asymptotic analysis of algorithms

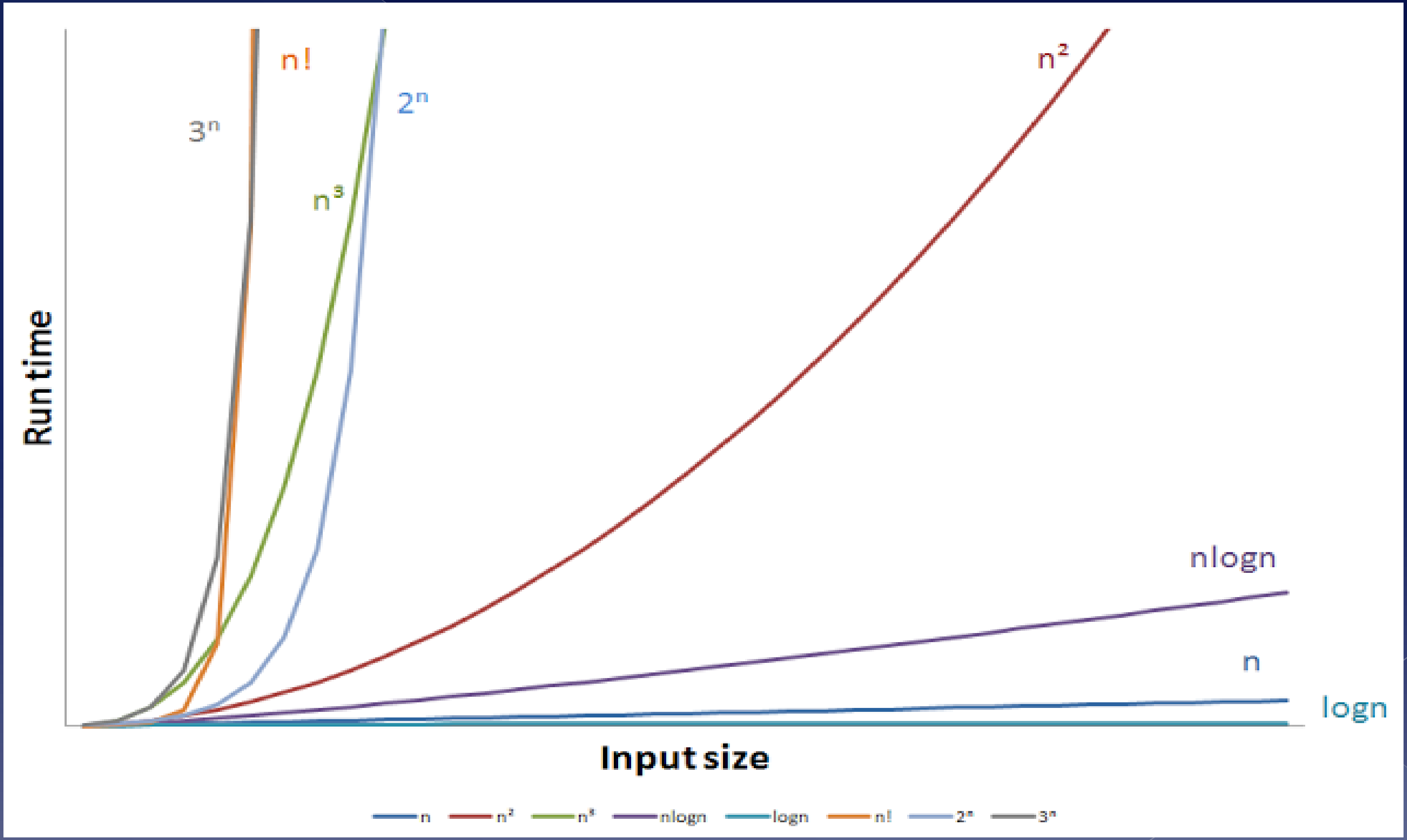
- Examples of Big-O
  - There is also running time of **O(1)**
    - **Means constant time** i.e. running time independent of input size
      - Whether you give input of size 1 or 10^{12} , algorithm will perform constant number of steps (=c).
      - E.g. assigning a number (value) to variable like x=123
    - **O()** notation is **not a tight bound!**
      - E.g. $T(n) = n+3 \Rightarrow T(n) = O(n)$ but also $T(n) = O(5^n)$
      - **But in general, it is used as a "tight bound"**
      - So when you see that an algorithm **has time complexity of $O(n^2)$** you **can assume that it will never execute more than cn^2 operations** if given an input size of n.

Asymptotic analysis of algorithms

- What is the constant, **c**, in the definition of Big-O representing?
  - E.g. in the definition on T(n) = O(g(n)) we have **c**g(n) <= T(n).
  - Intuitively: **represents the environment the algorithm runs on**
    - E.g. speed of computer, memory of computer, what other apps were running etc
      - Such **aspects are modelled**, but are **considered a constant, c.** Different computers will have different values of c.

Asymptotic analysis of algorithms

- Examples of **asymptotic time complexity and growth of functions**.

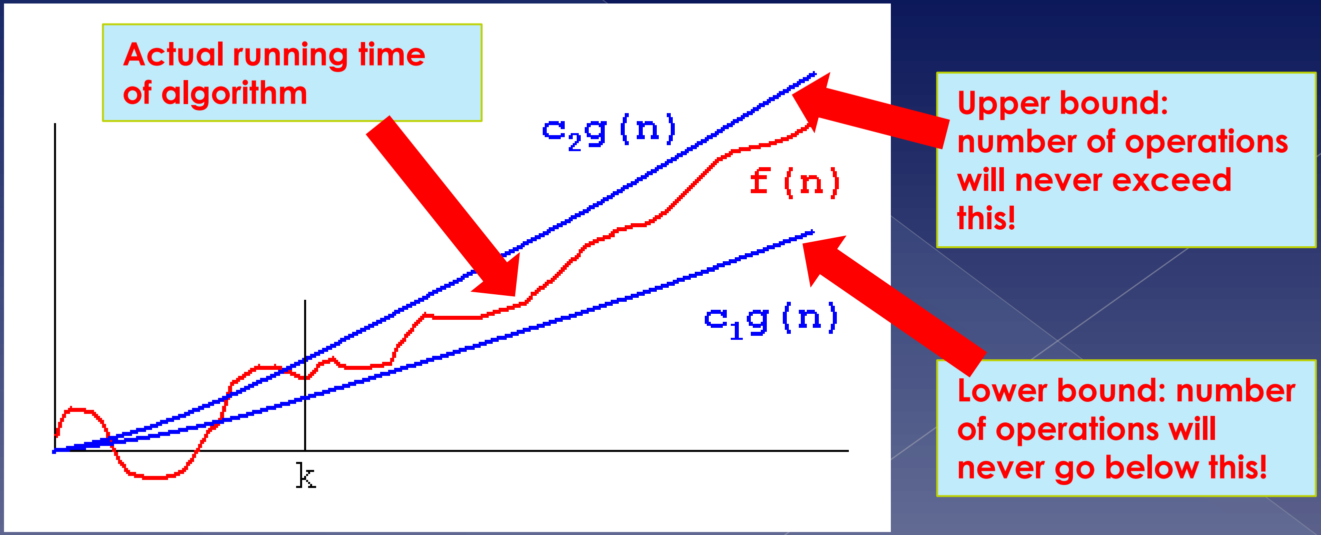


Asymptotic analysis of algorithms

- In general, Big-O helps in **grouping algorithms**
  - E.g. Class of algorithms with **O(n)** are said to be **linear**
  - E.g. Class of algorithms with **O(logn)** are said to be **logarithmic**
- From now on, you'll see **O() as a measure** of the running time of algorithms
  - For example when someone tells you that an algorithm has time complexity of **$O(n^3)$** then you can understand that running time is proportional to **n^3** of its input n
    - This means, running time can be **$T(n) = 2n^3$** or **$T(n) = 13n^3+3n^2+3$** but also **$T(n) = 97129n^3 +34n+1$**. But never faster growing than **n^3 !**

Asymptotic analysis of algorithms

- Definition **Θ() (Big-Theta notation)**
  - Let there be an algorithm with running time **$T(n)$**. We say that **$T(n) = \Theta(g(n))$** if there exist constants c_1, c_2 and a n_0 such that **$c_1 g(n) <= T(n) <= c_2 g(n)$ for every $n > n_0$**
    - This means that g(n) is upper and lower bounding T(n) (lower bound=gives also minimum number of steps to solve the problem).



Asymptotic analysis of algorithms

- In general, algorithms with **polynomial time complexities** are considered **fast and preferred**
  - Even with great exponent e.g. $O(n^{50})$
- Algorithms with **exponential time complexity are slow**.
  - E.g. **$O(3^n)$ is slow**
  - If an algorithm has time complexity of **$O(2^n)$**, then **if problem size is increased by one (n+1)** number of **operations double** (yup, that's sh*tty!).

Asymptotic analysis of algorithms

- Example algorithms
  - QuickSort:
    - Best case: $O(n \lg n)$
    - Average case: $O(n \lg n)$
    - Worst case: $O(n^2)$
  - MergeSort
    - Best case: $O(n \lg n)$
    - Average case: $O(n \lg n)$
    - Worst case: $O(n \lg n)$
  - All cryptographic algorithms
    - Exponential time complexity to crack password
  - Algorithm for making the course schedule for school/ university
    - Exponential time (that's why humans do it)

Asymptotic analysis of algorithms

- Example of time complexities of algorithms in data mining
  - **K-means**
    - If k and d (dimensions) fixed: **$O(n^{dk+1} \log n)$**, n number of objects/data to be clustered
    - **NP-hard** for general form of the problem
      - What is NP-hard? As hard/difficult as the hardest problems to solve
  - **Apriori**
    - **$O(mn + (1-R^M)/(1-R))$**, n=number of input transactions, m=threshold, R=number of unique elements.

About data

About data

- What is data? **A collection of objects and their attributes**
- An **attribute** is a **property or characteristic of an object**
  - Examples: eye color of a person, temperature, etc.
  - Attribute is also known as variable, field, characteristic, or feature
- A collection of attributes describe an object
  - Object is also known as *record*, *point*, *case*, *sample*, *entity*, or *instance*

Attributes

Objects, records, instances

Tid	**Refund**	**Marital Status**	**Taxable Income**	**Cheat**
1	Yes	Single	125K	**No**
2	No	Married	100K	**No**
3	No	Single	70K	**No**
4	Yes	Married	120K	**No**
5	No	Divorced	95K	**Yes**
6	No	Married	60K	**No**
7	Yes	Divorced	220K	**No**
8	No	Single	85K	**Yes**
9	No	Married	75K	**No**
10	No	Single	90K	**Yes**

About data

- **Attribute values?**
  - Numbers or symbols assigned to an attribute
- **Attribute vs Attribute values**
  - Same attribute can be mapped to different attribute values
    - E.g. height in feet or meters
  - Different attributes can be mapped to the same set of values
    - E.g. Attribute values for ID and age are integers
    - But with different properties: id's don't have limits, age has

About data

- There are different types of attributes (based on **how you can reason with these**):
  - **Nominal**
    - Examples: ID numbers, eye color, zip codes
  - **Ordinal**
    - Examples: rankings (e.g., taste of potato chips on a scale from 1-10 – Likert scale), grades, height in {tall, medium, short}
  - **Interval**
    - Examples: calendar dates, temperatures in Celsius or Fahrenheit.
  - **Ratio**
    - Examples: temperature in Kelvin, length, time, counts

About data

- The **type of an attribute** depends on which of the following properties it possesses (basically **what arithmetic operations** you can do with them):
  - **Distinctness:** = ≠
  - **Order:** < >
  - **Addition:** + -
  - **Multiplication:** * /

  - Nominal attribute: distinctness
  - Ordinal attribute: distinctness & order
  - Interval attribute: distinctness & order & addition
  - Ratio attribute: distinctness & order & addition & Multiplication

	Attribute Type	Description	Examples	Allowed Operations
Qualitative	**Nominal**	The values of a nominal attribute are just different names, i.e., nominal attributes provide only enough information to distinguish one object from another. (=, ≠)	zip codes, employee ID numbers, eye color, sex: {*male*, *female*}	mode, entropy, contingency correlation, χ^2 test
	Ordinal	The values of an ordinal attribute provide enough information to order objects. (<, >)	hardness of minerals, {good, better, best}, grades, street numbers, Likert scales	median, percentiles, rank correlation, run tests, sign tests
Quantitative	**Interval**	For interval attributes, the differences between values are meaningful, i.e., a unit of measurement exists. (+, -) but not (*, /) . E.g. 30°C is not twice as hot as 15°C	calendar dates, temperature in Celsius or Fahrenheit	mean, standard deviation, Pearson's correlation, t and F tests
	Ratio	For ratio variables, both differences and ratios are meaningful. (*, /)	temperature in Kelvin, monetary quantities, counts, age, mass, length, electrical current	geometric mean, harmonic mean, percent variation

Allowed transformation i.e. transformation that do not change the meaning of the attribute

Attribute Level	Allowed Transformation	Comments
Nominal	Any permutation of values	If all employee ID numbers were reassigned, would it make any difference?
Ordinal	An order preserving change of values, i.e., *new_value = f(old_value)* where *f* is a monotonic function.	An attribute encompassing the notion of good, better best can be represented equally well by the values {1, 2, 3} or by { 0.5, 1, 10}.
Interval	*new_value =a * old_value + b,* where a and b are constants	E.g. he Fahrenheit and Celsius temperature scales differ in terms of where their zero value is and the size of a unit (degree).
Ratio	*new_value = a * old_value*	Length can be measured in meters or feet.

Discrete and continuous

- **Discrete Attribute**
  - Has only a finite (or countable infinite set) of values (countable means can be ordered with a relationship)
  - 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 (cannot be ordered with a relationship)
  - 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.

Types of data sets

- Ways in which they are represented/structured
  - “Structured” data : ordered/grouped in some particular way
- **Record data**
  - Data Matrix
  - Document Data
  - Transaction Data
- **Graph data**
  - World Wide Web
  - Molecular Structures
- **Ordered data**
  - Spatial Data
  - Temporal Data
  - Sequential Data
  - Genetic Sequence Data

Important characteristics of structured data

- Dimensionality
  - How many dimensions the data has (here **dimensions**: number of features, attributes)
  - Dimensionality is a big problem (curse of dimensionality)
- Sparcity
  - How many values are present (or non-present/zero)?
- Resolution
  - Different patterns at different scales

Record data

- Record: a **fixed set of attributed**, handled as one entity
- Record data: collection of records

Tid	**Refund**	**Marital Status**	**Taxable Income**	**Cheat**
1	Yes	Single	125K	**No**
2	No	Married	100K	**No**
3	No	Single	70K	**No**
4	Yes	Married	120K	**No**
5	No	Divorced	95K	**Yes**
6	No	Married	60K	**No**
7	Yes	Divorced	220K	**No**
8	No	Single	85K	**Yes**
9	No	Married	75K	**No**
10	No	Single	90K	**Yes**

One record

Record data

Data matrix

- If data objects have the same fixed set of numeric attributes, then the data objects **can be thought of as points in a multi-dimensional space**, where each dimension represents a distinct attribute

- Such data set can be represented by an m by n matrix, where there are m rows, one for each object, and n columns, one for each attribute

Projection of x Load	Projection of y load	Distance	Load	Thickness
10.23	5.27	15.22	2.7	1.2
12.65	6.25	16.22	2.2	1.1

Document data

- Each document becomes a **`term' vector**,
  - each term is a component (attribute) of the vector,
  - the value of each component is the number of times the corresponding term occurs in the document.

Note: Search engines like google, Bing do this

Term/lemma/word '<u>team</u>' appears in '<u>Document 1</u>' 3 times

	team	coach	pla y	ball	score	game	wi n	lost	timeout	season
Document 1	3	0	5	0	2	6	0	2	0	2
Document 2	0	7	0	2	1	0	0	3	0	0
Document 3	0	1	0	0	1	2	2	0	3	0

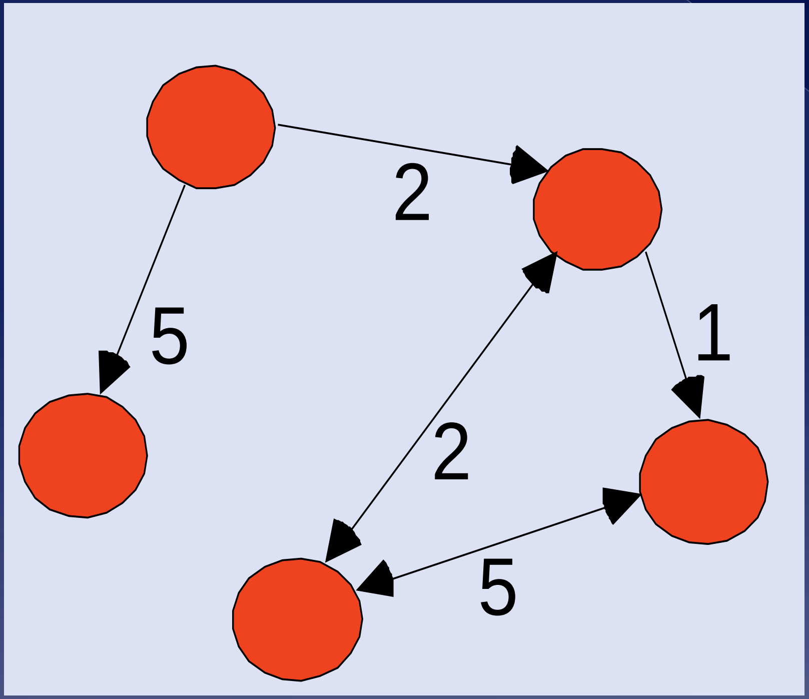
Transaction data

- A special type of record data, where
  - each record (transaction) involves a set of items.
  - For example, consider a **grocery store**. The set of products purchased by a customer during one shopping trip constitute a transaction, while the individual products that were purchased are the items.

TID	*Items*
1	Bread, Coke, Milk
2	Beer, Bread
3	Beer, Coke, Diaper, Milk
4	Beer, Bread, Diaper, Milk
5	Coke, Diaper, Milk

Graph data

- Data represented with nodes and links (=**graphs**)



- Examples
  - World wide web (pages, links)
  - References in scientific articles
    - Who references which paper (link)
  - Calculate
    - PageRank (google)
    - h-index
    - Hubs

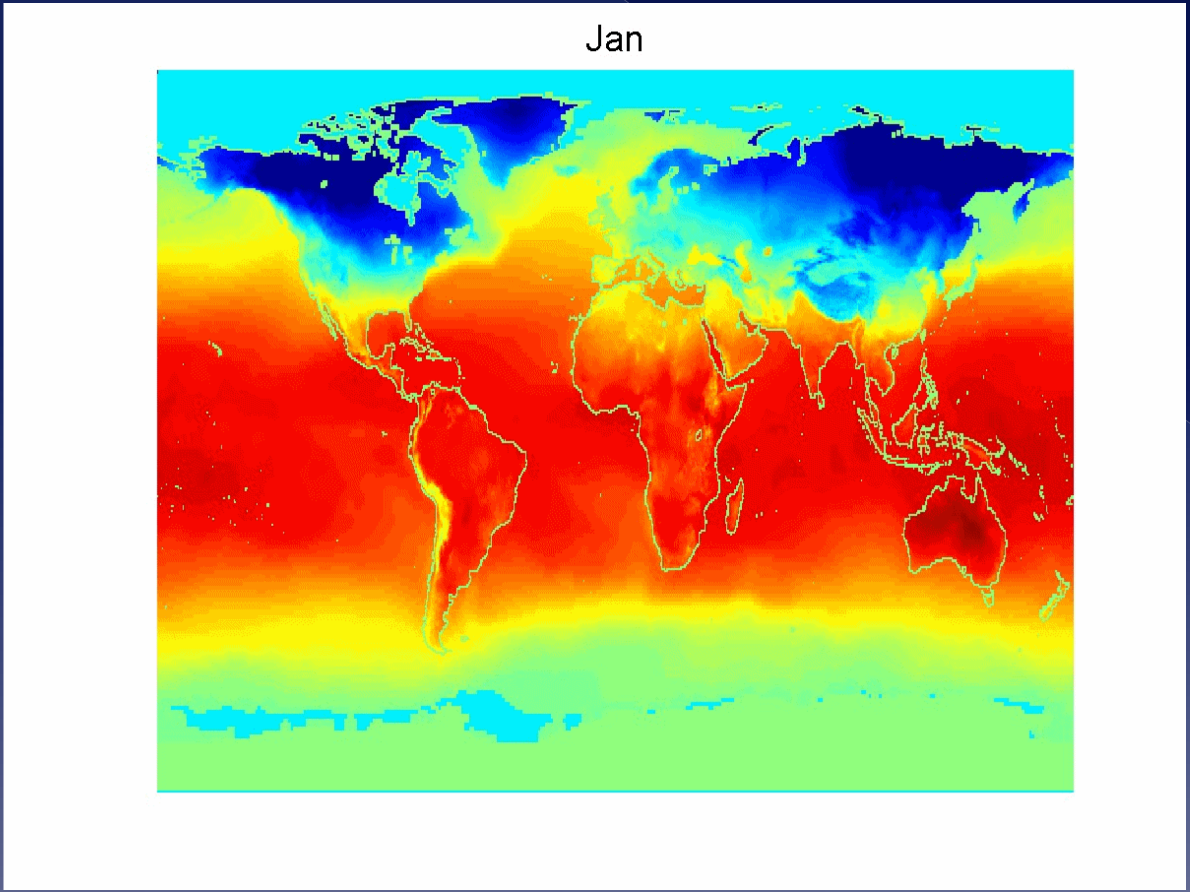
Ordered data

- Position/rank matters
  - E.g. genomic sequence

```
GGTTCCGCCTTCAGCCCCGCGCC
CGCAGGGCCCGCCCCGCGCCGTC
GAGAAGGGCCCGCCTGGCGGGCG
GGGGGAGGCGGGGCCGCCCGAGC
CCAACCGAGTCCGACCAGGTGCC
CCCTCTGCTCGGCCTAGACCTGA
GCTCATTAGGCGGCAGCGGACAG
GCCAAGTAGAACACGCGAAGCGC
TGGGCTGCCTGCTGCGACCAGGG
```

Ordered data

- Spatio-temporal data



Average Monthly Temperature of land and ocean

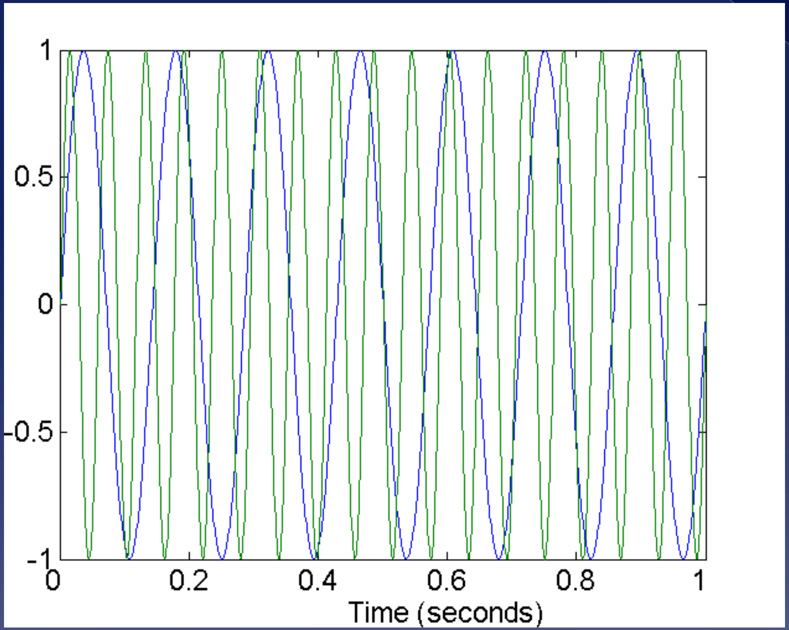
Data quality

Data quality

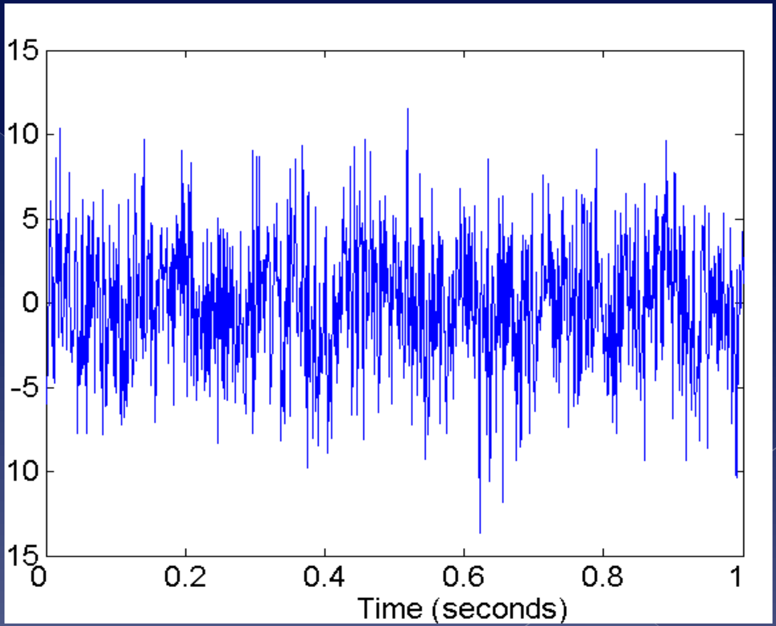
- Data quality?
  - The aspects of data sets that make it **suitable/useful** (or not) **for processing to achieve a goal**
  - Common data quality issue/problems
    - Noise and outliers
    - Missing values
    - Duplicate data

Noise

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



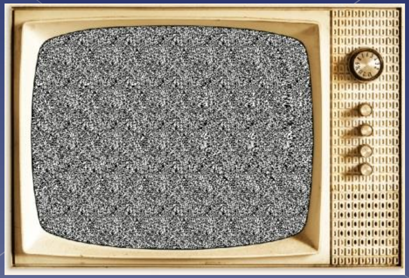
Two Sine Waves (voice)



Two Sine Waves + Noise (voice + distortion). Yup it's a miracle that you can hear a voice.

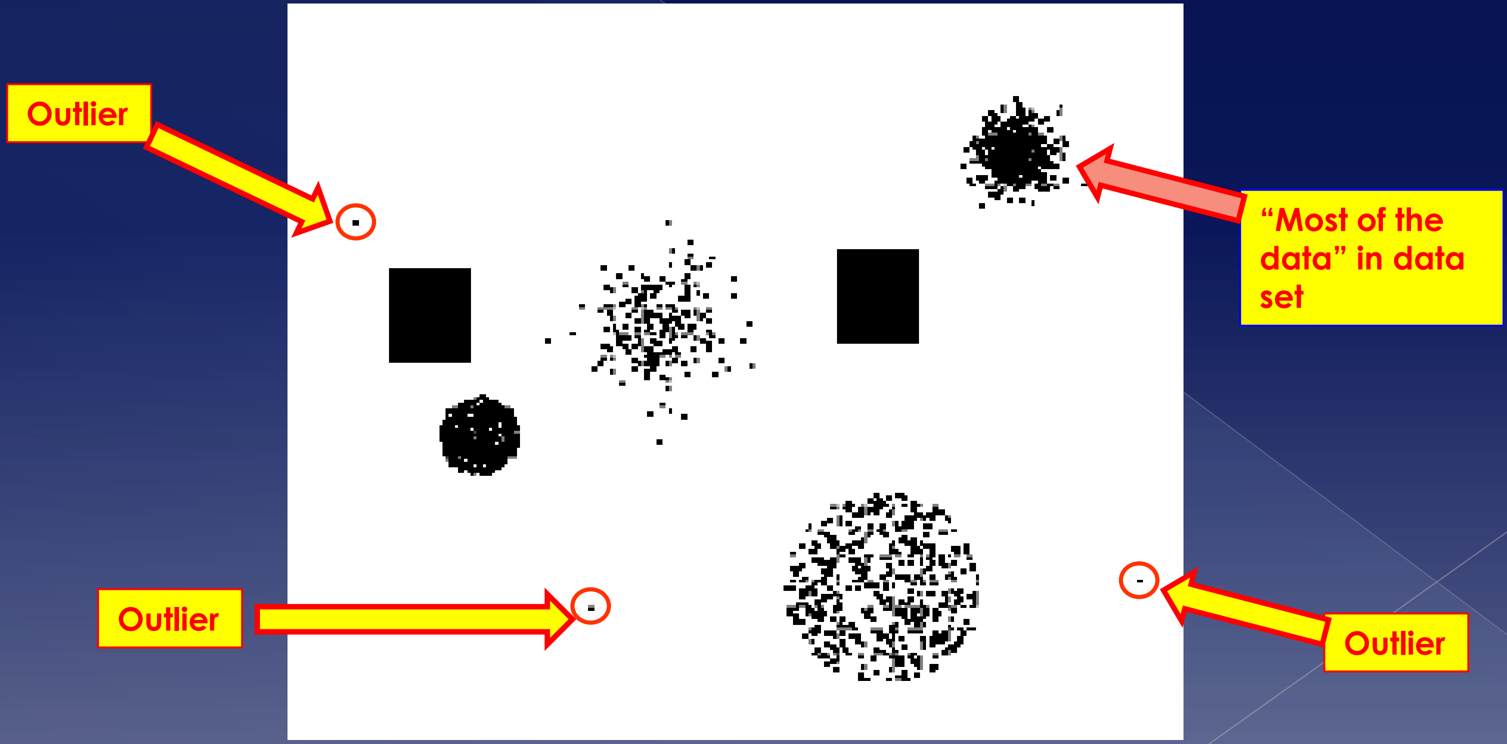
Noise

- Useless/funny bits of noise
  - Give rise to **information theory**
    - Claude Shannon aiming at separate voice (information) from not-voice (noise)
  - Noise **can be interesting**
    - "Snow" on old TVs is **~40% cosmic radiation (from Big Bang)**
      - Meaning the **"snow" that you saw**, was **the cosmos/universe on your TV**
        - Not anymore though due to digital TV.



Outliers

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



Outliers

- Can seriously distort your view

Person	Wealth (in Linden dollars)
Gianna	10000000000
Jim	19
John	20
Phil	25
Martha	16

(Naïve) average wealth:
2000000016 Linden dollars

#LOL, made everyone rich. No joke pal.

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)
  - Devices may be **faulty** (e.g. faulty thermometer)

- Handling missing values
  - Eliminate Data Objects (commonly used)
  - Estimate Missing Values
  - Ignore the Missing Value During Analysis
  - Replace with all possible values (weighted by their probabilities)

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 (typical in greek public sector)**
- Examples:
  - Same person with **multiple email addresses**
    - I know: what you do on facebook, twitter, insta etc.
- Data cleaning
  - Process of **dealing with duplicate data issues**
    - E.g. names: in greek Κων/νος, Κωνσταντίνος, Κώστας, Αγ. Βαρβάρα, Αγία Βαρβάρα etc

Data preprocessing

Data preprocessing

- Data preprocessing?
  - Steps that aim **making the data**, before their processing, **suitable for the desired processing**.
    - The issue here is to optimize various aspects that may affect processing, in particular
      - **Required space**
      - **Processing time, minimize running times i.e. O(g(n))**
    - Don't forget: we're **working with Big data!**
- Probably the most important step in data mining
- In general, **about 70%-80%** of total time is **consumed on data preprocessing tasks**
- Can definitely shoot your own foot
  - **Wrong preprocessing yields to wrong results.**

Data preprocessing

- Techniques/methods
  - Aggregation
  - **Sampling**
  - **Dimensionality reduction**
  - Feature subset selection
  - Feature creation
  - **Discretization**
  - Attribute transformation

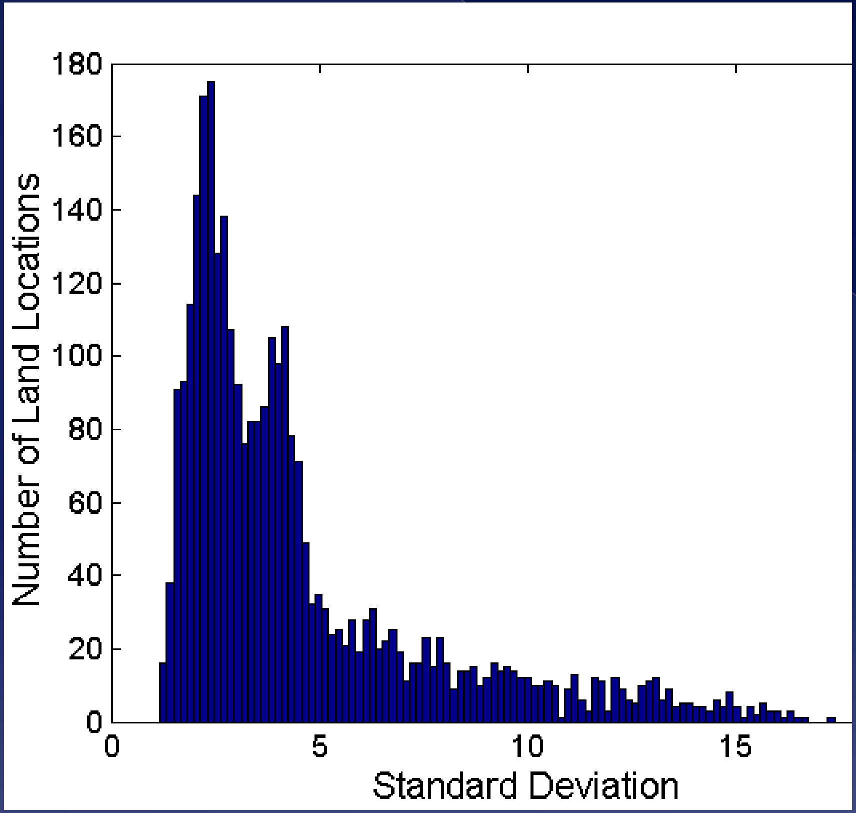
Aggregation

- Combining two or more attributes (or objects) into a single attribute (or object)

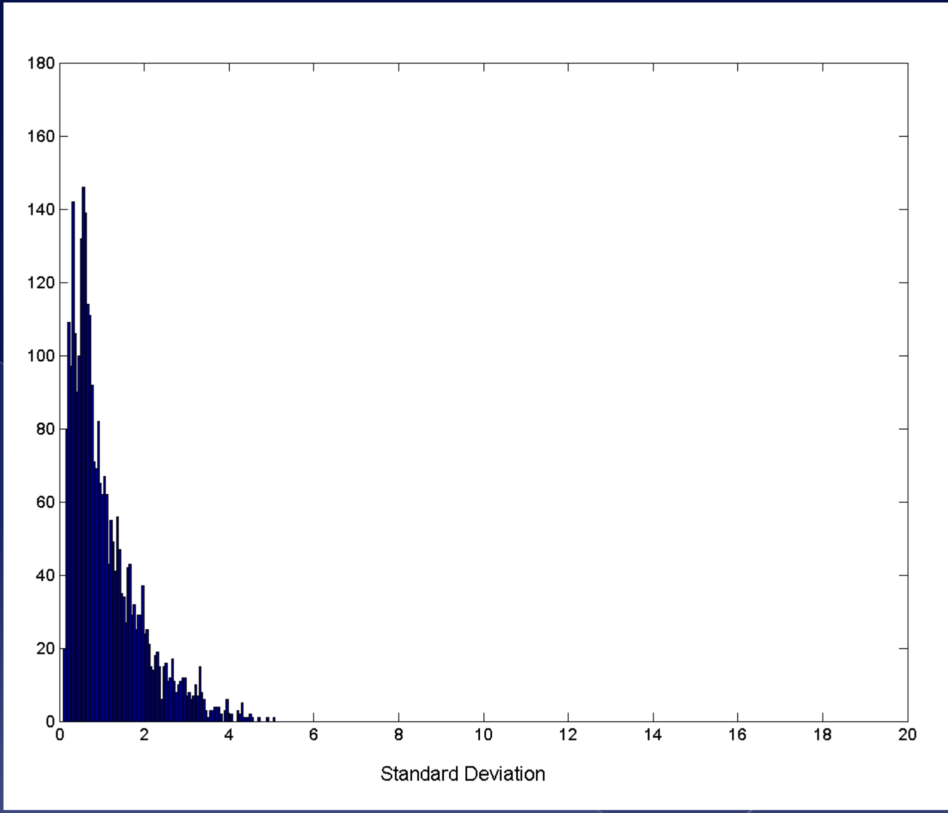
- Purpose
  - **Data reduction**
    - Reduce the number of attributes or objects
  - **Change of scale**
    - Cities aggregated into regions, states, countries, etc
  - **More “stable” data**
    - Aggregated data tends to have less variability

Aggregation

Variation of Precipitation in Australia



Standard Deviation of Average Monthly Precipitation



Standard Deviation of Average Yearly Precipitation – **aggregated** (note smaller variability)

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.
- Why sampling?
  - 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
    - In terms of its distribution

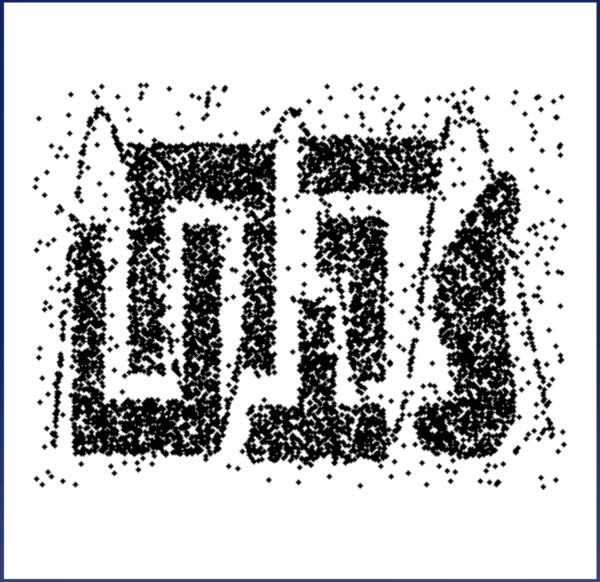
Sampling

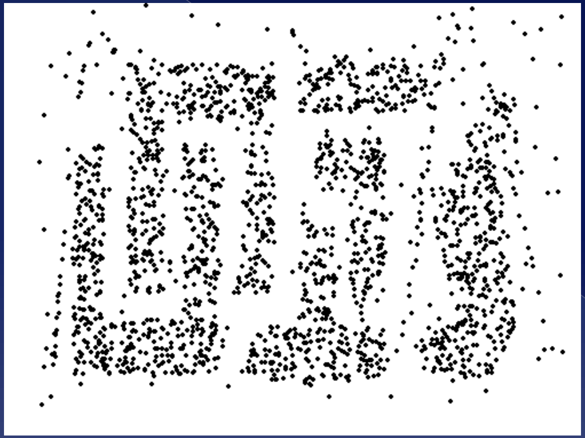
- **Simple Random Sampling**
  - There is an equal probability of selecting any particular item
- **Sampling without replacement**
  - As each item is selected, it is removed from the population
- **Sampling with replacement**
  - Objects are not removed from the population as they are selected for the 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

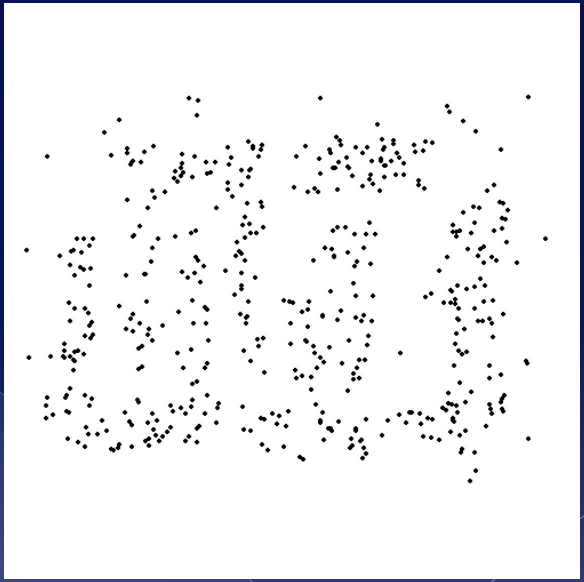
Sampling

- Effect of sample size?

Effects almost any type of data: e.g. when you talk on the phone and your voice is sent to other guy/girl


8000 points

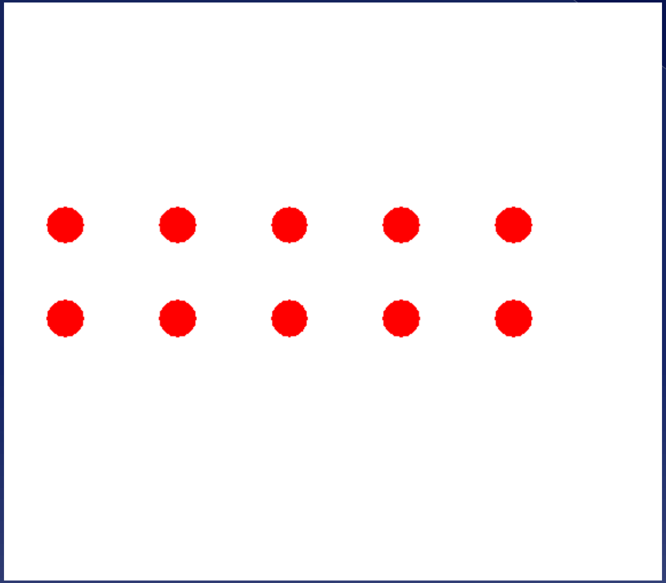

2000 Points


500 Points

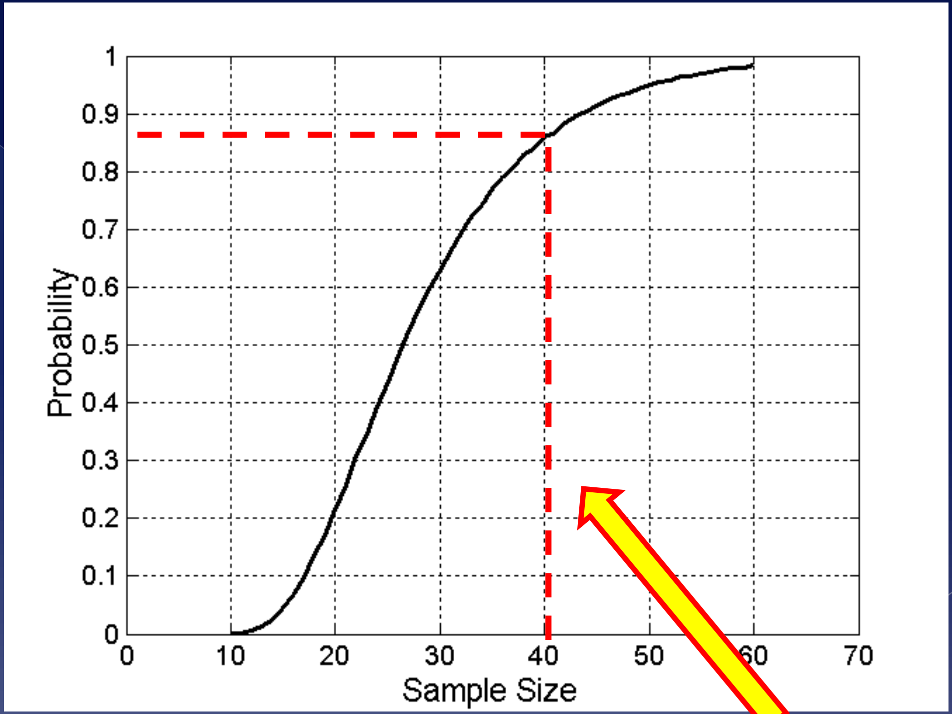
More objects/points/data is in general better. But more objects require more space, more time (preprocessing and analysis). Tradeoff.

Sampling

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



10 groups

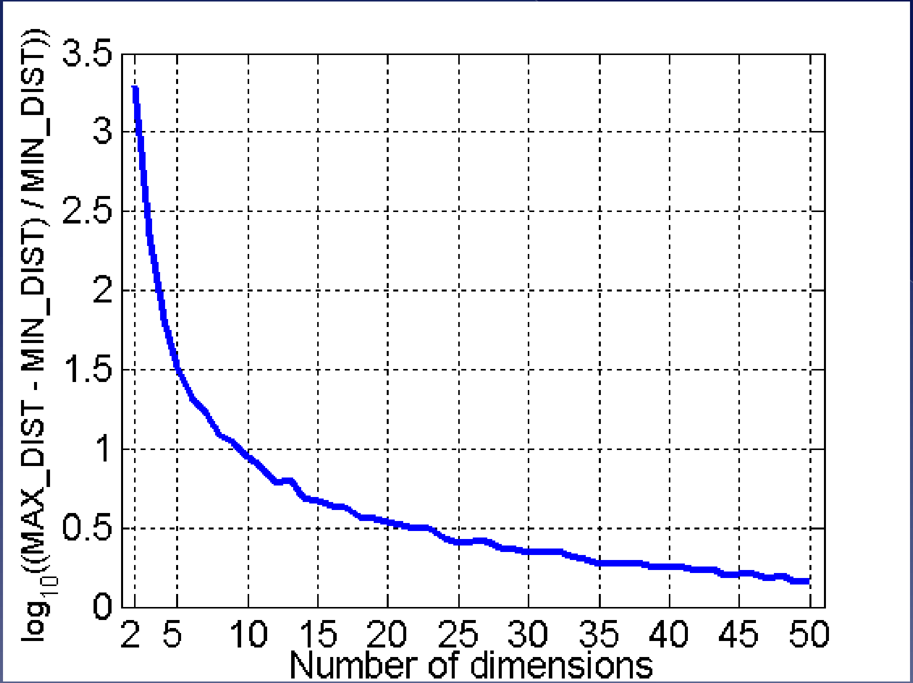


This graph will tell you. For example with a sample size of 40, the probability of having at least one from each group is ~0.87 .

Dimensionality reduction

- Curse of dimensionality
  - Remember: **dimensions = number of attributes**

- Randomly generate 500 points
- Compute difference between max and min distance between any pair of points
- Note: as dimensions increase, less meaningful distance **which causes problems when clustering**!



When **dimensionality increases**, data becomes increasingly sparse in the space that it occupies (i.e. many, many, missing or zero values)

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

Dimensionality reduction

- Purpose
  - Get rid of curse (**ha, take that!**)
  - **Reduce space and time required** by data mining algorithms
  - Facilitate easy visualization of data
  - May help in reducing noise
- Techniques/methods
  - **Principal Components Analysis (PCA)**
  - Singular Value Decomposition (SVD)
  - Supervised and non-supervised techniques

Data preprocessing
PCA – Principal Component Analysis

Principal Components Analysis (PCA)

- A quick look at PCA
  - What it aims for?
    - It aims to **expressing existing data with high dimensionality (attributes, n)** in the context of a new (optimal) axis system ("subspace") with fewer dimensions d, i.e. $d < n$.
      - **Goal of PCA**: capture most of the variation in original data set to bring out patterns.
      - **"fewer dimensions"** => reducing dimensionality and hence the curse of dimensionality
      - Basically we compress the data set.
      - Note: might lose some of variation of original data, and hence can't perfectly reproduce original data in the new subspace, but this variation is not important (due to being very small/insignificant).
      - This **new "subspace" comprises the Principal Components**

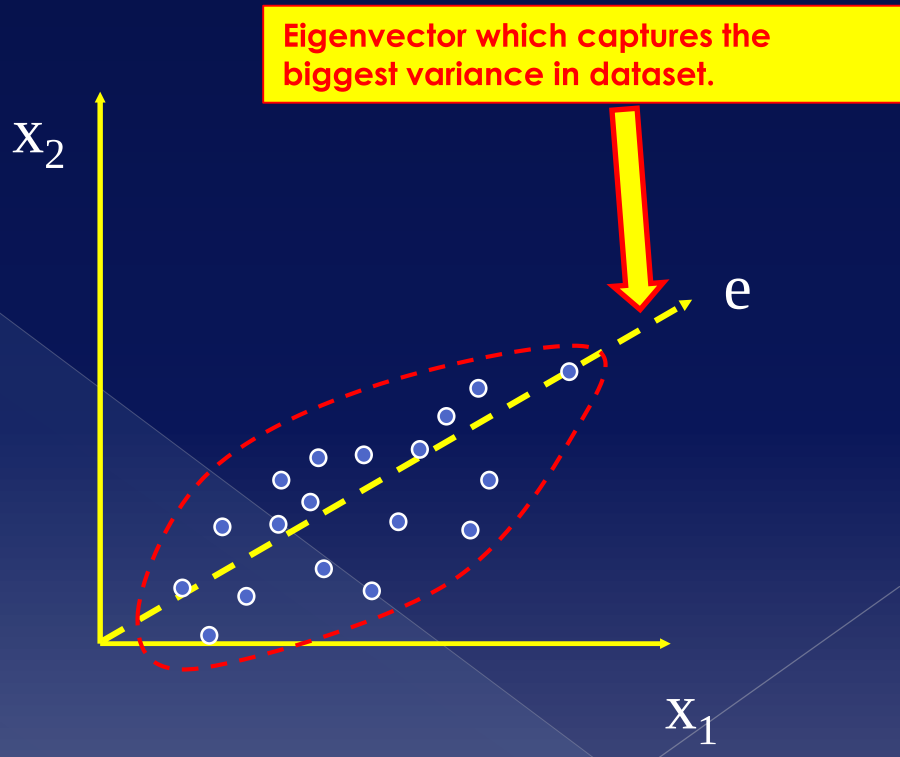
    - **<u>IMPORTANT: PCA works only with numerical vectors!</u>**

Principal Components Analysis (PCA)

- A quick look at PCA
  - Several issues with the new subspace
    - How to choose new dimension d ?
    - How to select feature space (“subspace”) that represents our data well (i.e. principal components)?

Principal Components Analysis (PCA)

- How to **find axes of new** space?
  - The **Eigenvectors, Eigenvalues** of the Covariance matrix define these spaces
    - Eigenvectors are linear independent



Principal Components Analysis (PCA)

- Steps to calculate Principal Components
  - Take whole dataset with n dimensions
  - Compute the dimensional mean-vector (i.e. mean for each dimension/attribute)
  - Subtract mean from each dimension (make variables have mean =0) – **Normalize the data**
  - Compute the covariance matrix
    - Indicating how each dimension/attribute varies with respect to all other
  - Compute Eigenvectors and Eigenvalues of the covariance matrix solving:
    - **$|\lambda I - A| = 0$, λ=eigenvalue, $| \ |$ = determinant, I = unit vector**
    - **$Av = lv$, v = eigenvector**
  - Choose k largest Eigenvalues and corresponding Eigenvectors
  - Use these Eigenvectors to form a d x k new matrix W of Eigenvectors
  - Use this d x k Eigenvector matrix to transform each object (vector) onto the new space, as follows:
    - **<New vector> = W^T x <old_vector>**

Principal Components Analysis (PCA) - Example

- Numerical Example
- Assume the following observations/data about different food items: vitamin C content, protein content)

Vitamin C	Protein
2.5	2.4
0.5	0.7
2.2	2.9
1.9	2.2
3.1	3.0
2.3	2.7
2	1.6
1	1.1
1.5	1.6
1.1	0.9

- Our goal/question to answer?
- **Reduce the number of variables while at the same time keep/explain most of the variance.**
  - **We have here only 2 variables, so this makes little sense. Imagine e.g. having 250 variables. In such cases you want to reduce the number of variables but "keep" the variance.**

Principal Components Analysis (PCA) - Example

- Calculate mean for each variable

Vitamin C	Protein
2.5	2.4
0.5	0.7
2.2	2.9
1.9	2.2
3.1	3.0
2.3	2.7
2	1.6
1	1.1
1.5	1.6
1.1	0.9

mean =1.81 **mean =1.91**

Principal Components Analysis (PCA) - Example

- Subtract mean from each value to normalize the data.

Vitamin C	Protein
2.5 – 1.81 = **0.69**	2.4 – 1.91 = **0.49**
0.5-1.81=-**1.31**	0.7 – 1.91 = **-1.21**
2.2-1.81=**0.39**	2.9 – 1.91 = **0.99**
1.9-1.81=**0.09**	2.2 -1.91=**0.29**
3.1-1.81=**1.29**	3.0 – 1.91 =**1.09**
2.3-1.81=**0.49**	2.7 -1.91 =**0.79**
2-1.81=**0.19**	1.6-1.91 = **-0.31**
1-1.81= **-0.81**	1.1 – 1.91 = **-0.81**
1.5-1.81=**-0.31**	1.6 – 1.91 = **-0.31**
1.1-1.81=**-0.71**	0.9 -1.91 = **-1.01**

mean =1.81 mean =1.91

NOTE: we will work from now on with the red values!

Hint: mean of both variables is now 0.

Principal Components Analysis (PCA) - Example

- Calculate the covariance matrix

	Vitamin C	Protein
Vitamin C	0.616	0.615
Protein	0.615	0.716

$$cov(VitaminC, Protein) = \frac{\sum_{i=1}^{10}\left(VitC_i - \overline{VitC}\right)\left(Prot_i - \overline{Prot}\right)}{9 = (10-1)}$$

NOTE: mean here is calculated on the normalized data (i,.e. mean = 0)

Principal Components Analysis (PCA) - Example

- Calculate **Eigenvalues and Eigenvectors of the Covariance matrix**
- Definition of Eigenvector v with Eigenvalue λ of the covariance matrix cov(VitC, Pr):
  - $cov(VitC, Pr)v = \lambda v \Rightarrow cov(Vit, Pr)v - \lambda v = 0 \Rightarrow$ $\boldsymbol{(cov(Vit, Pr) - \lambda I_2)v = 0}$
- Calculate **Eigenvalues first!**

Principal Components Analysis (PCA) - Example

- Calculate Eigenvalues first

$$(\boldsymbol{cov(Vit, Pr)} - \boldsymbol{\lambda I_2})\boldsymbol{v} = \mathbf{0}$$

$$\Downarrow$$

Note: 0 is the zero vector. We search for λ (eigenvalue) and corresponding v (eigenvector). Let's remember a little bit of linear algebra: In order for this to have non-zero vector v as solution, the determinant of $(\mathbf{cov(Vit, Pr)} - \boldsymbol{\lambda}\mathbf{I_2})$ **must be zero! Let's do it.**

Principal Components Analysis (PCA) - Example

- Calculate Eigenvalues

$$det(cov(Vit, Pr) - \lambda I_2) = 0$$

Covariance matrix

Identity matrix I_2

0.616	**0.615**
0.615	0.716

- λ

1	**0**
0	**1**

=

=

0.616 - λ	**0.615**
0.615	**0.716 - λ**

Determinant of this must be zero.

Principal Components Analysis (PCA) - Example

- Calculate Eigenvalues

$$\text{Det}\left(\begin{array}{|c|c|} \hline 0.616 - \lambda & 0.615 \\ \hline 0.615 & 0.716 - \lambda \\ \hline \end{array} \right) = 0 \Rightarrow$$

$$\Rightarrow (0.616-\lambda)*(0.716-\lambda) - 0.615 * 0.615 = 0 \Rightarrow \boxed{\lambda 1 = 0.0489,\ \lambda 2 = 1.283}$$

<u>**2 Eigenvalues calculated λ1, λ2 !**</u>

Principal Components Analysis (PCA) - Example

- Now, **for each Eigenvalue**, calculate the **Eigenvector V**.

For eingenvalue λ =0.0490

0.616 - λ	0.615
0.615	0.716 - λ

* V =

0
0

=>

0.616 – 0.0489 = 0.567	0.615
0.615	0.716 – 0.0489 = 0.667

* V =

0
0

=>

Principal Components Analysis (PCA) - Example

- For each Eigenvalue, calculate the Eigenvectors.

For eingenvalue λ =0.0490

$$\begin{bmatrix} 0.567 & 0.615 \\ 0.615 & 0.667 \end{bmatrix} * \begin{bmatrix} v1 \\ v2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Rightarrow$$

$$\left.\begin{array}{l} 0.567*v1 + 0.615*v2 = 0 \\ 0.615*v1 + 0.667*v2 = 0 \end{array}\right\}$$

Eigenvalue λ=0.049

Eigenvector = $\begin{bmatrix} -0.7351 \\ 0.6778 \end{bmatrix}$

Principal Components Analysis (PCA) - Example

- For each Eigenvalue, calculate the Eigenvectors.

For Eigenvalue λ =1.284

0.616 - λ	0.615
0.615	0.716 - λ

* V =

0
0

=>

0.616 – 1.284 = -0.668	0.615
0.615	0.716 – 1.284 = -0.568

* V =

0
0

=>

Principal Components Analysis (PCA) - Example

- For each Eigenvalue, calculate the Eigenvectors.

For Eigenvalue λ =1.284

$$\begin{bmatrix} -0.668 & 0.615 \\ 0.615 & -0.568 \end{bmatrix} * \begin{bmatrix} v1 \\ v2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Rightarrow$$

$$\left.\begin{aligned} -0.668*v1 + 0.615*v2 &= 0 \\ 0.615*v1 + 0.568*v2 &= 0 \end{aligned}\right\}$$

Eigenvalue λ=1.284

Eigenvector = $\begin{bmatrix} -0.6778 \\ -0.7351 \end{bmatrix}$

Principal Components Analysis (PCA) - Example

- We found 2 Eigenvalue/Eigenvector pairs

Eigenvalue λ=1.284

Eigenvector = $\begin{bmatrix} -0.6778 \\ -0.7351 \end{bmatrix}$

Eigenvalue λ=0.049

Eigenvector = $\begin{bmatrix} -0.7351 \\ 0.6778 \end{bmatrix}$

- Notice how **one Eigenvalue is greater than the other ? 1.284 > 0.049**.
  - This means that **the Eigenvector with λ = 1.284 captures most variance of the dataset!**

Principal Components Analysis (PCA) - Example

- **How much variance** does the greatest Eigenvector explain?
  - Use $\frac{\lambda_k}{\sum_{i=1}^{n} \lambda_i}$ where n= number of eigenvalues/eigenvectors - to see how muck variance Eingenvector with Eigenvalue λ_k explains
  - In our case Eigenvector with **λ=1.284** explains **1.284 / (1.284+0.049) = 0.96** or **96% of the variance** in the data
  - In the general case, what you do is **select the k largest Eigenvalues (and corresp. Eigenvectors)** until you are happy with the variance explained – **The selected Eigenvalues/Eigenvectors are the Principal Components!**
    - In this case the explained variance is $\frac{\sum_{i=1}^{k} \lambda_i}{\sum_{j=1}^{n} \lambda_j}$
    - Empirical: **aiming at explaining >70% or variance**

Principal Components Analysis (PCA) - Example

- If we are happy with the variance explained, do the following:
  - Map the original data to the selected k Eigenvectors with the k greatest eigenvalues -in our example, lets say we select only 1 Eigenvalue/Eigenvector pair – the one with the largest Eigenvalue :

Vitamin C	Protein
2.5	2.4
0.5	0.7
2.2	2.9
1.9	2.2
3.1	3.0
2.3	2.7
2	1.6
1	1.1
1.5	1.6
1.1	0.9

$\Rightarrow$

Map this data to this feature vector defined by the Eigenvector

Eigenvalue λ=1.284

Eigenvector = $\begin{bmatrix} -0.6778 \\ -0.7351 \end{bmatrix}$

We aim to do this => Express data solely <u>in terms of the selected Eigenvectors!</u>

Principal Components Analysis (PCA)

- A more complex example:
- *"In the Places Rated Almanac, Boyer and Savageau rated 329 communities according to the following nine criteria:*
  - *Climate and Terrain*
  - *Housing*
  - *Health Care & the Environment*
  - *Crime*
  - *Transportation*
  - *Education*
  - *The Arts*
  - *Recreation*
  - *Economics*

  Note that within the dataset, except for housing and crime, the higher the score the better. For housing and crime, the lower the score the better. Where some communities might do better in the arts, other communities might be rated better in other areas such as having a lower crime rate and good educational opportunities."

  Objective: Search for relationships (correlation) between these variables.

Principal Components Analysis (PCA)

- In order to do this you need to check all combination of variables and expect a linear correlation
  - In this 9-dimensional space, observation which are correlated will appear closely together
  - **Difficult to see**: too many scatterplots of variables against each other, how to draw a 9-dimensional space etc.
- Or you could **do a PCA**, find principal components and project data onto these
  - Such projection **gives you a quick view of the grouping** which implies correlation.

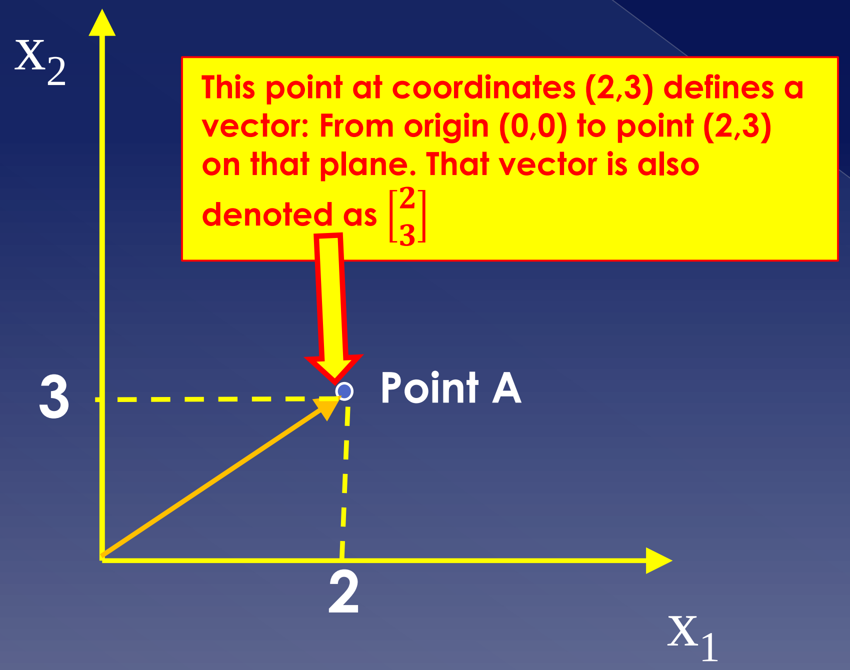
Principal Components Analysis (PCA)

- Some Notes!
- Principal Component Analysis - PCA
  - **When to use it?**
    - When number of dimensions (attributes) in dataset is very large (say >100) and you want to reduce the number of dimensions while still explaining great amount of variance in the data
  - **On what kind of attributes/data does it work?**
    - PCA works **only on Ratio attributes.**
    - Variations of PCA to work in interval data available.
  - **PCA can make use of the Correlation matrix instead of the Covariance matrix**
    - Important when implementing PCA in R
      - Look at the appropriate parameters!

Data preprocessing
PCA – Sorry, I still don't get it!

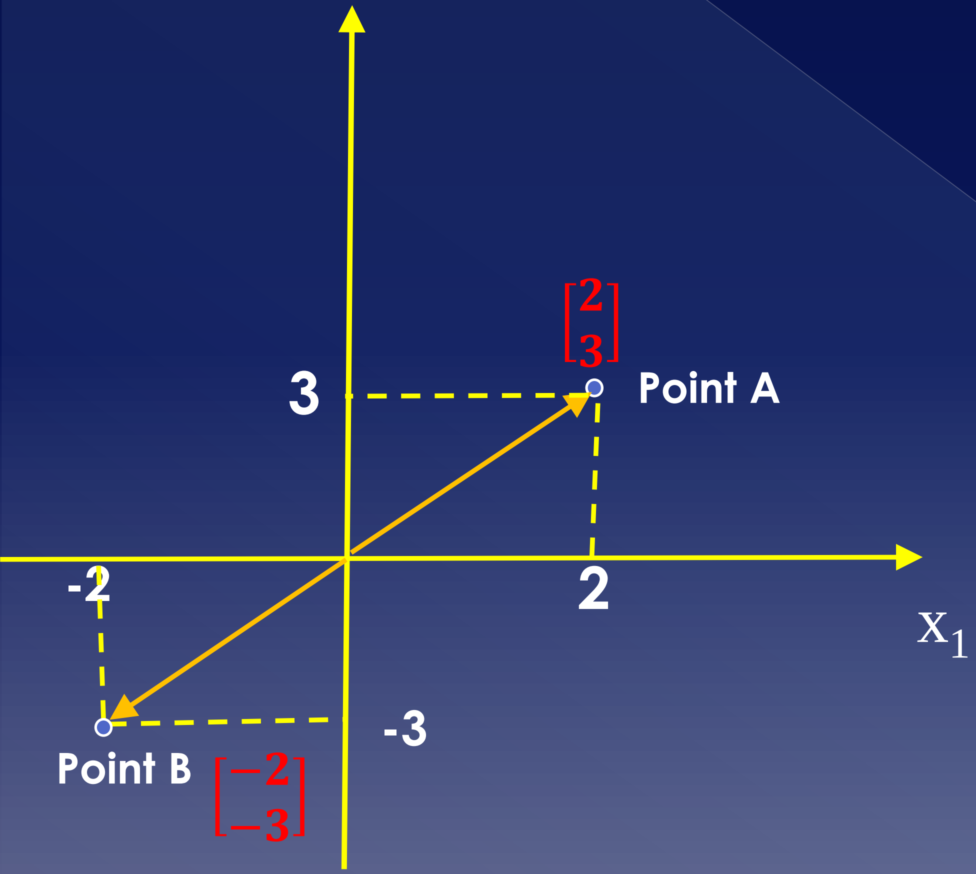
Principal Components Analysis (PCA) – I don't get it

- I'm sorry, I still don't get PCA. Get you draw it for me? Ok, first some basics.


x_2
This point at coordinates (2,3) defines a vector: From origin (0,0) to point (2,3) on that plane. That vector is also denoted as $\begin{bmatrix}2\\3\end{bmatrix}$
Point A
3
2
x_1

Principal Components Analysis (PCA)

- Notice how point B is a reflection of Point A on the origin (0,0)?



$\begin{bmatrix}2\\3\end{bmatrix}$
3
Point A
-2
2
x_1
-3
Point B
$\begin{bmatrix}-2\\-3\end{bmatrix}$

The question is now: how can we calculate the reflection of any point P in the origin?

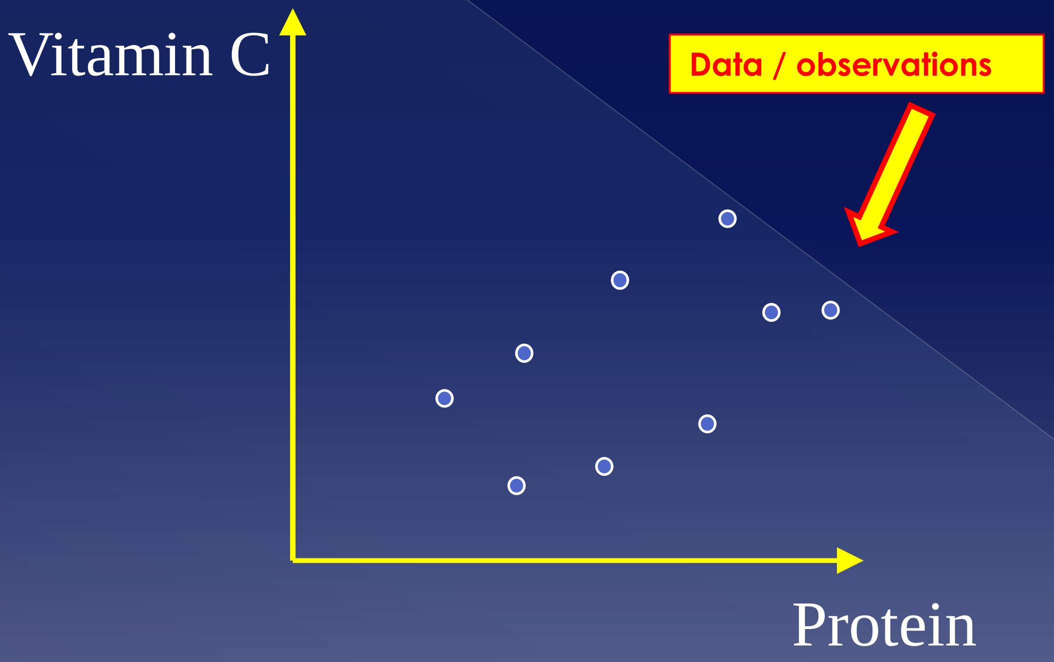
Easy: Just multiply the vector with the matrix $\begin{bmatrix}-1 & 0\\0 & -1\end{bmatrix}$ this will calculate the vector that is the reflection of the original e.g.

$$\begin{bmatrix}-1 & 0\\0 & -1\end{bmatrix}\begin{bmatrix}2\\3\end{bmatrix} = \begin{bmatrix}-2\\-3\end{bmatrix}$$

From this, please take away the following important message: Matrix multiplication is simply Vector TRANSFORMATIONS (i.e. move vector elsewere)! Note: you can define matrices for any transformation. If you multiply matrices A and B with vector $\begin{bmatrix}-2\\-3\end{bmatrix}$ i.e. A*B* $\begin{bmatrix}-2\\-3\end{bmatrix}$ that means: transform vector $\begin{bmatrix}-2\\-3\end{bmatrix}$ according to B and the result according to A. This may indicate e.g. Rotate and Mirror vector.

Principal Components Analysis (PCA)

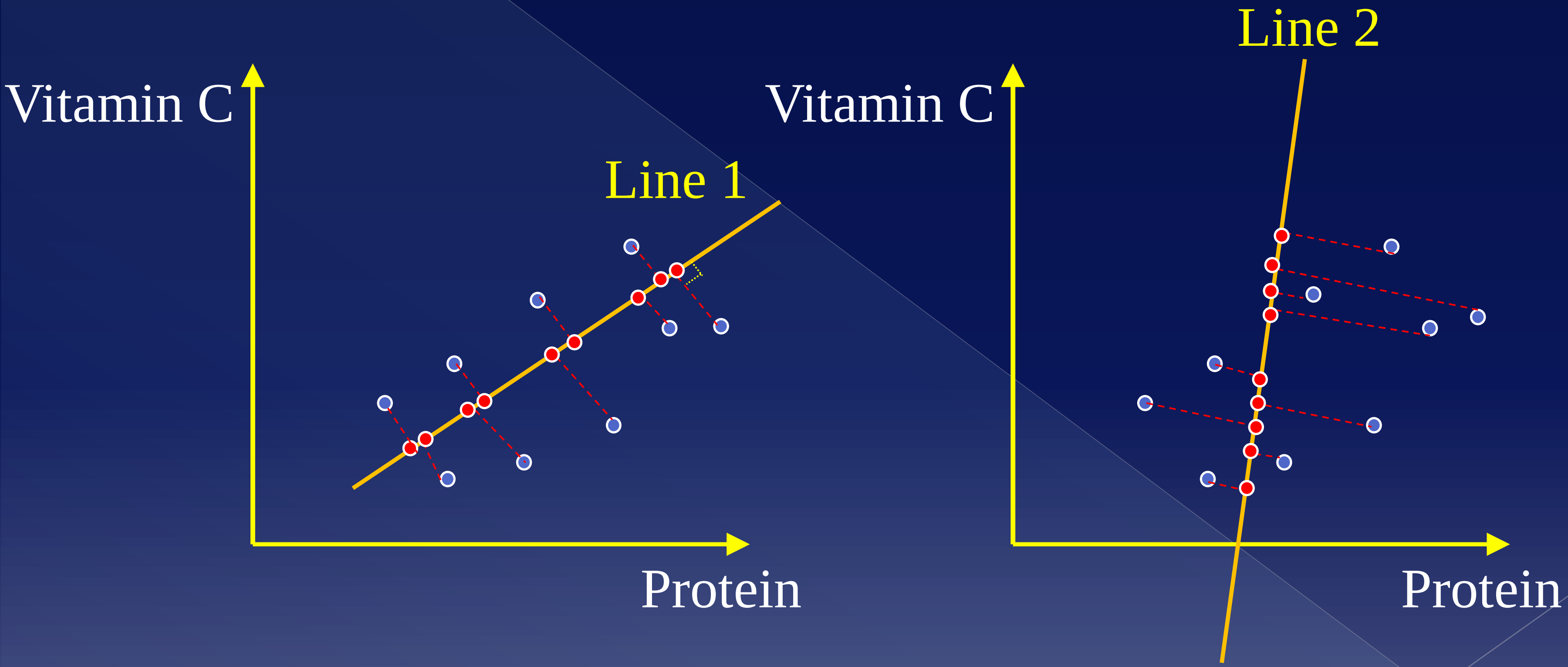
- Let’s assume we have some data.



Principal Components Analysis (PCA)

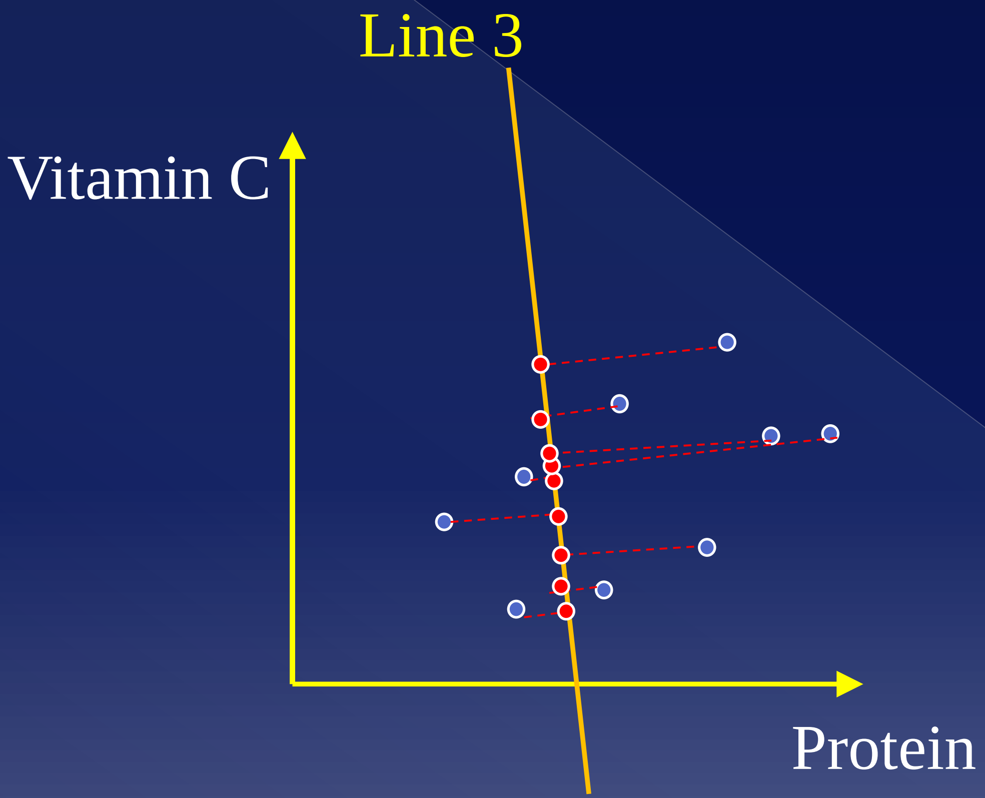
- Let’s do the following now: **Draw random lines** on the plane of your data **and project the data on that line.** How does this look like?

Principal Components Analysis (PCA)



Note: Red dots on Line 1 and Line 2 are the projections of the data on each line. Projections are perpendicular to the lines. HINT: Notice how the "spread" (aka variance) of the red dots on these lines (Line1, Line2) differ?

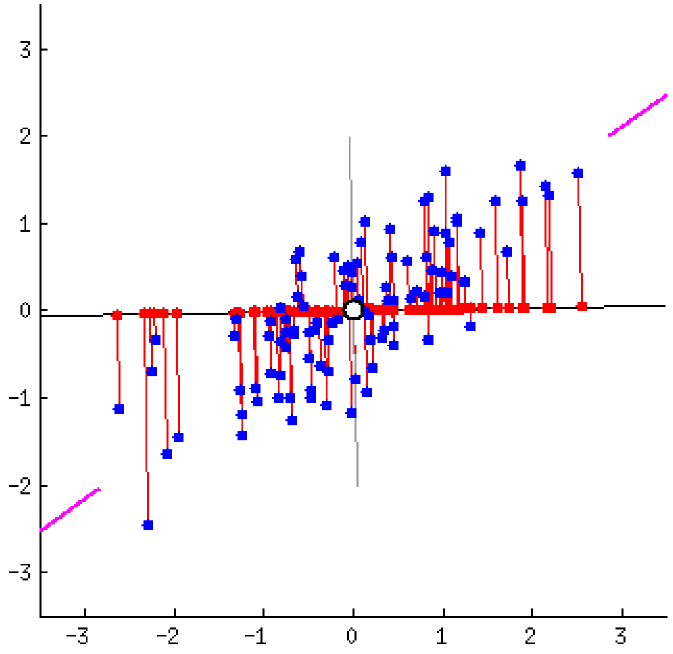
Principal Components Analysis (PCA)



Compare the spacing of the red dots (variance) on Line 3 to Line 1 and 2. See how the spread of red dots on Line 3 is well…. Smaller than on Lines 2 and 3? That means smaller variance of red dots!

Principal Components Analysis (PCA)

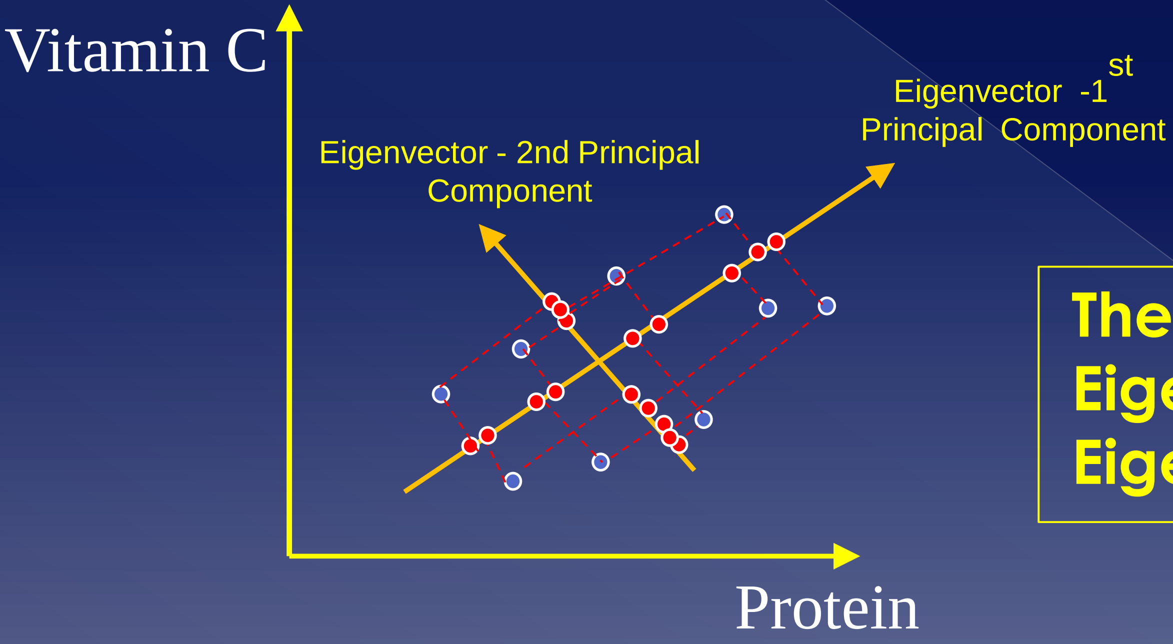
You can draw indefinitely many such lines (see rotating line) and project the data onto them. On some lines, the "spread" of red dots i.e. variance of red dots on the line will be greater than on others. These are the Eigenvectors!



For animated version see file: PCA-Eigenvector-Illustration.gif

Principal Components Analysis (PCA)

- The line where the red dots have **the greatest variance (biggest spread)**, is an **Eigenvector** and the **First Principal Component** of our data! The **variance (spread) of red dots are the Eigenvalues of the Eigenvectors!**
  - The line with **the second biggest spread** is the **second Principal Component**, the line with the **third biggest spread** is the **Third Principal Component** etc.


Vitamin C
Eigenvector -1st Principal Component
Eigenvector - 2nd Principal Component
Protein

The length of the Eigenvector is its Eigenvalue λ

Principal Components Analysis (PCA)

- Using **Eigenvalues/Eigenvectors** is **one way to do PCA**
- **Other ways** also available
  - E.g. **using Single Value Decomposition – SVD**
- Both methods **yield to similar results**
  - i.e. not much difference.

Principal Components Analysis (PCA)

- **PCA in R: the Iris dataset – 1/3**

```
####################################################################################
#                                                    #
# A simple example of Principal Component Analysis on the build in iris dataset.          #
#                                                    #
# Iris is a dataset that contains observations of three iris varieties                 #
# (Iris setosa, Iris virginica, Iris Versicolor ) recording five features              #
# for each observaion: Sepal length, Sepal width, Pedal lentgh, Pedal width and          #
# the species it belongs to (Setosa, Virginica, Versicolor )                            #
#                                                    #
#  For a picture of the Iris plant and what is recorded in the dataset see:             #
#  http://5047-presscdn.pagely.netdna-cdn.com/wp-content/uploads/2015/04/iris_petal_sepal.png    #
#                                                    #
# The Iris dataset contains a total of 150 observations, 50 from each variety.          #
#                                                    #
# The aim of the code is to perform Principal Component Analysis on the Iris dataset.      #
# Please note that this may not make sense for only 5 variables as PCA is mostly used in     #
# situations where the number of variables must be reduces, if these are large (dimensionality).   #
#                                                    #
####################################################################################

# Let's take a quick look at the Iris dataset, by displaying the first 6 observations in the dataset.
# Note: you can peek at more data by supplying a second argument like this: head(iris, 10) which
# means show the first 10 observations of the iris dataaset.
head(iris)

# By peeking at the dataset we see that it has 5 variables, of which the first 4 looks to be numerical values
# and the last one (Species) nominal i.e. not numerical.

# Let's take a summary of the iris data. This will show some fisrt desctiptive statistics.
summary(iris)
```

# cont…

PCA in R: the Iris dataset – 2/3

```
# Since the variable 'Species' has nominal values, we can't use them for PCA. PCA works only
# on numerical values. Hence, get rid of the  column 'Species' and keep just the other ones.
# This can be done using the following command: iris[, 1:4] => This means from the iris dataset
# return  all rows, but only columns 1 until 4 (i.e. exluding column 5 which is the 'Species' variable).
# We store this data in a new variable data pcaData.
# NOTE: We could also do the following: pcaData <- iris[, -5] which means all rows and all columns except
# column 5.

pcaData<-iris[,1:4]

# Let's take a look to see if everything is ok
head(pcaData, 12)


# Yep, looks ok. Now, we need to make sure that there are no
# missing values (that are displayed as NA).
# PCA does not work if there are missing values in any column/variable.
# Let's check this.

# Does variable Sepal.Length have any (at least 1) missing (na) value?
if (any(is.na(pcaData[,"Sepal.Length"]))) {
  sprintf("Sepal.Length has NA values")
} else
  sprintf("Sepal.Length is ok! ")


# Does variable Sepal.Width have any (at least 1) missing (na) value?
if (any(is.na(pcaData[,"Sepal.Width"]))) {
  sprintf("Sepal.Width has NA values")
} else
   sprintf("Sepal.Width is ok! ")


# Does variable Petal.Length have any (at least 1) missing (na) value?
if (any(is.na(pcaData[,"Petal.Length"]))){
  sprintf("Petal.Length has NA values")
} else
   sprintf("Petal.Length is ok! ")


# Does variable Petal.Width have any (at least 1) missing (na) value?
if (any(is.na(pcaData[,"Petal.Width"]))){
  sprintf("Petal.Width has NA values")
} else
   sprintf("Petal.Width is ok! ")
```

#cont…

PCA in R: the Iris dataset – 3/3

```
#
# OK, our data (pcaData) is ok. Now ready to execute PCA
#


# R's princomp() function is one way of executing PCA (there are also other functions available e.g. prcomp() ).
# We use princomp() because it can be configured to use the Covariance matrix to calculate Eigenvalues/Eigenvectors
# Please note that princomp() supports also performing PCA by using a Correlation matrix and SVD. This all depends
# on the parameters that you will provide.
#
# First parameter is our data (pcaData). Since we'll use the Covariance matrix and we signify this by setting
# the parameter cor equal to FALSE. Set to TRUE, princomp() will calculate the Covariance matrix. However you can
# provide yourself the Covariance matrix by setting the covmat parameter.
# If you set parameter cor to TRUE, the Correlation matrix will be used instead.
# Parameter score=TRUE tells princomp to transform each original observation to the new system defined by the principal
# components. Remember that principal components define a new coordinate system and the original data MUST be mapped
# properly onto this new coordinate system.
principalComponents<-princomp(pcaData, cor=FALSE, score=TRUE)

# Ok, done. Now the result of the princomp() function is a new object -that we store in a new variable
# called principalComponents- that has inside all necessary information. This object has attributes that
# you can access.
# But first, let's see what attributes it has.
attributes(principalComponents)

#You can see attributes such sdev, scores etc. You can display their values.
# Here, we display the calculated scores
principalComponents$scores

# Or, you can display a summary, which gives you a better overview.
summary(principalComponents)

# You may also plot the principal components to see the variances of each principal component
# in decreasing order
plot(principalComponents)

# Or you can plot the original data on a coordinate system defined by the two biggest principal
# components (note the bi- in biplot). Note that eigenvectors are the vertical and horizontal axes.
# The red vectors you see are pointing in the direction of the variables, as projected
# into the 2-d plane of the biplot.
biplot(principalComponents)
```

PCA in Python: the Iris dataset

```
#
# Principal Component Analysis in Python
#


#
# Load the required libraries.
# Make sure that you installed properly the sklearn module that contains
# the required functions and datasets
#


#Next two lines required to load the PCA function
from sklearn import decomposition
from sklearn.decomposition import PCA

# sklearn comes with datasets. Make them available to this program
from sklearn import datasets

# Load the iris dataset
iris = datasets.load_iris()

# Get the data of the iris dataset into a new variable
irisDataset = iris.data

# Initialize the PCA function of the sklearn module.
# Here, we say how many principal components we want. We will require
# 2 principal components
pca = decomposition.PCA(n_components=2)

# Here we actually apply PCA to the iris dataset.
# After executing PCA on the dataset, you can examine the properties
# of the pca object to get the necessary information
pca.fit(irisDataset)

# Now transform the data of the iris dataset to the new coordinate system,
# defined by the two Eigenvectors that resulted from PCA
transformedIrisDataset = pca.transform(irisDataset)
```

Discretization

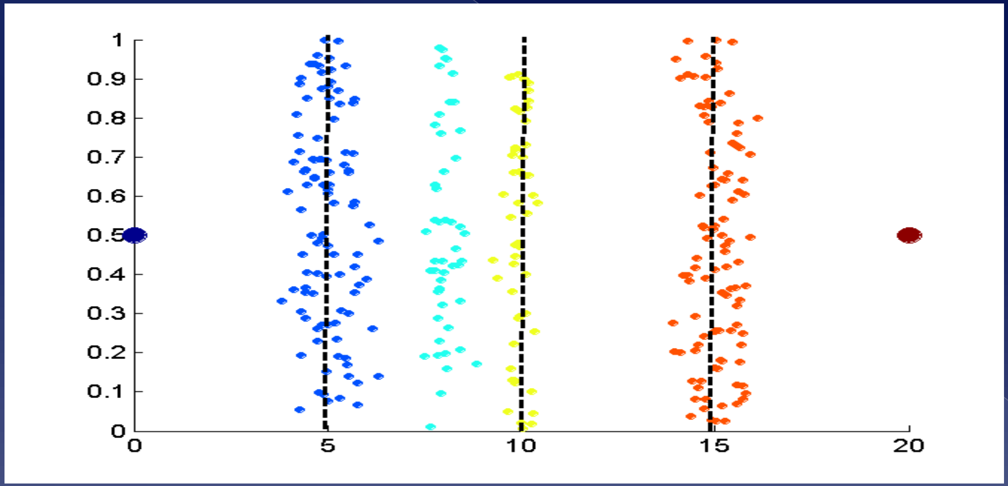
- Discretization?
  - **Divide the range of a continuous** attribute **into intervals**
  - Some classification algorithms only accept categorical attributes.
  - **Reduce data size by discretization**
  - Prepare for further analysis
  - Used in problems that require categorization and correlation analysis

Discretization

- Two ways to discretization
  - **Unsupervised**
    - Don’t take into consideration the classes in which the data item belong
  - **Supervised**
    - Take into consideration the classes in which data items belong

Discretization

- Unsupervised methods
  - **Equal interval width :** Split range in **n equal spaces** by specifying **n-1 split points**



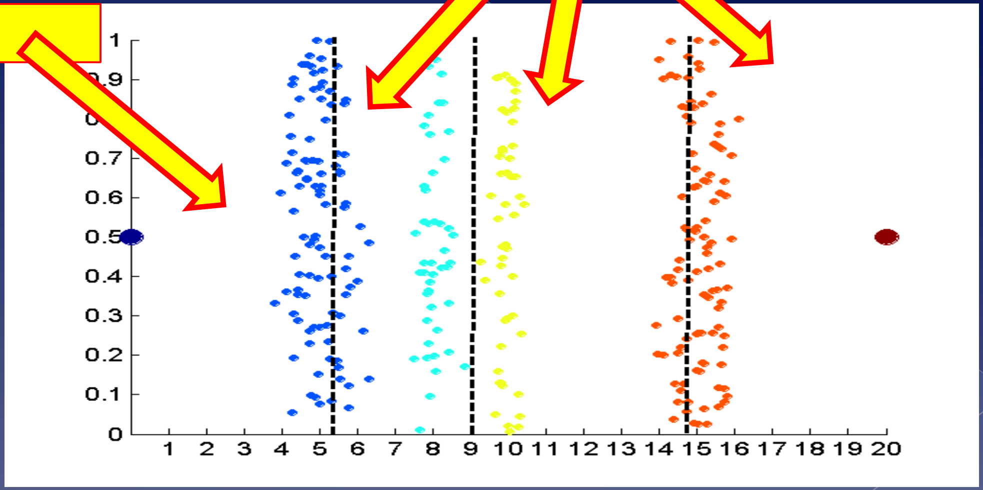
Equal interval width

Discretization

- Unsupervised methods
  - **Equal frequency**: Split range in spaces so **that equal number of data objects are in each space/bin**

Number of objects in this bin…

…equal to number of objects in these bins



Equal frequency

Discretization

- Supervised methods
  - Here **we look at some attribute (class)** of the data and try to take this into consideration when building the bins (hence supervised). Try to **improve quality of bins wrt class**.
  - Bottom-up approach
    - Each item belongs to its own bin. Then try to produce bigger bins by evaluating some metrics
  - Goal: create **bins that are as “clean” as possible wrt an attribute**, i.e. minimize “chaos”/”unorderly-ness” in each bin in terms of the class the items belong.

Discretization

- Can we **measure "chaos"/"unorderly-ness"** in each bin?
  - Yup, that is what **Entropy** does
  - Measuring entropy of bin e_i:

$$e_i = \sum_{i=1}^{k} \frac{m_{i,j}}{m_i} log_2 \frac{m_{i,j}}{m_i}$$

…where k the number of different bins/classes, m_i the number of items in class i, m_{ij} the number of items that are in class j found in bin i. m_{ij}/m_i is the probability of class j in bin i.

Discretization

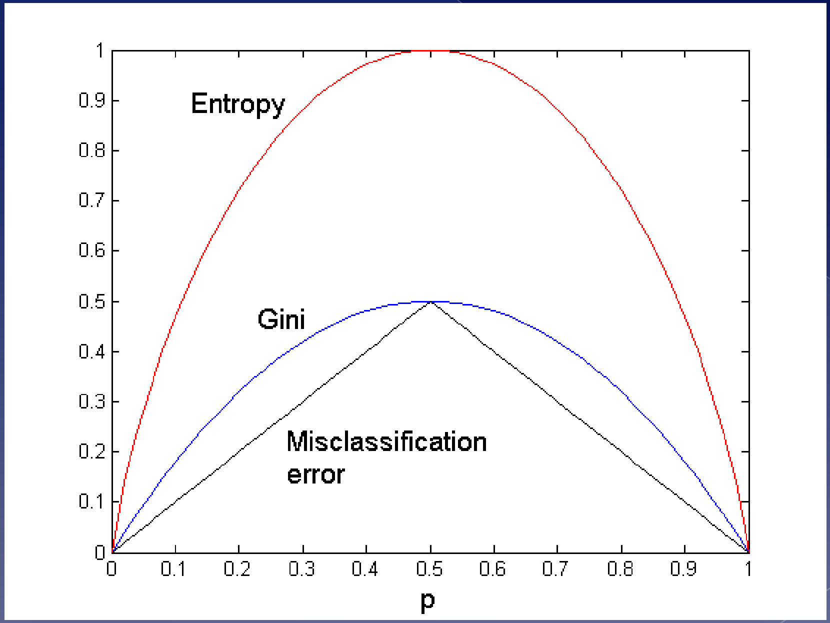
- Total entropy e of the spaces/partitioning is defined as

$$e = \sum_{i=1}^{n} \frac{m_i}{m} e_i$$

…where m total number of data items, m_i the number of data items in bin I (defined in terms of class)

Discretization

- Some notes on Entropy
  - **If Entropy = 0** => no chaos, perfect order, clean space/partition. **Minimum entropy**
  - **If Entropy = 1** => biggest chaos, greatest "unorder", most unclean space/partition. **Maximum entropy**



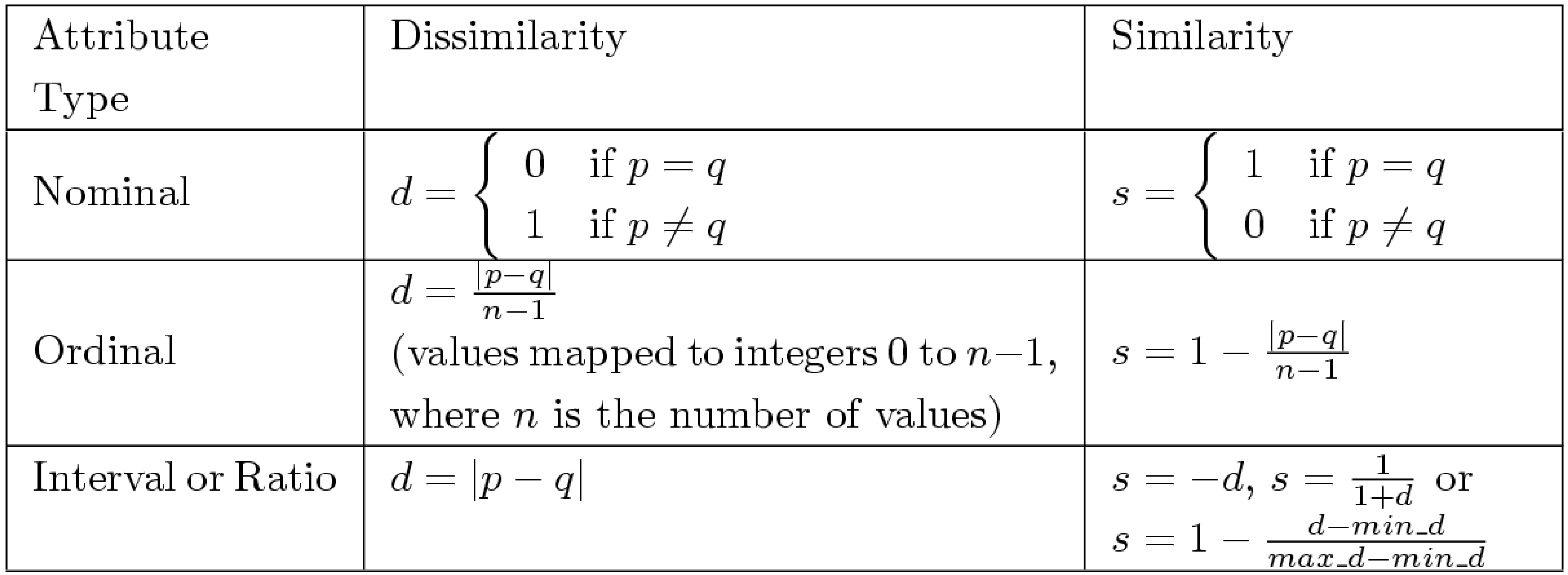
Similarity and dissimilarity measures

Similarity and dissimilarity measures

- **Similarity**
  - Numerical measure of how alike two data objects are.
  - Is higher when objects are more alike.
  - Often falls in the range [0,1]
- **Dissimilarity**
  - Numerical measure of how different two data objects are
  - Lower when objects are more alike
  - Minimum dissimilarity is often 0
  - Upper limit varies
- **Proximity** refers to a similarity or dissimilarity

Similarity and dissimilarity measures

- For simple attributes
  - **Note: q, p below are attribute values for two data objects**
  - **s, d below stand for (s)imilarity and d(istance)**



Attribute Type	Dissimilarity	Similarity
Nominal	$d = \begin{cases} 0 & \text{if } p = q \\ 1 & \text{if } p \neq q \end{cases}$	$s = \begin{cases} 1 & \text{if } p = q \\ 0 & \text{if } p \neq q \end{cases}$
Ordinal	$d = \frac{\lvert p-q \rvert}{n-1}$ (values mapped to integers 0 to $n-1$, where n is the number of values)	$s = 1 - \frac{\lvert p-q \rvert}{n-1}$
Interval or Ratio	$d = \lvert p - q \rvert$	$s = -d$, $s = \frac{1}{1+d}$ or $s = 1 - \frac{d - min\_d}{max\_d - min\_d}$

Table 5.1. Similarity and dissimilarity for simple attributes

Similarity and dissimilarity measures

- Distance
  - is an **dissimilarity measure**
  - Observe that **Dissimilarity and Distance** are same things
    - You use distance to measure similarity/dissimilarity
    - You **transform distance** in order to calculate similarity/dissimilarity e.g. $\boldsymbol{similarity = \frac{1}{distance(p_1,p_w)}}$ **or** $\boldsymbol{similarity = \frac{1}{e^{distance(p_1,p_2)}}}$, etc. In general you choose the proper formula.
- Different ways to measure distance
  - **Euclidian** distance
  - **Minkowski** distance
  - **Mahalanobis** distance

Similarity and dissimilarity measures

- You can define **your own distance measure.**
- However, in order to be considered a proper distance measure, it must be a metric. Or more clearly **it has to have the following properties:**

1. $d(x,y) \geq 0$
2. $d(x,y) = 0 \text{ iff } x = y$
3. $d(x,y) = d(y,x)$
4. $d(x,z) \leq d(x,y) + d(y,z)$

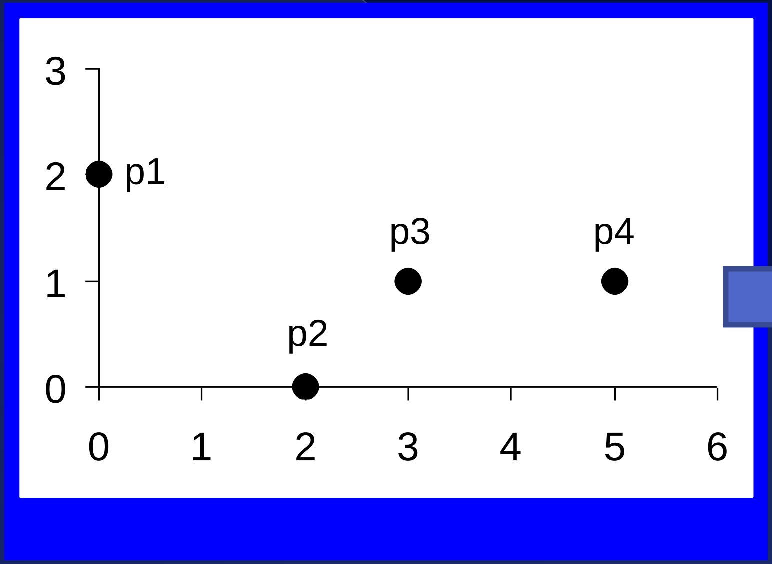
Euclidian Distance

- **"Works" for points x, y** in **one, two, three or more dimensions**
- (known) Formula

$$d(x,y) = \sqrt{\sum_{k=1}^{n} (x_k - y_k)^2}$$

…where *n* is the number of dimensions (attributes) and x_k and y_k are, respectively, the kth attributes (components) or data objects x and *y*.

Euclidian Distance



point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

Data objects

	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

Euclidean Distance Matrix

Minkowski distance

- Minkowski distance **is a generalization of Euclidean Distance**

$$d(x,y) = \sqrt[r]{\sum_{k=1}^{n} |(x_k - y_k)|^r}$$

…where *r* is a parameter, ***n*** is the number of dimensions (attributes) and **x_k** and **y_k** are, respectively, the **kth attributes** (components) or **data objects x and *y***.

Minkowski distance

- **Special cases of the Minkowski distance:**
- ***r* = 1**. City block (Manhattan distance, taxicab, L_1 norm) distance.
  - A common example of this is the **Hamming distance**, which is just the number of bits that are different between two binary vectors
- ***r* = 2**. Euclidean distance
- $r \rightarrow \infty$. "Supremum" (L_{max} norm, L_∞ norm) distance.
  - This is the maximum difference between any component of the vectors
- **IMPORTANT!** Do not confuse *r* with *n*, i.e., all these distances are defined for all numbers of dimensions.

Minkowski distance

Manhattan distance, r=1

L1	p1	p2	p3	p4
p1	0	4	4	6
p2	4	0	2	4
p3	4	2	0	2
p4	6	4	2	0

Euclidean distance, r=2

L2	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

Distance $r \to \infty$, L_∞ norm

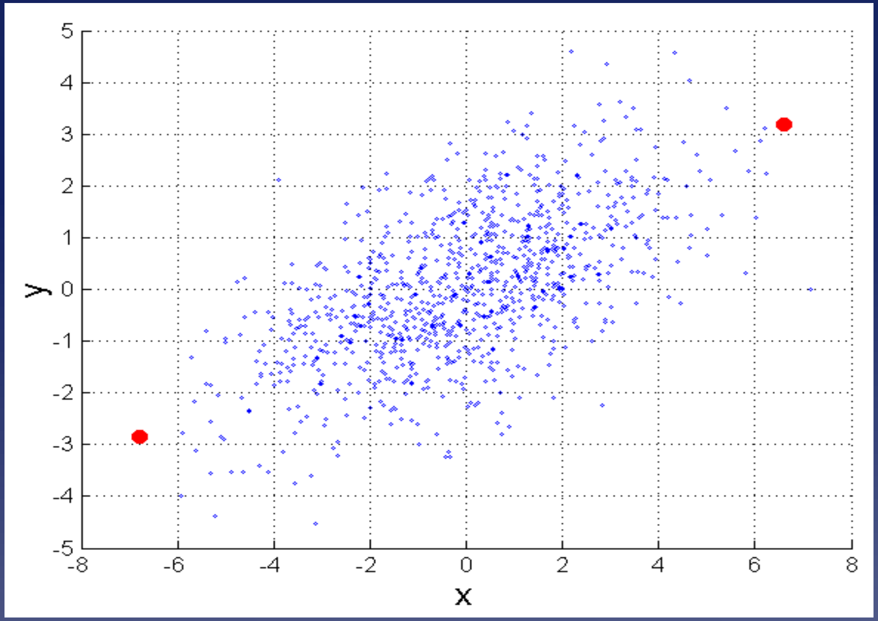
L_∞	p1	p2	p3	p4
p1	0	2	3	5
p2	2	0	1	3
p3	3	1	0	2
p4	5	3	2	0

point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

Distance Matrices

Mahalanobis distance

- Is the distance **between a point p and a distribution D**
  - **If Mahalanobis distance = 0**, then point is at the mean of D



$$d(x,y) = (p-q)\Sigma^{-1}(p-q)^T$$

Σ is the covariance matrix of the input data *X*

$$\Sigma_{\iota,\kappa} = \frac{1}{n-1}\sum_{i=1}^{n}(X_{ij}-\bar{X}_k)(X_{ik}-\bar{X}_k)$$

For red points, the Euclidean distance is 14.7, Mahalanobis distance is 6.

Cosine similarity

- **Applies to document data**

- If d_1 and d_2 are two document vectors, then

  cos(d_1, d_2) = ($d_1 \bullet d_2$) / ||d_1|| ||d_2|| ,

  where $\bullet$ indicates vector dot product and || *d* || is the length of vector *d*.

- Example:

  d_1 = **(3, 2, 0, 5, 0, 0, 0, 2, 0, 0)**
  d_2 = **(1, 0, 0, 0, 0, 0, 0, 1, 0, 2)**

$d_1 \bullet d_2$= 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5

$||d_1||$ = $(3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)^{0.5}$ = $(42)^{0.5}$ = 6.481

$||d_2||$ = $(1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{0.5}$ = $(6)^{0.5}$ = 2.245

Hence, cos(d_1, d_2) = .3150

Summary

Summary

- **Running time** of algorithms is characterized in terms of **number of steps they take to solve a problem**
  - Number of steps expressed as a function of the problem size, T(n) (in general **polynomial time alg = good! Exponential time algorithm = bad!**)
    - **Problem size**: aspect of input data that will influence number of steps
    - Use of asymptotic notations to characterize **running time** (referred to as **time complexity**): **O(), Θ()**
- Data has different types of attributes depending on the type of values they may take

Summary

- **Different types** imply **different methods of analysis**
  - Different methods of analysis work for on different types of data
- **Preprocessing** is one of the most important steps in data mining
  - Consumes most of the time (70-80% of dm tasks)
- There are **different objectives** when preprocessing data
  - Reducing dimensions
  - Sampling
  - Discretization

Summary

- **PCA** most powerful way **to reduce dimensions of the dataset (curse of dimensionality) which causes problems in Big Data**
  - Used in many-many Big Data environments
- There are also **different distance metrics**
  - Depending on objective of task at hand
- In general, **choose wisely, the appropriate, types of values, preprocessing methods and distance metrics**
  - Will **influences** your data mining **results**!

Appendices

APPENDIX A: Related Bibliography

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