FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG
NATURWISSENSCHAFTLICHE
FAKULTÄT

# Introduction

Lecture “Mathematics of Learning (Maths of Data Science 1)”

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Winter semester 2022

WIRTSCHAFTS
MATHEMATIK

# Preliminaries

- These lecture notes are based on the material by Frauke Liers from the summer semester 2022. It is a compilation from different sources that will be mentioned for further references during the lecture.
- Among the different sources: *Many thanks to Frauke Liers, Martin Burger, Daniel Tenbrinck, and Philipp Wacker for allowing me to use their material from earlier lectures!*
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- Exercises: Jan Krause and Ehsan Waiezi, take place online in the first week

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- Students need to pass a written exam in presence at the end of the semester.
- Passing this course is mandatory for Master Data Science.

# What is Data Science?

- relatively **new field** due to recent boost in digital transformation → *digitization, IoT, paperless office, ...*
- needs mathematics, computer science, and domain knowledge
- well-known examples for successfully harvesting and interpreting data:
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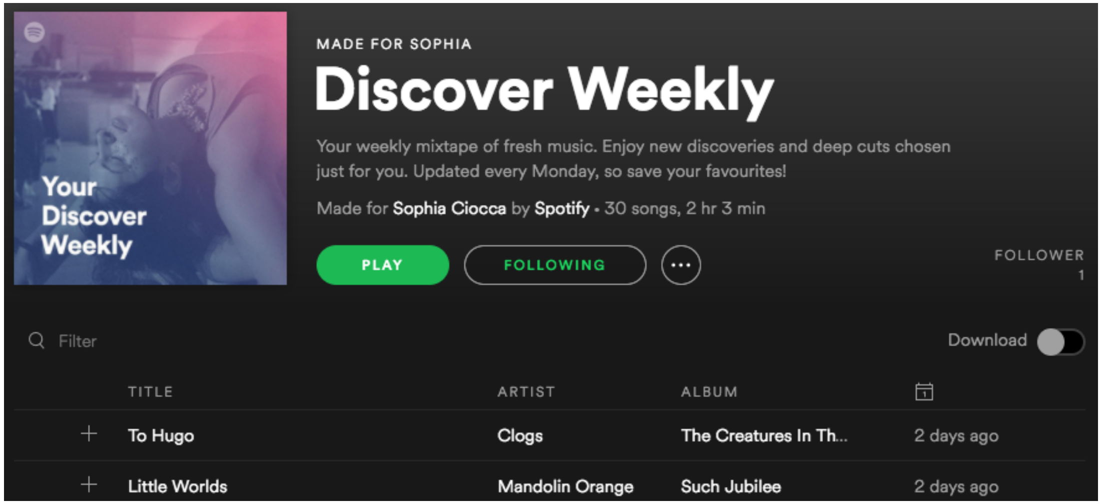

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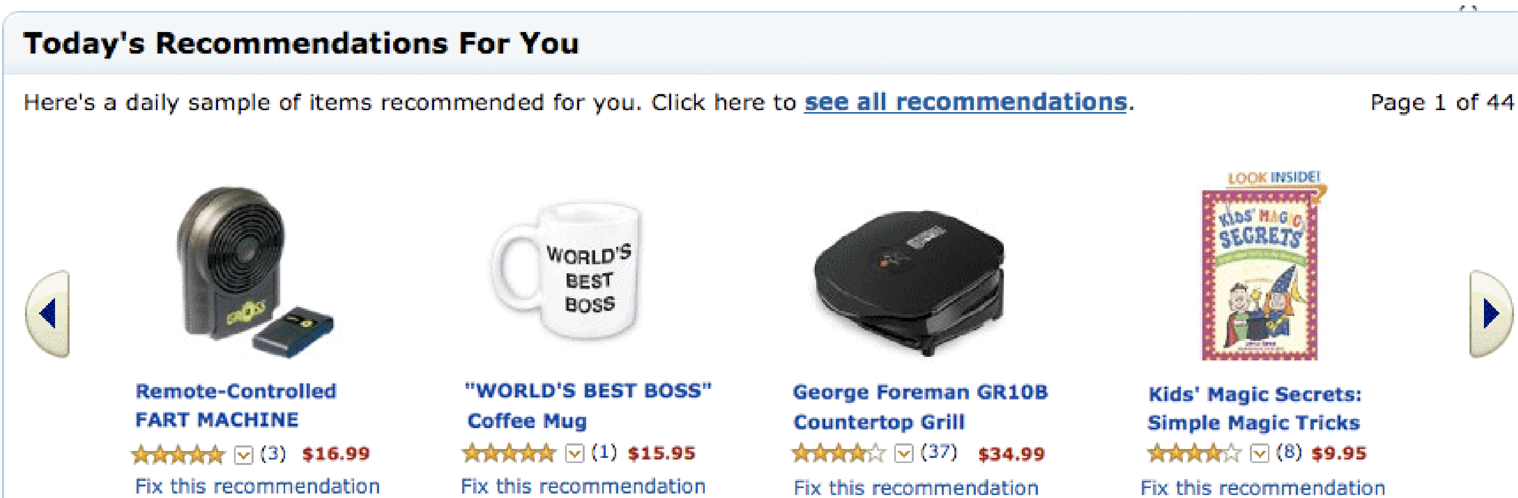

# Data Science Cycle

**iteratively...**

1. extract and process / correct data
2. extract hypotheses
3. *develop approaches, models, algorithms, implementations (from statistics, optimization, numerics and simulation, math theory, databases, AI,...)*
4. use approaches to explore and understand data
5. derive predictions, decisions, consequences, recommendations for application domain
6. visualize data and results, possibly iterate

Your study programme covers these aspects, with specializations possible.

Many applications: logistics, mobility, health care, energy networks, ...

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**Goals of this course**

- learn fundamental math-based data science concepts and algorithms, know where to look it up
- understanding the underlying mathematical reasons why certain algorithms work well and others do not
- solve realistic problems

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**Topics: unsupervised learning and supervised learning methods, e.g.**

- clustering
- PCA, kernel methods, kernel-PCA
- statistical methods
- machine learning via neural networks
- graphical models,...

# Some Data Science Examples

- prediction of solar injection in energy networks
  and best-possible curtailment decisions beforehand
  to avoid breakdown of the network
- learn customer / market preferences, produce accordingly
  and forecast price developments
- predict shelf life of food
- forecast development of chronic diseases,
  determine best possible medication and treatment
- forecast development of Covid-19, determine best possible reactions
- many more

# Further Reading

- Hastie, Tibshirani, Friedman: The Elements of Statistical Learning: Data Mining, Inference, and Prediction, Springer
- www.deeplearningbook.org

# Excursion: Some Background in Algorithms

This excursion is meant to give some brief and abstract introduction into algorithms. Further reading, e.g.:

- Thomas Cormen, Charles Leiserson, Ronald Rivest, and Cliff Stein: Introduction to Algorithms, MIT Press
- Thomas Ottmann and Peter Widmayer: Algorithmen und Datenstrukturen,
- Robert Sedgewick, Kevin Wayne: Algorithms, Addison-Wesley,
- Donald Knuth: The Art of Computer Programming,

and many others.

For exemplary purposes, we consider a basic operation: sorting numbers.

# Sorting: Notation

Sorting is a basic operation in computer science.

- **Input:** $n$ numbers $\langle a_1, a_2, \ldots, a_n \rangle$.
- **Output:** permutation $\langle a'_1, a'_2, \ldots, a'_n \rangle$ such that $a'_1 \leq a'_2 \leq \ldots \leq a'_n$.

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- How many elements?
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$\vdots$

An algorithm is called **correct**, if it **terminates** for all instances with a correct solution. It then **solves** the problem.

# Insertion Sort


Figure 2.1 Sorting a hand of cards using insertion sort.

Aus: Cormen et al. (2001) "Algorithms", chpt. 2;
MIT Press, Cambridge (MA)

# Insertion Sort

As parameters, it has the array `A` and its length `length(A)`. In the for-loop, the *j*-th element of the sequence is inserted in the correct position that is determined by the while-loop. In the latter we compare the element to be inserted (`key`) from 'right' to 'left' with each element from the sorted subsequence stored in `A[0],...,A[j-1]`. If `key` is smaller, it has to be insert further left. Therefore, we move `A[i]` one position to the right and decrease `i` by one in line 7. If the while-loop stops, `key` is inserted.

```
insertion_sort(A)
  for j = 1 to (length(A)-1) do
    key = A[j]
    // insert A[j] into the sorted sequence A[1...j-1]
    i = j
    while (i > 0 and (A[i-1] > key) ) do
      A[i] = A[i-1]
      i = i-1
    end while
    A[i] = key
    end for
```

# Insertion sort for the example sequence $\langle 5, 2, 4, 6, 1, 3 \rangle$

| A[1] | A[2] | A[3] | A[4] | A[5] | A[6] |
|---|---|---|---|---|---|
| 5 | 2 | 4 | 6 | 1 | 3 |
| 2 | 5 | 4 | 6 | 1 | 3 |
| 2 | 4 | 5 | 6 | 1 | 3 |
| 2 | 4 | 5 | 6 | 1 | 3 |
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- When the `for`-loop stops, we have `j=n` and `A[0..n-1]` is sorted.
- Termination: The `while`- and the `for`-loop always terminate.

# Used Ressources

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Question: Does the worst-case running time of insertion_sort grow linearly, quadratically, . . ., or even exponentially in $n$?

# Running Time Insertion Sort

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**For a sequence sorted in reverse order (worst case):**

- The `while`-loop stops only when $i = 0$
- $j = 1$: 1 assignment $A[i] = A[i-1]$
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in total: $\sum_{i=1}^{n-1} i = \frac{n(n-1)}{2}$ many assignments; quadratically many

# ...more formally

## Worst-Case Running Time

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## Worst-Case Running Time

Idea: Consider only the characteristic behaviour as a function of the input size; ignore constants and terms of lower order.
If the values of a function $f$ are "less" than those of another function $g$ for all $n$ larger than some constant $n_0$ (up to a constant factor $c$), then asymptotically $g$ is an upper bound for $f$, denoted by $f \in O(g)$.

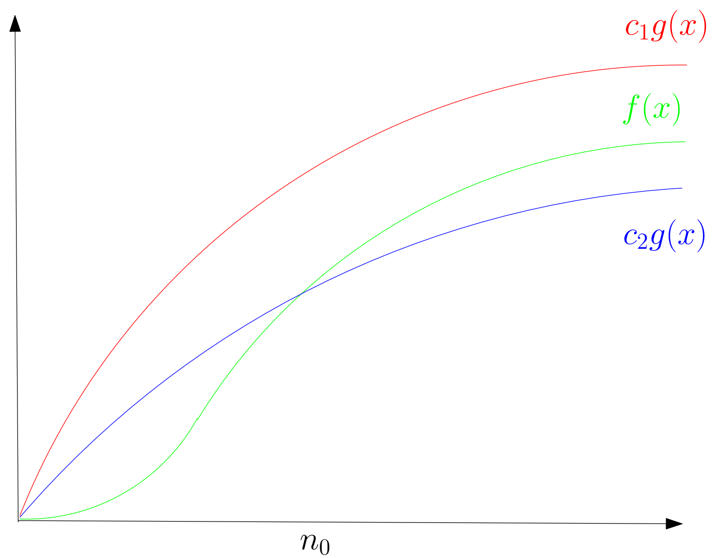
More generally, the following symbols are often used for a function $g \colon \mathbb{N} \to \mathbb{R}$ (for upper bounds $O$, for lower bounds $\Omega$ and for equally fast growth $\Theta$):

$$O(g) := \{f \colon \mathbb{N} \to \mathbb{R} \mid (\exists c, n_0 > 0)(\forall n \geq n_0) : 0 \leq f(n) \leq cg(n)\}$$

$$\Omega(g) := \{f \colon \mathbb{N} \to \mathbb{R} \mid (\exists c, n_0 > 0)(\forall n \geq n_0) : 0 \leq cg(n) \leq f(n)\}$$

$$\Theta(g) := \{f \colon \mathbb{N} \to \mathbb{R} \mid (\exists c_1, c_2, n_0 > 0)(\forall n \geq n_0) : c_1 g(n) \leq f(n) \leq c_2 g(n)\}$$

# Worst-Case Running Time




- The *worst case* running time of insertion sort is $O(n^2)$.

# Design of Algorithms

insertion sort: *incremental method.*
different principle: *'divide and conquer'*

- **divide** problem in subproblems
- **conquer** the subproblems through recursive solution. (If small enough, solve them directly.)
- **combine** the solutions of the subproblems to a solution for the original problem.

# Merge Sort

- **divide:** divide sequence of $n$ numbers in the middle into two sub sequences.
- **conquer:** sort the subsequences recursively using *merge sort*.
- **combine:** merge the two subsequences to a sorted sequence.

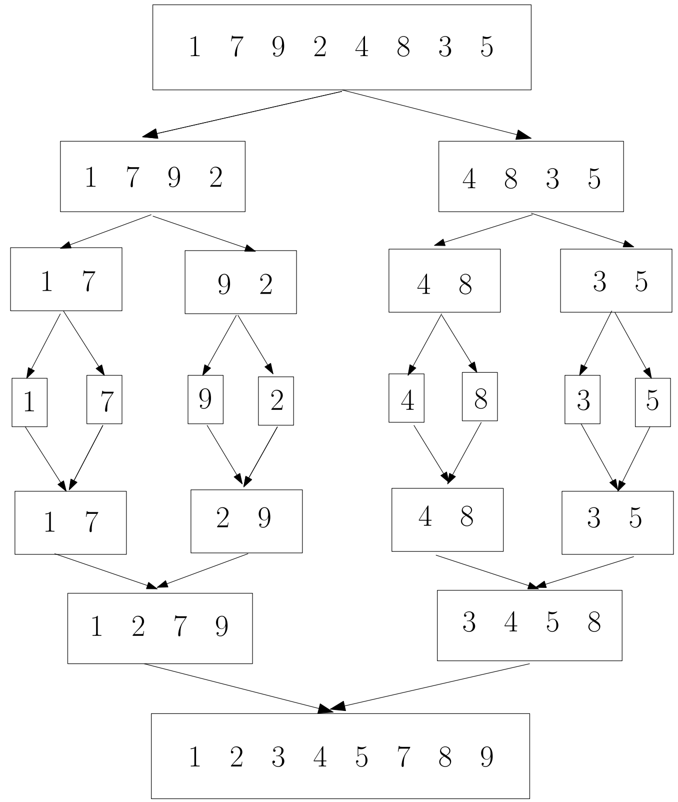
$\longrightarrow$ for sequences containing one element only nothing has to be done.

# Merge sort

Sort the sequence stored in `A[p]...A[r]`:

```
void merge_sort(int[] A, int p, int r) {
  int q; /* Middle of the sequence */
  if (p < r) {  /* if p = r: only 1 element */
    q = p+((r-p)/2);
    merge_sort (A, p, q);  /* left subsequence */
    merge_sort (A, q+1, r);  /* right subsequence */
    merge (A, p, q, r);  /* merge subsequences */
  }
}
```

# Illustration of Merge Sort



# Merge Sort

It can be shown: worst-case running time of merge sort is $O(n \log n)$ (better than insertion sort)

In fact: any algorithm for sorting $n$ numbers that uses only comparisons and moves of numbers needs at least $\Omega(n \log n)$.

BTW: try the shell-command **sort**!

This is the end of our excursion.
We will now return to the introduction of learning methods.