Principles of Computer Science II

Algorithms for BioInformatics

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Lecture 5

Recursion Coding Style

Recursion is a way of programming or coding a problem, in which a function calls itself one or more times in its body. Usually, it is returning the return value of this function call. If a function definition fulfils the condition of recursion, we call this function a recursive function.

Termination condition:

- A recursive function has to terminate to be used in a program.
- A recursive function terminates, if with every recursive call the solution of the problem is downsized and moves towards a base case.
- A base case is a case, where the problem can be solved without further recursion.

Factorial Computation: Using Iteration

```python
def iterative_factorial(n):
    result = 1
    for i in range(2,n+1):
        result *= i
    return result
```

Factorial Computation: Using Recursion

```python
def factorial(n):
    if n == 1:
        return 1
    else:
        return n * factorial(n-1)
```

Factorial Computation

```
def factorial(n):
    print("factorial has been called with n = " + str(n))
    if n == 1:
        return 1
    else:
        res = n * factorial(n-1)
        print("intermediate result for ", n, " * factorial(" ,n-1, "):
        return res

print(factorial(5))
```

Fibonacci Numbers

The Fibonacci numbers are defined by:
$F_n = F_{n-1} + F_{n-2}$
where $F_0 = 0$ and $F_1 = 1$

- 0,1,1,2,3,5,8,13,21,34,55,89, ...

Factorial Computation: Using Recursion

```
def fib(n):
    if n == 0:
        return 0
    elif n == 1:
        return 1
    else:
        return fib(n-1) + fib(n-2)
```

Factorial Computation: Using Iteration

```
def fibi(n):
    a, b = 0, 1
    for i in range(n):
        a, b = b, a + b
    return a
```

Measure Performance

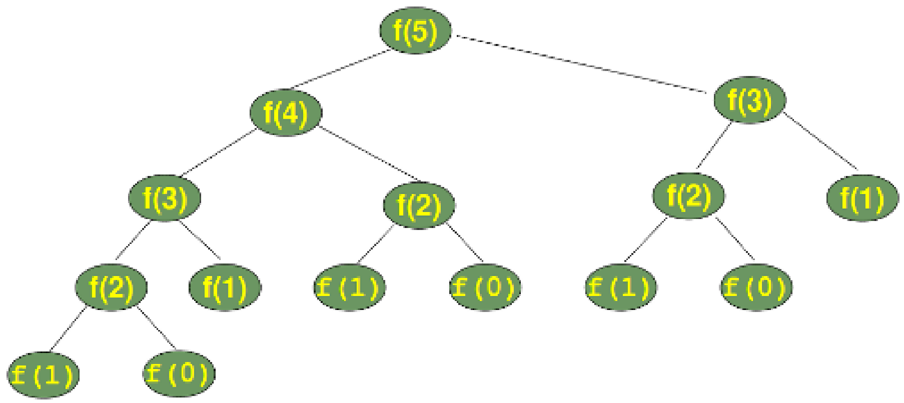
```python
import time

for i in range(1,41):
        t1 = time.perf_counter()
        s = fib(i)
        t2 = time.perf_counter() - t1

        t3 = time.perf_counter()
        s = fibi(i)
        t4 = time.perf_counter() - t3

        print(f"n={i}, fib: {t2:.2f}, fibi: {t1:.2f}, percent: {t2/t4:.
```

Fibonacci Numbers



Factorial Computation: Using Recursion and Memory

```python
memo = {0:0, 1:1}
def fibm(n):
    if not n in memo:
        memo[n] = fibm(n-1) + fibm(n-2)
    return memo[n]
```

Pebble Game

- Game played in turns by 2 players.
- Two piles of equal number of pebbles.
- Each turn a player may either
  - take 1 pebble **from a single pile**, or
  - take 1 pebble **from both piles**.
- The player that takes the last pebble wins.

Best Strategy for Winning the Pebble Game

- Does the first player always have an advantage?
- Let's consider the most simplified version.
  - Pebbles = 2 – we call this the 2×2 game.
  - Is there a winning strategy?
  - What is the winning strategy?

Generaled Strategy for Winning the Pebble Game

- Can we generalize the strategy of the 2×2 game?
- What about the 3×3 game?
  - Consider different game sequences.
- Consider the $n \times n$ game.
  - Is there only one winning strategy?
  - How easy it is to describe our strategy?
  - Quality of solution.

We build a matrix for all game combinations. Four actions:

1. $\uparrow$ take one pebble from pile A.
2. $\leftarrow$ take one pebble from pile B.
3. $\nwarrow$ take one pebble from each pile.
4. * ignore game.

	0	1	2	3	4	5	6	7	8	9	10
0											
1											
2											
3											
4											
5											
6											
7											
8											
9											
10											

- The first player always loses the 2×2.
- Clearly also for 0×2, 0×4, ...
- Can we generalize for all games where each pile has an even number of pebbles?

	0	1	2	3	4	5	6	7	8	9	10
0	*		*		*		*		*		*
1											
2	*		*								
3											
4	*										
5											
6	*										
7											
8	*										
9											
10	*										

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	0	1	2	3	4	5	6	7	8	9	10
0	*		*		*		*		*		*
1											
2	*		*		*		*		*		*
3											
4	*		*		*		*		*		*
5											
6	*		*		*		*		*		*
7											
8	*		*		*		*		*		*
9											
10	*		*		*		*		*		*

- Only 1 option for all 0×1, 0×3, ...and 1×0, 3×0, ...

	0	1	2	3	4	5	6	7	8	9	10
0	*		*		*		*		*		*
1											
2	*		*		*		*		*		*
3											
4	*		*		*		*		*		*
5											
6	*		*		*		*		*		*
7											
8	*		*		*		*		*		*
9											
10	*		*		*		*		*		*

- Only 1 option for all 0×1, 0×3, ...and 1×0, 3×0, ...

	0	1	2	3	4	5	6	7	8	9	10
0	*	←	*	←	*	←	*	←	*	←	*
1	↑										
2	*		*		*		*		*		*
3	↑										
4	*		*		*		*		*		*
5	↑										
6	*		*		*		*		*		*
7	↑										
8	*		*		*		*		*		*
9	↑										
10	*		*		*		*		*		*

- Only 1 option for all 0×1, 0×3, ...and 1×0, 3×0, ...
- Can we generalize for other columns/rows where one pile has an odd number of pebbles and the other an even?

	0	1	2	3	4	5	6	7	8	9	10
0	*	←	*	←	*	←	*	←	*	←	*
1	↑		↑		↑		↑		↑		↑
2	*	←	*	←	*	←	*	←	*	←	*
3	↑		↑		↑		↑		↑		↑
4	*	←	*	←	*	←	*	←	*	←	*
5	↑		↑		↑		↑		↑		↑
6	*	←	*	←	*	←	*	←	*	←	*
7	↑		↑		↑		↑		↑		↑
8	*	←	*	←	*	←	*	←	*	←	*
9	↑		↑		↑		↑		↑		↑
10	*	←	*	←	*	←	*	←	*	←	*

- Only 1 option for all 0×1, 0×3, ... and 1×0, 3×0, ...
- Can we generalize for other columns/rows where one pile has an odd number of pebbles and the other an even?
- What about the other rows/columns?

	0	1	2	3	4	5	6	7	8	9	10
0	*	←	*	←	*	←	*	←	*	←	*
1	↑	↖	↑	↖	↑	↖	↑	↖	↑	↖	↑
2	*	←	*	←	*	←	*	←	*	←	*
3	↑	↖	↑	↖	↑	↖	↑	↖	↑	↖	↑
4	*	←	*	←	*	←	*	←	*	←	*
5	↑	↖	↑	↖	↑	↖	↑	↖	↑	↖	↑
6	*	←	*	←	*	←	*	←	*	←	*
7	↑	↖	↑	↖	↑	↖	↑	↖	↑	↖	↑
8	*	←	*	←	*	←	*	←	*	←	*
9	↑	↖	↑	↖	↑	↖	↑	↖	↑	↖	↑
10	*	←	*	←	*	←	*	←	*	←	*

An algorithmic approach for winning the Pebble Game

- How can we build the matrix for any game size, e.g., 20×20
- What is the algorithm for winning the game?

An algorithmic approach for winning the Pebble Game

- How can we build the matrix for any game size, e.g., 20×20
- What is the algorithm for winning the game?
- Why should I care?

An algorithmic approach for winning the Pebble Game

- How can we build the matrix for any game size, e.g., 20×20
- What is the algorithm for winning the game?
- Why should I care?
- It is the sequence alignment problem.
- The computational idea used to solve both problems is the same.
- We need to understand how algorithms work.

Methodology of solving a computational problem

- What is the problem at hand ?
  - Identify & Understand assumptions.
  - What is our goal ?
  - Identify similar problems/solutions in the bibliography
  - What are the theoretical foundation ?
  - Can we formulate the problem in a unambiguous and precise way ?
- What is the Input that we have ?
  - Do we have enough data or should we try to collect?
  - Open data sets ?
  - Can we synthesize input data ?
- What is the expected Output ?

Solution Sketch

- Do we have a rough idea of a solution ?
- Do we have identified an approach to solving the problem ?
  - think again !
  - go through the definition – maybe we overlooked something ?
- Write down a solution sketch
  - check if it adheres to the initial assumptions
  - can you try it out with a small input ?
- Is the solution correct ? can we provide some arguments ?
- What is the performance of the solution ?
- Can we think of a more efficient solution ?

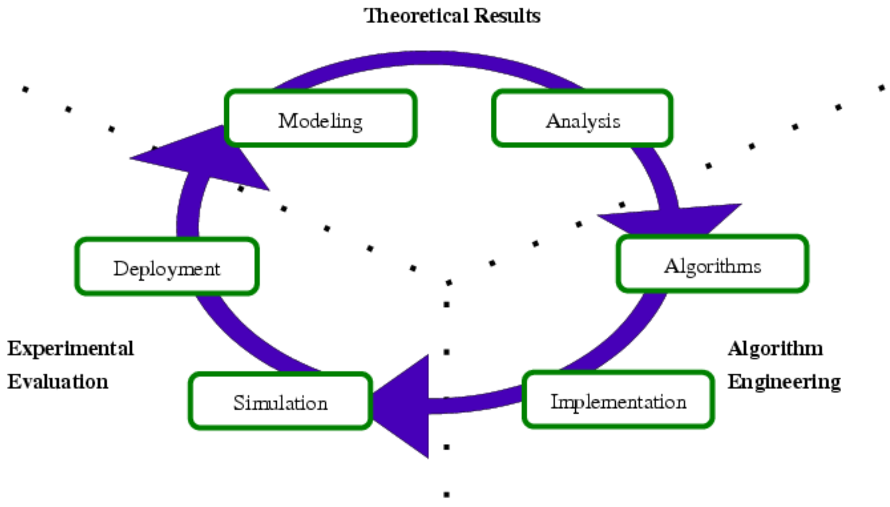
Implement the first version

- Pick your programming language of choice.
- Implement your solution
  - No need to try to make it elegant / fast.
  - Remember Donalt Knuth: There is no such thing as early optimization.
- Get some input data
  - Open datasets
  - Small size
- Limited Evaluation
  - does it work ?
  - do you need to make any modifications ?
  - are there special cases that you missed ?

Iterative approach

- Step-by-step development
  - Continuous development.
  - Agile methodology.
- Identify issues in previous version
  - Code beautification.
  - Bug fixes.
  - Performance improvements.
  - Additional functionalities.
- Implement improvements
  - Make sure code is always clean + easy to maintain.
  - Keep detailed records of changes.
  - Always keep history of source code evolution.
- Performance Evaluation
  - bigger input.
  - scalability ?

Theoretical – Practical Approach Cycle



Quality of Code

John Woods

Always code as if the guy who ends up maintaining your code will be a violent psychopath who knows where you live.

Measuring Performance

- Performance of an algorithm?
  - Speed/Computational Time
  - Memory/Space
  - Robustness/Failures
  - Network/Communication
  - Consumption/Energy
  - ...
- How can we measure the speed/memory/robustness/...of an algorithm?
- How much performance degrades when the amount of input data increases?

Computational Time Complexity

Computational Complexity

Describes the change in the runtime of an algorithm, depending on the change in the input data's size.

- Measures the speed of an algorithm.
- How much additional time it requires when the amount of input data increases.
- Examples:
  - How much longer does it take to find an element within an unsorted array when the size of the array doubles?
  - How much longer does it take to find an element within a sorted array when the size of the array doubles?

Space Complexity

Computational Complexity

Describes the requirements in terms of memory of an algorithm, depending on the size of the input data.

- Measures the memory requirements of an algorithm.
- Without considering the size of the input data.
- Additional memory is used by:
  - Helper variables within loops.
  - Temporary data structures.
  - Call stack.
  - ...

Complexity Classes – Big O Notation

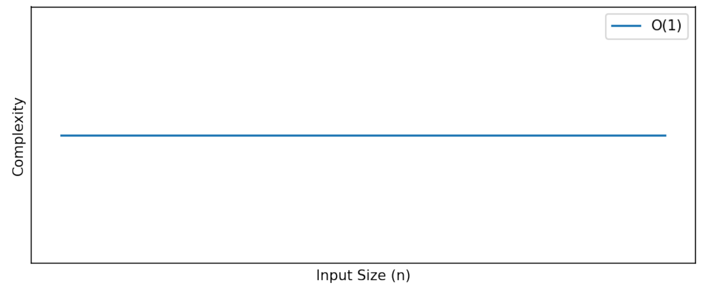
- We organize algorithms into Complexity Classes
- A complexity class is noted using the Bachmann-Landau symbol $\mathcal{O}$ ("big O")
- Let f the function to be estimated
- Let g the comparison function
- We write $f(x) = \mathcal{O}(g(x))$ as $x \to \infty$
- f is bounded above by g (up to constant factor) asymptotically.
- We do not measure the exact running time rather we classify the behaviour when n is sufficiently large.

Complexity Classes – Asymptotic behaviour

- An algorithm may contain sub-components of different complexity.
- For large inputs, the behaviour will be dominated by the part of the complexity that grows fastest.
  - Complexity function $g(n) = 100 \times n^2 + 10000 \times n + 840$ grows like $\mathcal{O}(n^2)$
  - Complexity function $g(n) = 0.33 \times n^3$ grows like $\mathcal{O}(n^3)$
- If $f(x)$ is a sum of several terms: we keep the one with the largest growth rate.
- If $f(x)$ is a product of several factors, any constants can be omitted.

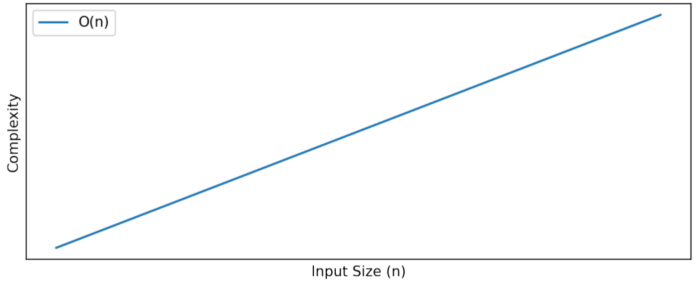
Constant Time – $\mathcal{O}(1)$

- Pronounced: "Order 1", "O of 1", "big O of 1"
- The runtime is constant.
- Independent of the number of input elements n.
- Examples
  - Accessing a specific ellement of an array of size n.
  - Inserting an element at the beginning of a list.



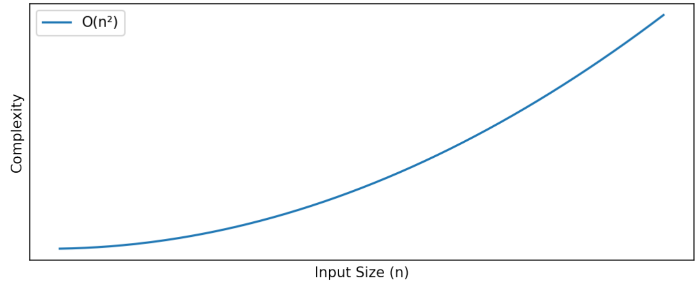
Linear Time – $\mathcal{O}(n)$

- Pronounced: "Order n", "O of n", "big O of n"
- Runtime grows linearly with the number of input elements n.
- If n doubles, then the runtime approximately doubles, too.
- Examples
  - Finding a specific ellement in an array of size n.
  - Summing up all elements of an array.



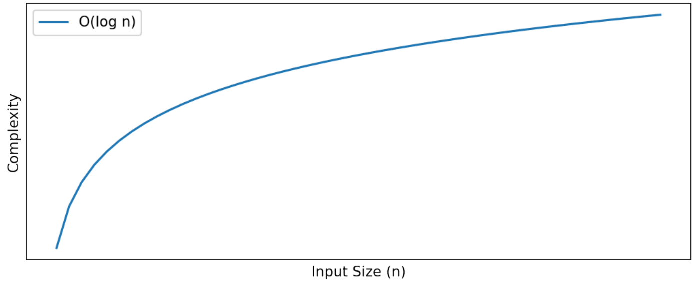
Quadratic Time – $\mathcal{O}(n^2)$

- Pronounced: "Order n squared", "O of n squared", "big O of n squared"
- Runtime grows linearly to the square of the number of input elements n.
- If n doubles, then the runtime approximately quadruples.
- Examples
  - Simple sorting algorithms (e.g., Insertion Sort).



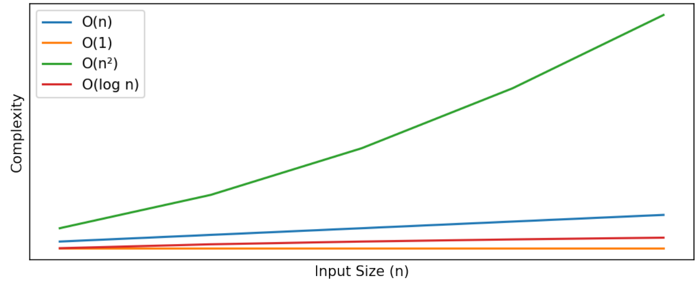
Logarithmic Time – $\mathcal{O}(\log n)$

- Pronounced: "Order log n", "O of log n", "big O of log n"
- Runtime increases by a constant amount when the number of input elements n doubles.
- Examples
  - Binary search.



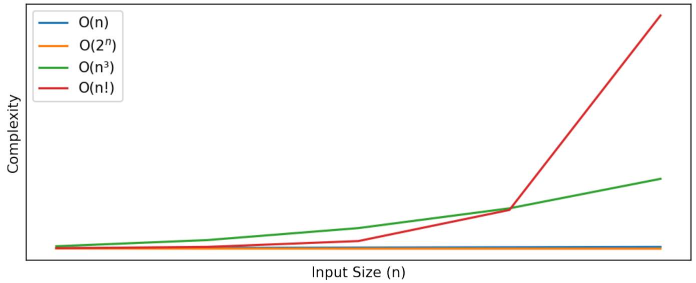
Big O Notation Order

- $\mathcal{O}(1)$ – constant time
- $\mathcal{O}(\log n)$ – logarithmic time
- $\mathcal{O}(n)$ – linear time
- $\mathcal{O}(n \log n)$ – quasilinear time
- $\mathcal{O}(n^2)$ – quadratic time



Other Complexity Classes

- $\mathcal{O}(n^m)$ – polynomial time
- $\mathcal{O}(2^n)$ – exponential time
- $\mathcal{O}(n!)$ – factorial time
- ...



Little-oh and Big-Theta notations

- We write $f(x) = o\left(g(x)\right)$ – read "$f(x)$ is little-oh of $g(x)$"
  - $g(x)$ grows much faster than $f(x)$
  - f is dominated by g asymptotically.
  - $\mathcal{O}$ has to be true for at least one constant M, little-o holds for every postivie constant ϵ, however small.
- We write $f(x) = \Theta\left(g(x)\right)$ – read "$f(x)$ is big-theta of $g(x)$"
  - f is bounded both above and below by g asymptotically.
- Consider $T(n) = 73n^3 + 22n^2 + 58$, all the following are generally acceptable:
  - $T(n) = \mathcal{O}(n^{100})$ – grows asymptotically no faster than $n^1 00$
  - $T(n) = \mathcal{O}(n^3)$ – grows asymptotically no faster than n^3
  - $T(n) = \Theta(n^3)$ – grows asymptotically as fast as n^3