

Principles of Computer Science II

Algorithms for Bioinformatics

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Lecture 5



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?



Generalized 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. \swarrow 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 $0 \times 2, 0 \times 4, \dots$
- ▶ 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 $0 \times 1, 0 \times 3, \dots$ and $1 \times 0, 3 \times 0, \dots$

	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 $0 \times 1, 0 \times 3, \dots$ and $1 \times 0, 3 \times 0, \dots$
- ▶ 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 $0 \times 1, 0 \times 3, \dots$ and $1 \times 0, 3 \times 0, \dots$
- ▶ 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 ?



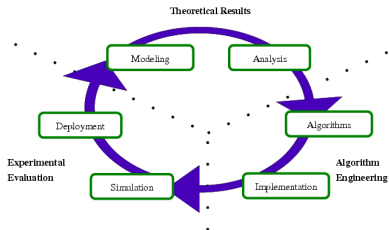
Implement the first version

- ▶ Pick your programming language of choice.
- ▶ Implement your solution
 - ▶ No need to try to make it elegant / fast.
 - ▶ Remember Donald 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.

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

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



Factorial Computation: Using Recursion

```
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, "):", res)
    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

```
import time

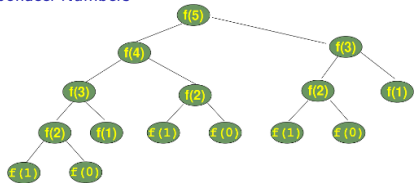
for i in range(1,41):
    t1 = time.perf_counter()
    s = fib(i)
    t2 = time.perf_counter() - t1

    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:.2f}")
```



Fibonacci Numbers



Factorial Computation: Using Recursion and Memory

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

