Algorithms and Data Structures in Biology

Algorithms and Their Complexity

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Section 1

Defining The Algorithm

The Rock Pile Game

- Alice and Bob play a game, starting from two rock piles, each containing 10 rocks.
- In turn Alice and Bob either pick **one** rock from one of the two piles, or **two** rocks, one from each pile.
- *Who wins*? Whomever manage to remove *the last* pile.
- Alice starts.
- Is there a winning strategy?
- Bob realizes that if the rocks were just 2, he could easily win, independently on Alice's moves.
- But how about the general case?

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	0	1	2	3	4	5	6	7	8	9	10
0	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$
1	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$
2	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$
3	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$
4	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$
5	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$
6	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$
7	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$
8	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$
9	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$	$\nwarrow$	$\uparrow$
10	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$	$\leftarrow$	$*$

But What if…

- What if the number of **rocks** we start from is higher than 10?
- And what if the number of **piles** is higher than 2?
- How could we determine the next move to make depending on the current state of the game (i.e., number of piles, number of rocks on each pile)?
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Defining Combinatorial Problems

- A **combinatorial problem** is a *unambiguous* and *precise* problem concerning the production of some *outputs* from some *inputs*.
  - The *class* of possible input must be clearly specified.
  - *Which* output one gets from each input must itself be itself specified without any ambiguity.
  - Specifying *how* to obtain the output from the input is not part of the problem's definition.
- **Example**: The $n \times n$ rock pile problem
  - Input: n, and a state (m, k).
  - Output: a move that a player should make in (m, k) in order to win, *if possible*.

Defining Algorithms

- An **algorithm** is a sequence of instructions that one performs to *solve* a combinatorial problem.
- How should we *specify* an algorithm?
  - We could be *programming-language* dependent.
  - Or we could try to be *more abstract*.
- In this course, algorithms will be specified by way of **pseudocode**, namely by a notation which can be easily translated to concrete programming languages, including `Python`.
- We will not follow specific rules as for how pseudocode is specified. Rather, we will fit it to our needs whenever possible.
  - One should be **precise** without being **formal**.
  - The following basic requirements should be satisfied: *determinism*, *finiteness*, *unambiguity*.
  - There are certain constructions which are very common in pseudocode.

Assignment

Format: $a \leftarrow b$

Effect: Sets the variable a to the value b.

Example: $b \leftarrow 2$

$a \leftarrow b$

Result: The value of a is 2

Arithmetic

Format: $a + b$, $a - b$, $a \cdot b$, a/b, a^b

Effect: Addition, subtraction, multiplication, division, and exponentiation of numbers.

Example: $\textsc{Dist}(x1, y1, x2, y2)$

$dx \leftarrow (x2 - x1)^2$

$dy \leftarrow (y2 - y1)^2$

return $\sqrt{(dx + dy)}$

Result: $\textsc{Dist}(x1, y1, x2, y2)$ computes the Euclidean distance between points with coordinates $(x1, y1)$ and $(x2, y2)$. $\textsc{Distance}(0, 0, 3, 4)$ returns 5.

Conditional

Format:

```
if A is true
    B
else
    C
```

Effect: If statement A is true, executes instructions **B**, otherwise executes instructions **C**. Sometimes we will omit "**else C**," in which case this will either execute **B** or not, depending on whether A is true.

Example: $\textsc{Max}(a, b)$

```
if a < b
    return b
else
    return a
```

Result: $\textsc{Max}(a, b)$ computes the maximum of the numbers a and b. For example, $\textsc{Max}(1, 99)$ returns 99.

`for` loops

Format: **for** $i \leftarrow a$ **to** b

$\quad\quad\mathbf{B}$

Effect: Sets i to a and executes instructions $\mathbf{B}$. Sets i to $a+1$ and executes instructions $\mathbf{B}$ again. Repeats for $i = a+2, a+3, \ldots, b-1, b$.[3]

Example: SUMINTEGERS(n)

```
sum ← 0
for i ← 1 to n
    sum ← sum + i
return sum
```

Result: SUMINTEGERS(n) computes the sum of integers from 1 to n. SUMINTEGERS(10) returns $1 + 2 + \cdots + 10 = 55$.

`while` loops

Format: **while** A is true
    B

Effect: Checks the condition A. If it is true, then executes instructions **B**. Checks A again; if it's true, it executes **B** again. Repeats until A is not true.

Example: ADDUNTIL(b)

```
i ← 1
total ← i
while total ≤ b
    i ← i + 1
    total ← total + i
return i
```

Result: ADDUNTIL(b) computes the smallest integer i such that $1 + 2 + \cdots + i$ is larger than b. For example, ADDUNTIL(25) returns 7, since $1+2+\cdots+7 = 28$, which is larger than 25, but $1+2+\cdots+6 = 21$, which is smaller than 25.

Array access

Format: a_i

Effect: The ith number of array $\mathbf{a} = (a_1, \ldots a_i, \ldots a_n)$. For example, if $\mathbf{F} = (1, 1, 2, 3, 5, 8, 13)$, then $F_3 = 2$, and $F_4 = 3$.

Example: FIBONACCI(n)

$F_1 \leftarrow 1$
$F_2 \leftarrow 1$
for $i \leftarrow 3$ **to** n
    $F_i \leftarrow F_{i-1} + F_{i-2}$
return F_n

Result: FIBONACCI(n) computes the nth Fibonacci number. FIBONACCI(8) returns 21.

United States Change Problem:
Convert some amount of money into the fewest number of coins.

Input: An amount of money, M, in cents.

Output: The smallest number of quarters q, dimes d, nickels n, and pennies p whose values add to M (i.e., $25q + 10d + 5n + p = M$ and $q + d + n + p$ is as small as possible).

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```
USChange(M)
while M > 0
    c ← Largest coin that is smaller than (or equal to) M
    Give coin with denomination c to customer
    M ← M − c
```

Algorithm Correctness

- Are we sure that USCHANGE *indeed solves* the combinatorial problem it is supposed to solve, namely that it is **correct**?
- There are two ways one can use to convince herself of the correctness of an algorithm:
  1. **Testing** the algorithm.
     - Just check that the algorithm transforms inputs to outputs correctly.
     - This is an experimental methodology.
     - It is impossible to test an algorithm on *all* of the input instances.
  2. **Proving** the algorithm correct.
     - One needs to find a mathematical proof of the fact that the algorithm indeed does what it is supposed to do.
     - This is an analytical methodology.
     - Computer science has devised along the years so many methodology for proving algorithms correct.

Change Problem:
Convert some amount of money M into given denominations, using the smallest possible number of coins.

> **Input:** An amount of money M, and an array of d denominations $\mathbf{c} = (c_1, c_2, \ldots, c_d)$, in decreasing order of value ($c_1 > c_2 > \cdots > c_d$).
>
> **Output:** A list of d integers $i_1, i_2, \ldots, i_d$ such that $c_1 i_1 + c_2 i_2 + \cdots + c_d i_d = M$, and $i_1 + i_2 + \cdots + i_d$ is as small as possible.

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```
BetterChange(M, c, d)
r ← M
for k ← 1 to d
      i_k ← r/c_k
      r ← r − c_k · i_k
return (i_1, i_2, ..., i_d)
```

Ouch!

- Unfortunately, algorithm BetterChange is simply **incorrect**, although being a generalisation of a correct algorithm.
  - Consider the case in whih $\mathbf{c} = (25, 20, 10, 5)$ and the amount of money M is 40. The algorithm would return the list $1, 0, 1, 1$, while there is a shorter one, namely $0, 2, 1, 1$.
  - What's the deep reason why the algorithm is not correct?
- Sometime, if one is not sure about the correctenss of the algorithm she has in mind, it is better to start with an algorithm which is **trivially correct**, although having perhaps other problems…

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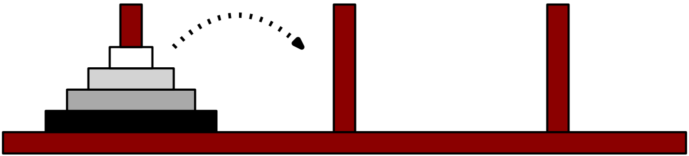
```
BruteForceChange(M, c, d)
  smallestNumberOfCoins ← ∞
  for each (i_1, ..., i_d) from (0, ..., 0) to (M/c_1, ..., M/c_d)
      valueOfCoins ← Σ_{k=1}^{d} i_k c_k
      if valueOfCoins = M
          numberOfCoins ← Σ_{k=1}^{d} i_k
          if numberOfCoins < smallestNumberOfCoins
              smallestNumberOfCoins ← numberOfCoins
              bestChange ← (i_1, i_2, ..., i_d)
  return (bestChange)
```

Direct Proofs of Correctness

- Sometimes, the correctness of an algorithm can be proved by simply observing some simple facts, without any complicated mathematical arguments.
- This is the case of the algorithm BruteForceChange:
  - Any correct solution, and in particular, the optimal one, can be seen as a sequence between $(0, \ldots, 0)$ to $(M/c_1 \ldots, M/c_d)$.
  - The algorithm, simply, consider all such sequences one after the other.
  - At any iteration, the algorithm checks that the considered sequence indeed sums up to M.
  - It also keep track of *the best* sequence, namely the one with the fewest coins. This is done by two variables, *smallestNumberOfCoins* and **BestChange**. These are updated only when appropriate.

The Hanoi Puzzle



- One piece at a time.
- Never a larger piece stands above a smaller piece.

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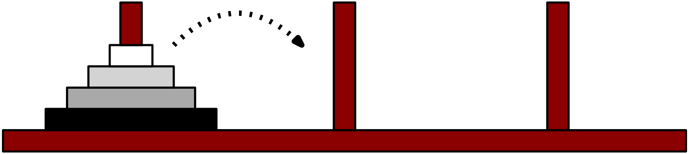

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Output a list of moves that solves the Towers of Hanoi.

Input: An integer n.

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HANOITOWERS(n − 1, unusedPeg, toPeg)
return
```

Proving the Correctness of Recursive Algorithms

- Recursively defined algorithm, like HanoiTowers, are particularly fit to be proved correct.
- The proof follows the structure of the algorithm, and consists in proving that:
  1. **Base Case**. Whenever the algorithm *does not* make any recursive call, it is correct.
  2. **Inductive Case**. If the algorithm *do make* recursive calls, it is correct *provided* all the recursive calls are themselves correct.
- It is of course crucial, in the inductive case, that the fact all the recursive calls are correct (called the **inductive hypothesis**) is *sufficient* to prove the algorithm correct.
  - Sometime this is not the case, and it is thus necessary to prove *a stronger* claim.

Proving the Correctness of HanoiTowers

- We can start by proving that HanoiTowers($n, \mathit{fromPeg}, \mathit{toPeg}$) correctly solves the Hanoi Problem, by induction on n
  1. The **base case** is easy.
  2. The inductive case fails, because the statement is too weak.
- We need a stronger statement, namely that HanoiTowers($n, \mathit{fromPeg}, \mathit{toPeg}$) correctly moves n (stacked) disks in *fromPeg* to *toPeg* *whenever* all the other disks in the three Peg are correctly stacked and of size higher than n.
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Fibonacci Problem:
Calculate the nth Fibonacci number.

Input: An integer n.

Output: The nth Fibonacci number $F_n = F_{n-1} + F_{n-2}$ (with $F_1 = F_2 = 1$).

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```
RecursiveFibonacci(n)
if n = 1 or n = 2
    return 1
else
    a ← RecursiveFibonacci(n − 1)
    b ← RecursiveFibonacci(n − 2)
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Fibonacci(n)
F_1 ← 1
F_2 ← 1
for i ← 3 to n
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return F_n
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Correctness through Invariants

- The correctness of RECURSIVEFIBONACCI is very easy to be proved, since the algorithm's structure perfectly matches the definition of Fibonacci numbers.
  - There is not so much left to be proved.
- The algorithm FIBONACCI, is not recursive but rather *iterative*. Its proof of correctness is more delicate.
  - We need to find a statement, called an **invariant**, which is true before the *first* iteration of the **for** loop, which stays true after the execution of *any* such iteration, and which *implies* the correctness of the algorithm *as a whole*.
  - In our case such a statement can be

$$\forall j < i.F_j \text{ is a the } j\text{-th Fibonacci number.}$$

  - Could we find something slightly weaker?
- Why using FIBONACCI, then? Simply because it is *more efficient*!

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Another Example

Sorting Problem:
Sort a list of integers.

Input: A list of n distinct integers $\mathbf{a} = (a_1, a_2, \dots, a_n)$.

Output: Sorted list of integers, that is, a reordering $\mathbf{b} = (b_1, b_2, \dots, b_n)$ of integers from $\mathbf{a}$ such that $b_1 < b_2 < \cdots < b_n$.

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```
SELECTIONSORT(a, n)
for i ← 1 to n − 1
        a_j ← Smallest element among a_i, a_{i+1}, ... a_n.
        Swap a_i and a_j
return a
```

Fast and Slow Algorithms

- Different (correct) algorithms for the same problem can behave *very differently* when implemented as programs, even when using the same programming language and the same machine.
  - One can take much longer than the other to be executed!
  - The amount of memory one algorithm needs is perhaps much larger then the one the other needs.
- We will see in the Lab Module that a **purely empirical** approach to the benchmarking of algorithms makes a lot of sense.
- Benchmarking, being genuinely experimental, cannot however be exhaustive. Could we rather proceed analitically?

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Measuring an Algorithm's Complexity

- With the (time) **complexity** of a given algorithm, A what we mean is an abstract measure of the execution time of A.
- An algorithm's complexity, being *a model*, is measured following a number of principles, namely the model's **axioms**:
  1. The complexity of A is simply the **number** of **basic** instructions which are executed when A is run on any of its instances. Each instruction costs *the same*.
  2. Since the number of instructions A executes may vary depending on the input, one expresses A's complexity as a function of some **parameters** of the input (typically, its *size*).
  3. In doing so, one is allowed to slightly **overapproximate** the amount of instructions involved in A's execution, for the sake of having simple expressions.
  4. Multiplicative and additive constants are typically **elided** themselves, and only the asymptotic behaviour of the involved functions matters.

Asymptotic Notation

- A function $f : \mathbb{N} \to \mathbb{N}$ is $O(g)$ if there are positive real constants c and x_0 such that $f(x) \leq c \cdot g(x)$ for all values of $x \geq x_0$.
  - **Example**: the function $n \mapsto 3 \cdot n^2 + 4 \cdot n$ is $O(n^2)$, but also $O(n^3)$, and certainly $O(2^n)$. It is not, however, $O(n)$.
- A function $f : \mathbb{N} \to \mathbb{N}$ is $\Omega(g)$ if there are positive real constants c and x_0 such that $f(x) \geq c \cdot g(x)$ for all values of $x \geq x_0$.
  - **Example**: the function $n \mapsto 3 \cdot n^2 + 4 \cdot n$ is $\Omega(n^2)$, but also $\Omega(n)$, but not $\Omega(n^3)$.
- A function f is $\Theta(g)$ if f is both $O(g)$ and $\Omega(g)$.

```
HanoiTowers(n, fromPeg, toPeg)
if n = 1
    output "Move disk from peg fromPeg to peg toPeg"
    return
unusedPeg ← 6 − fromPeg − toPeg
HanoiTowers(n − 1, fromPeg, unusedPeg)
output "Move disk from peg fromPeg to peg toPeg"
HanoiTowers(n − 1, unusedPeg, toPeg)
return
```

$$O(4^n)$$

HanoiTowers(n, $fromPeg$, $toPeg$)

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    output "Move disk from peg $fromPeg$ to peg $toPeg$"
    return
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output "Move disk from peg $fromPeg$ to peg $toPeg$"
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SelectionSort($\mathbf{a}$, n)

for $i \leftarrow 1$ **to** $n - 1$
    $a_j \leftarrow$ Smallest element among $a_i, a_{i+1}, \ldots a_n$.
    Swap a_i and a_j
return a

$$O(n^2)$$

Thank You!

Questions?