

Algorithms and Complexity

Selected Topics in Computer Intelligence - 2015

Bioinformatics Programming

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What is an Algorithm?

A sequence of instructions that we perform in order to solve a well-formulated problem



- A method of translating the inputs into outputs
- We can use pseudocode to describe algorithms
 - Operations can be grouped into subroutines that solve problems
 - Covers concepts of variables, arrays, and arguments

Examples

Euclidean distance

```
DIST(x1, y1, x2, y2)

1 dx \leftarrow (x2 - x1)^2

2 dy \leftarrow (y2 - y1)^2

3 return \sqrt{(dx + dy)}
```

- Result: the Euclidean distance between points with coordinates (x1,y1) and (x2,y2)
- Maximum

$$Max(a, b)$$
1 if $a < b$
2 return b
3 else
4 return a

Result: the maximum of the numbers a and b

Examples

Sum Integers

```
SUMINTEGERS(n)

1 sum \leftarrow 0

2 for i \leftarrow 1 to n

3 sum \leftarrow sum + i

4 return sum
```

- \blacksquare Result: sum of integers from 1 to n
- Fibonacci

```
FIBONACCI(n)

1 F_1 \leftarrow 1

2 F_2 \leftarrow 1

3 for i \leftarrow 3 to n

4 F_i \leftarrow F_{i-1} + F_{i-2}

5 return F_n
```

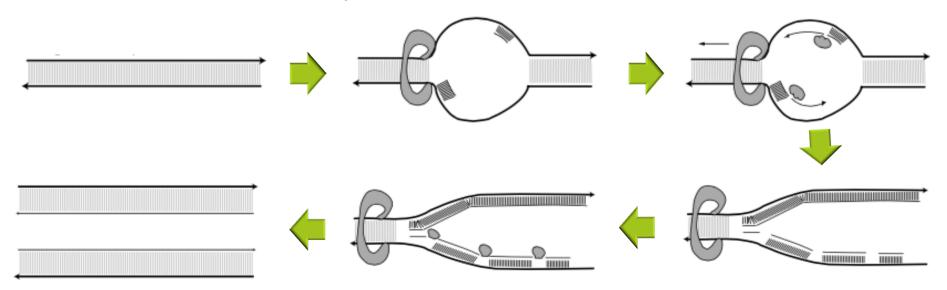
 \blacksquare Result: the n^{th} Fibonacci number

Biological vs. Computer Algorithms

■ DNA Replication Process



- Uses algorithm-like procedures to solve this problem
- Before a cell can divide, it must first make a copy of its genetic material
- Requires an elaborate cooperation between different types of molecules and enzymes



Biological vs. Computer Algorithms

■ In Computer Domain

- \bigcirc
- "String Duplication Problem"
 - Given a string of letters, return a copy
- STRINGCOPY(\mathbf{s}, n)

 1 for $i \leftarrow 1$ to n2 $t_i \leftarrow s_i$ 3 return t
- A trivial algorithm but may require the number of operations
- We have invented programming language to solve the problem quite easily
- Biologist have not yet invented a similar "language" to describe biological algorithms working in the cell...

- To solve computational problem we need to ...
 - Identify precisely what the problem is then we can devise an algorithms that solves it
 - Two important questions:
 - Does it work correctly?
 - How long will it take?
 - The Change Problem
 - How to make change in the least annoying way.
 - Minimize the number of coins returned
 - Is it specific to a certain country? (generalization?)





Returning coins in US currency

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).

USCHANGE(M)

- $1 \quad r \leftarrow M$
- 2 q ← r/25
- $3 \quad r \leftarrow r 25 \cdot q$
- 4 $d \leftarrow r/10$
- 5 $r \leftarrow r 10 \cdot d$
- 6 n ← r/5
- 7 $r \leftarrow r 5 \cdot n$
- 8 $p \leftarrow r$
- 9 return (q, d, n, p)

Problem?

- unlimited supply of each coin
- lacks generality

Returning coins in ANY currency

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 $\mathbf{c} = (c_1, c_2, \dots, c_d)$, 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 $c_1i_1+c_2i_2+$ $\cdots + c_d i_d = M$, and $i_1 + i_2 + \cdots + i_d$ is as small as possible.

- Correct algorithm
 - Can it translate EVERY input instance into the correct output
- Incorrect algorithm
 - At least one input instance does not produce the correct output

```
BetterChange(M, \mathbf{c}, d)
     r \leftarrow M
     for k \leftarrow 1 to d
          i_k \leftarrow r/c_k
           r \leftarrow r - c_k \cdot i_k
     return (i_1, i_2, \ldots, i_d)
```

Problem?

- changing 40 cents
- -c = (25, 20, 10, 5, 1)

- Returning coins in ANY currency (cont.)
 - Brute force algorithm

```
BRUTEFORCECHANGE(M, \mathbf{c}, d)

1 smallestNumberOfCoins \leftarrow \infty

2 \mathbf{for} \mathbf{each} (i_1, \dots, i_d) \mathbf{from} (0, \dots, 0) \mathbf{to} (M/c_1, \dots, M/c_d)

3 valueOfCoins \leftarrow \sum_{k=1}^d i_k c_k

4 \mathbf{if} valueOfCoins = M

5 numberOfCoins \leftarrow \sum_{k=1}^d i_k

6 \mathbf{if} numberOfCoins < smallestNumberOfCoins

7 smallestNumberOfCoins \leftarrow numberOfCoins

8 \mathbf{bestChange} \leftarrow (i_1, i_2, \dots, i_d)

9 \mathbf{return} (\mathbf{bestChange})
```

Recursive

- An algorithm is recursive if it calls itself
- Calculates Factorial and Fibonacci numbers
- Towers of Hanoi puzzle introduced in 1883



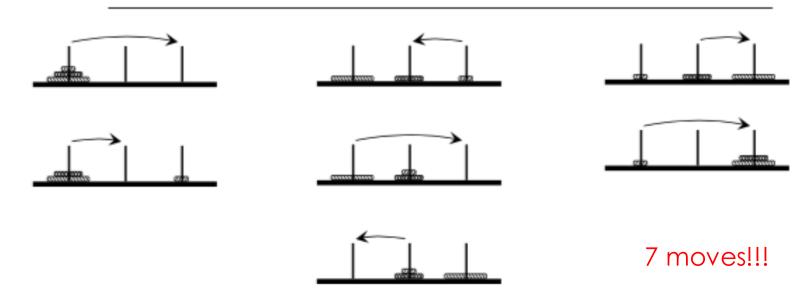
Recursion - Towers of Hanoi (cont.)

Towers of Hanoi Problem:

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

Input: An integer n.

Output: A sequence of moves that will solve the *n*-disk Towers of Hanoi puzzle.



- Recursion Towers of Hanoi (cont.)
 - Cannot complete the game without moving the largest disk
 - \blacksquare How many steps for 4 disks (n=4)
 - \square move top 3 (n-1) disks to an empty peg 7 moves
 - \square Move the largest disk, n^{th} disk, to the destination peg
 - Move again the 3 (n-1) disks from the temp peg to the destination peg 7 moves



Recursion - Towers of Hanoi (cont.)

```
Hanoitowers(n, fromPeg, toPeg)

1 if n = 1

2 output "Move disk from peg fromPeg to peg toPeg"

3 return

4 unusedPeg \leftarrow 6 - fromPeg - toPeg

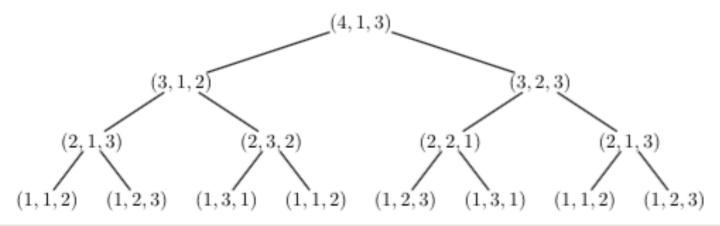
5 Hanoitowers(n - 1, fromPeg, unusedPeg)

6 output "Move disk from peg fromPeg to peg toPeg"

7 Hanoitowers(n - 1, unusedPeg, toPeg)

8 return
```

fromPeg	toPeg	unusedPeg
1	2	3
1	3	2
2	1	3
2	3	1
3	1	2
3	2	1



- Iterative vs. Recursive Algorithm
 - Most recursive algorithm can be rewritten in iterative loops

Exponential-time

linear-time

Complexity

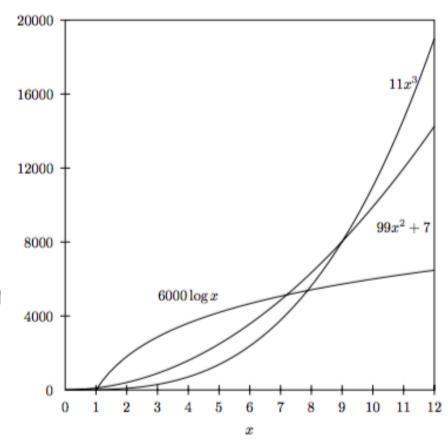
■ Fast vs. Slow algorithm

■ It's about total number of operations that an algorithm perform

to describe the running time

Algorithm complexity

- Logarithmic
- Quadratic
- Cubic
- What else?
- The behavior of algorithms on small inputs does NOT matter



Complexity

Big-O Notation

- Describe the running time of an algorithm
- Considering the term that grows the fastest with respect to n

Definition 2.1 A function f(x) is O(g(x)) if there are positive real constants c and x_0 such that $f(x) \leq cg(x)$ for all values of $x \geq x_0$. Upper bound

Definition 2.2 A function f(x) is $\Omega(g(x))$ if there are positive real constants c and x_0 such that $f(x) \ge cg(x)$ for all values of $x \ge x_0$. Lower bound

Definition 2.3 A function f(x) is $\Theta(g(x))$ if f(x) = O(g(x)) and $f(x) = \Omega(g(x))$. Tight bound

Complexity

- Big-O Notation (cont.)
 - Worst case efficiency the largest amount of time taking to solve the worst possible of input of a given size (n)
 - E.g. measure sorting algorithm (min to max)
 - Given that the input of size n with max to min order

Algorithm Design Techniques

- Exhaustive Search (aka. Brute force)
- Branch-and-Bound (aka. Pruning)
 - Brute force with a bit of common sense
- □ Greedy iterative procedure
 - Choosing the most attractive choice in each iteration
- Dynamic Programming
 - Organize computations to avoid computing known values
- Divide-and-Conquer
 - Splitting problem into smaller subproblems and combining the results
- Machine Learning
 - Based their strategies on the computation analysis of previous collected data