



CEITEC

Central European Institute of Technology
BRNO | CZECH REPUBLIC

Introduction to Bioinformatics (LF:DSIB01)

Week 2 : Algorithm Basics

Basics of Algorithms

- Definition of an algorithm
- Pseudocode Notation
- Exercise: The Coin Change Problem
- Brute force, Iterative, Recursive
- Big-O notation

What is an algorithm

- A sequence of instructions one must perform to **solve** a well formulated problem
- A step-by-step method of **solving** a problem
- A set of instructions designed to **perform** a specific task

Sequence of instructions
Step-by-step method
Set of instructions

Solve
Perform

Well formulated problem
Specific task

Sequence of instructions
Step-by-step method
Set of instructions

Solve
Perform

Well formulated problem
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MAKE PUMPKIN PIE

1 $\frac{1}{2}$ cups canned or cooked pumpkin
1 cup brown sugar, firmly packed
 $\frac{1}{2}$ teaspoon salt
2 teaspoons cinnamon
1 teaspoon ginger
2 tablespoons molasses
3 eggs, slightly beaten
12 ounce can of evaporated milk
1 unbaked pie crust

Combine pumpkin, sugar, salt, ginger, cinnamon, and molasses. Add eggs and milk and mix thoroughly. Pour into unbaked pie crust and bake in hot oven (425 degrees Fahrenheit) for 40 to 45 minutes, or until knife inserted comes out clean.



Pseudocode Notation

```
MAKEPUMPKINPIE(pumpkin, sugar, salt, spices, eggs, milk, crust)
1  PREHEATOVEN(425)
2  filling ← MIXFILLING(pumpkin, sugar, salt, spices, eggs, milk)
3  pie ← ASSEMBLE(crust, filling)
4  while knife inserted does not come out clean
5      BAKE(pie)
6  output "Pumpkin pie is complete"
7  return pie
```

Pseudocode Notation

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

Pseudocode Notation

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: $\text{MAX}(a, b)$
1 **if** $a < b$
2 **return** b
3 **else**
4 **return** a

Pseudocode Notation

for loops

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

Effect: Sets i to a and executes instructions **B**. Sets i to $a + 1$ and executes instructions **B** again. Repeats for $i = a + 2, a + 3, \dots, b - 1, b$.

Example: SUMINTEGERS(n)
1 $sum \leftarrow 0$
2 **for** $i \leftarrow 1$ **to** n
3 $sum \leftarrow sum + i$
4 **return** sum

Pseudocode Notation

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*)
1 *i* ← 1
2 *total* ← *i*
3 **while** *total* ≤ *b*
4 *i* ← *i* + 1
5 *total* ← *total* + *i*
6 **return** *i*

Pseudocode Notation

Array access

Format: a_i

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

Example: FIBONACCI(n)

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

Pseudocode vs Computer Code

If you were to build a machine that follows these instructions, you would need to make it specific to a particular kitchen and be tirelessly explicit in all the steps (e.g., how many times and how hard to stir the filling, with what kind of spoon, in what kind of bowl, etc.)

This is exactly the difference between pseudocode (the abstract sequence of steps to solve a well-formulated computational problem) and computer code (a set of detailed instructions that one particular computer will be able to perform).

Pseudocode Exercise: Coin Change (Euro coins)

Convert an amount of money into the fewest number of coins

Input: Amount of money (M)

Output: the smallest number of 50c (a), 20c (b), 10c (c), 5c (d), 2c (e) and 1c (f) such that $50a+20b+10c+5d+2e+1f = M$

```
1  while  $M > 0$ 
2       $c \leftarrow$  Largest coin that is smaller than (or equal to)  $M$ 
3      Give coin with denomination  $c$  to customer
4       $M \leftarrow M - c$ 
```

Try: $M=60c$; $M=55c$; $M=40c$

Pseudocode Exercise: Coin Change (Generalised)

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 ($c_1 > c_2 > \dots > c_d$).

Output: A list of d integers i_1, i_2, \dots, i_d such that $c_1 i_1 + c_2 i_2 + \dots + c_d i_d = M$, and $i_1 + i_2 + \dots + i_d$ is as small as possible.

Pseudocode Exercise: Coin Change (US 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 ($c_1 > c_2 > \dots > c_d$).

Output: A list of d integers i_1, i_2, \dots, i_d such that $c_1i_1 + c_2i_2 + \dots + c_di_d = M$, and $i_1 + i_2 + \dots + i_d$ is as small as possible.

BETTERCHANGE(M, \mathbf{c}, d)

```
1  $r \leftarrow M$ 
2 for  $k \leftarrow 1$  to  $d$ 
3      $i_k \leftarrow r/c_k$ 
4      $r \leftarrow r - c_k \cdot i_k$ 
5 return  $(i_1, i_2, \dots, i_d)$ 
```

NB: Division = "floor"

Try

$M = 40$; $c_1=25$, $c_2=10$, $c_3=5$, $c_4=1$



Pseudocode Exercise: Coin Change (US 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 ($c_1 > c_2 > \dots > c_d$).

Output: A list of d integers i_1, i_2, \dots, i_d such that $c_1 i_1 + c_2 i_2 + \dots + c_d i_d = M$, and $i_1 + i_2 + \dots + i_d$ is as small as possible.

BETTERCHANGE(M, \mathbf{c}, d)

```
1  $r \leftarrow M$ 
2 for  $k \leftarrow 1$  to  $d$ 
3    $i_k \leftarrow r / c_k$ 
4    $r \leftarrow r - c_k \cdot i_k$ 
5 return  $(i_1, i_2, \dots, i_d)$ 
```

NB: Division = "floor"



$M = 40$; $c_1=25$, $c_2=20$, $c_3=10$, $c_4=5$, $c_5=1$



Discontinued
1875
for being too
confusing

Pseudocode Exercise: Coin Change (US 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 ($c_1 > c_2 > \dots > c_d$).

Output: A list of d integers i_1, i_2, \dots, i_d such that $c_1 i_1 + c_2 i_2 + \dots + c_d i_d = M$, and $i_1 + i_2 + \dots + i_d$ is as small as possible.

BETTERCHANGE(M, \mathbf{c}, d)

```
1  $r \leftarrow M$ 
2 for  $k \leftarrow 1$  to  $d$ 
3      $i_k \leftarrow r/c_k$ 
4      $r \leftarrow r - c_k \cdot i_k$ 
5 return  $(i_1, i_2, \dots, i_d)$ 
```

BetterChange

40=
1x25 + 1x10 + 1x5=
3 coins

Incorrect!
40 = 2x20=
2 coins



$M = 40$; $c_1=25$, $c_2=20$, $c_3=10$, $c_4=5$, $c_5=1$



Discontinued
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NB: Division = "floor"

Pseudocode Exercise: Coin Change

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 ($c_1 > c_2 > \dots > c_d$).

Output: A list of d integers i_1, i_2, \dots, i_d such that $c_1i_1 + c_2i_2 + \dots + c_di_d = M$, and $i_1 + i_2 + \dots + i_d$ is as small as possible.

Tries every combination
Guaranteed to find optimal
Slow

Brute Force Algorithm

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 ($c_1 > c_2 > \dots > c_d$).

Output: A list of d integers i_1, i_2, \dots, i_d such that $c_1 i_1 + c_2 i_2 + \dots + c_d i_d = M$, and $i_1 + i_2 + \dots + i_d$ is as small as possible.

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

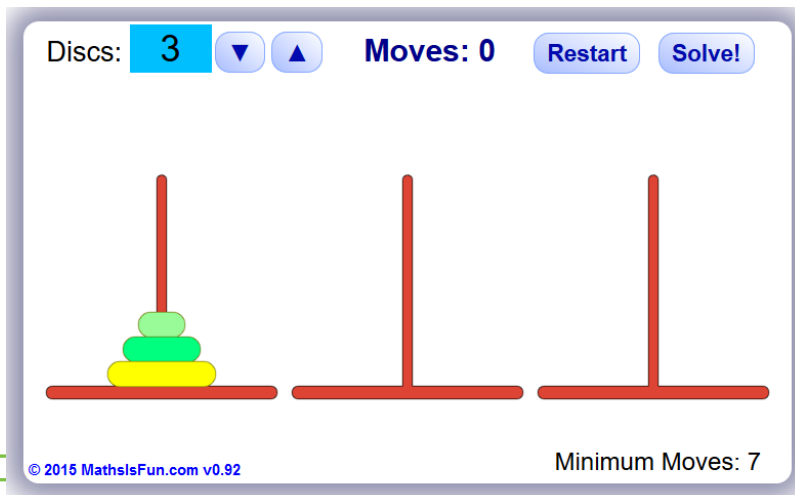
```
1  smallestNumberOfCoins  $\leftarrow \infty$ 
2  for each  $(i_1, \dots, i_d)$  from  $(0, \dots, 0)$  to  $(M/c_1, \dots, M/c_d)$ 
3    valueOfCoins  $\leftarrow \sum_{k=1}^d i_k c_k$ 
4    if valueOfCoins =  $M$ 
5      numberOfCoins  $\leftarrow \sum_{k=1}^d i_k$ 
6      if numberOfCoins < smallestNumberOfCoins
7        smallestNumberOfCoins  $\leftarrow$  numberOfCoins
8        bestChange  $\leftarrow (i_1, i_2, \dots, i_d)$ 
9  return (bestChange)
```

Tries every combination
Guaranteed to find optimal
Slow

Spoiler: (There is a better solution: Stay tuned for Week 4)

Recursive Algorithms

The *Towers of Hanoi* puzzle, introduced in 1883 by a French mathematician, consists of three pegs, which we label from left to right as 1, 2, and 3, and a number of disks of decreasing radius, each with a hole in the center. The disks are initially stacked on the left peg (peg 1) so that smaller disks are on top of larger ones. The game is played by moving one disk at a time between pegs. You are only allowed to place smaller disks on top of larger ones, and any disk may go onto an empty peg. The puzzle is solved when all of the disks have been moved from peg 1 to peg 3.



1 disc = 1 move

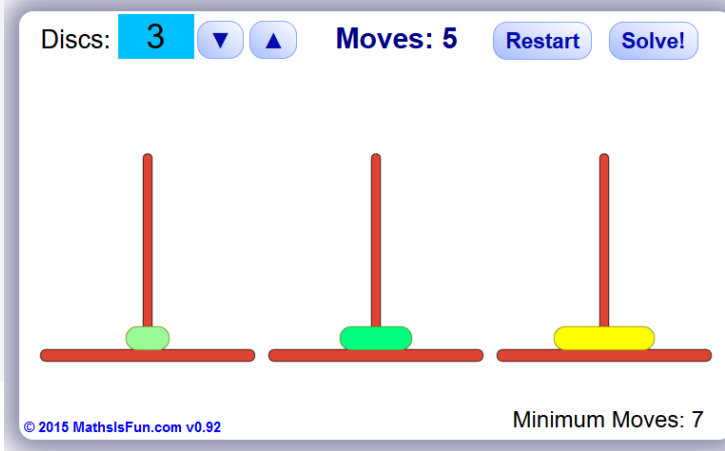
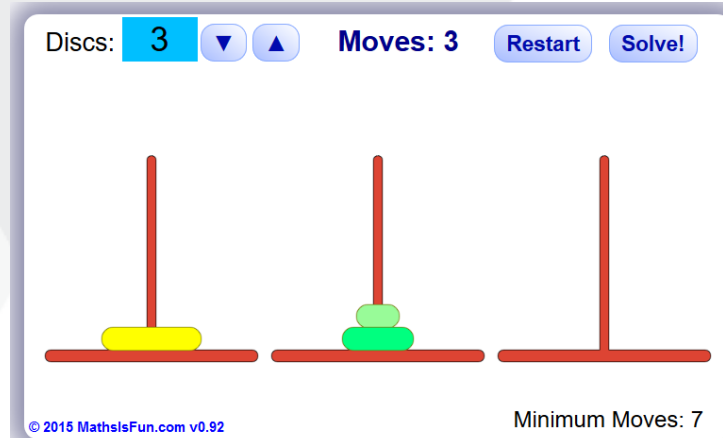
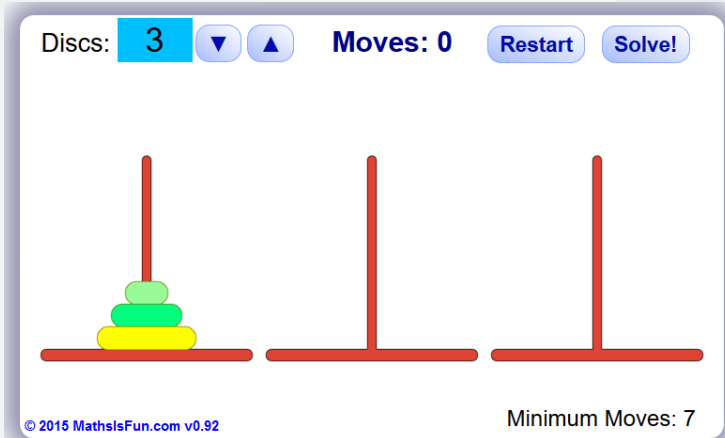
2 discs = 3 moves (1-2, 1-3, 2-3)

3 discs = 7 moves (1-3, 1-2, 3-2, 1-3, 2-1, 2-3, 1-3)

...

Towers of Hanoi (3 disks)

7 moves (1-3, 1-2, 3-2, 1-3, 2-1, 2-3, 1-3)

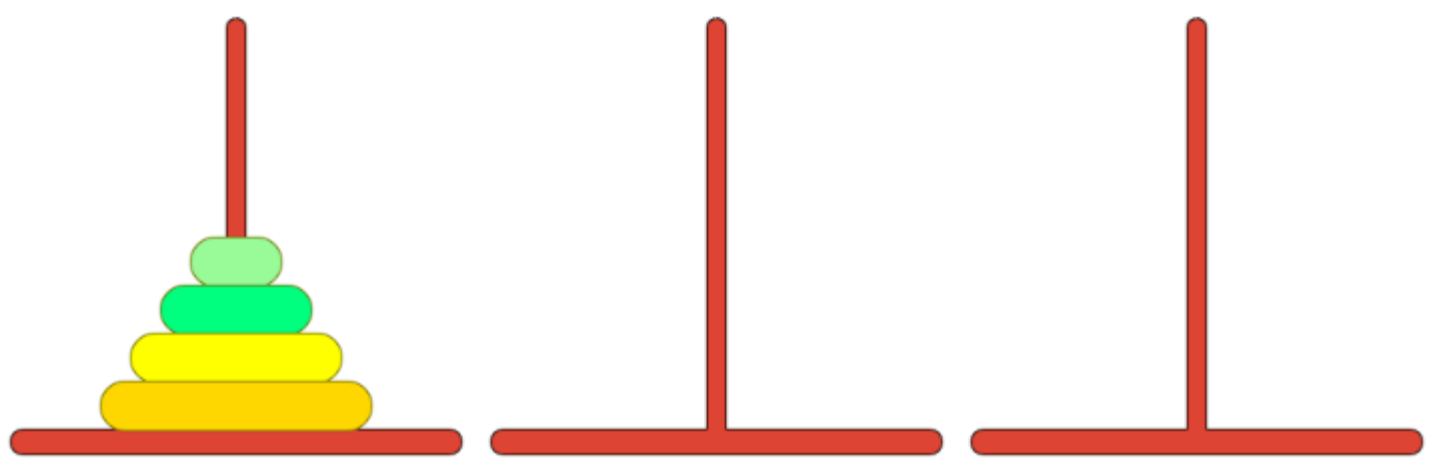


More generally, to move a stack of size n from the **left** to the **right** peg, you first need to move a stack of size $n - 1$ from the **left** to the **middle** peg, and then from the middle peg to the right peg once you have moved the n th disk to the right peg.

To move a stack of size $n - 1$ from the **middle** to the **right**, you first need to move a stack of size $n - 2$ from the **middle** to the **left**, then move the $(n - 1)$ th disk to the right, and then move the stack of $n - 2$ from the left to the right peg, and so on.

Towers of Hanoi: N disks

Discs: **4** ▼ ▲ Moves: 0 Restart Solve!



© 2015 MathsIsFun.com v0.92 Minimum Moves: ?

The image shows a digital interface for the Towers of Hanoi puzzle. At the top, it displays 'Discs: 4' in a blue box, with up and down arrow buttons. To the right, it shows 'Moves: 0' and two buttons labeled 'Restart' and 'Solve!'. The main area features three vertical red towers. The leftmost tower has four disks stacked on it, colored from top to bottom: light green, green, yellow, and orange. The other two towers are empty. At the bottom left, there is a copyright notice '© 2015 MathsIsFun.com v0.92'. At the bottom right, it says 'Minimum Moves: ?' with a question mark inside a small box.

Towers of Hanoi: N disks

<i>fromPeg</i>	<i>toPeg</i>	<i>unusedPeg</i>
1	2	3
1	3	2
2	1	3
2	3	1
3	1	2
3	2	1

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
6
7
8  return
```


Towers of Hanoi: N disks

<i>fromPeg</i>	<i>toPeg</i>	<i>unusedPeg</i>
1	2	3
1	3	2
2	1	3
2	3	1
3	1	2
3	2	1

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($n - 1$, $fromPeg$, $unusedPeg$)

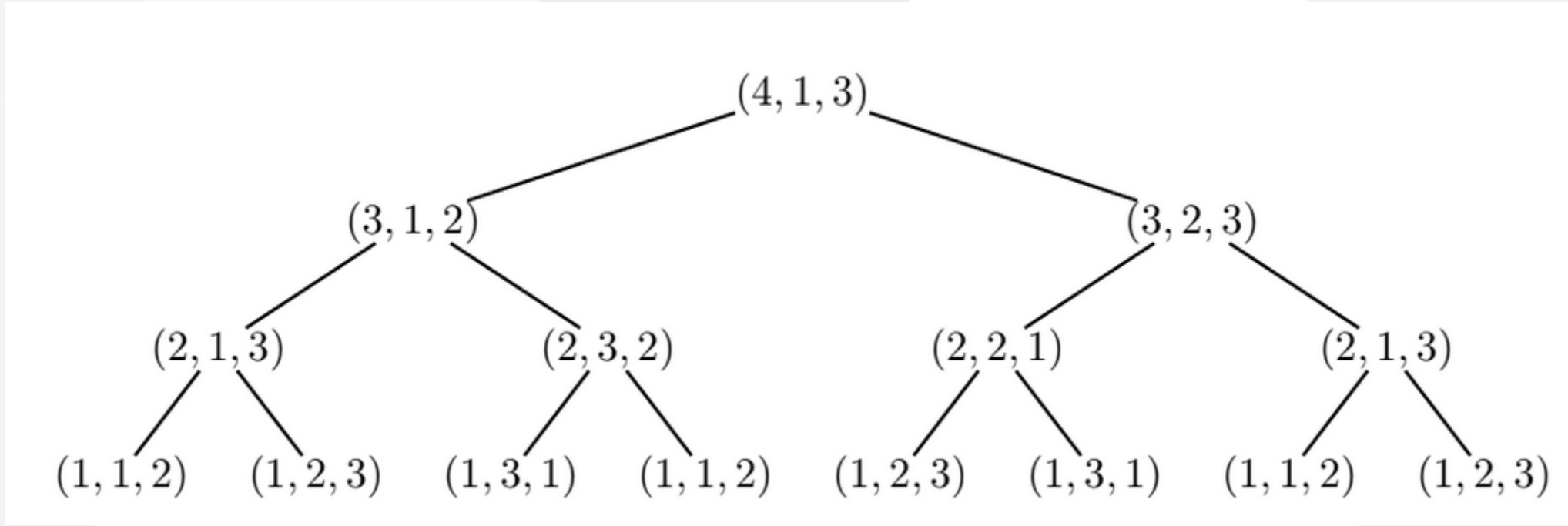
6 **output** "Move disk from peg $fromPeg$ to peg $toPeg$ "

7 HANOITOWERS($n - 1$, $unusedPeg$, $toPeg$)

8 **return**

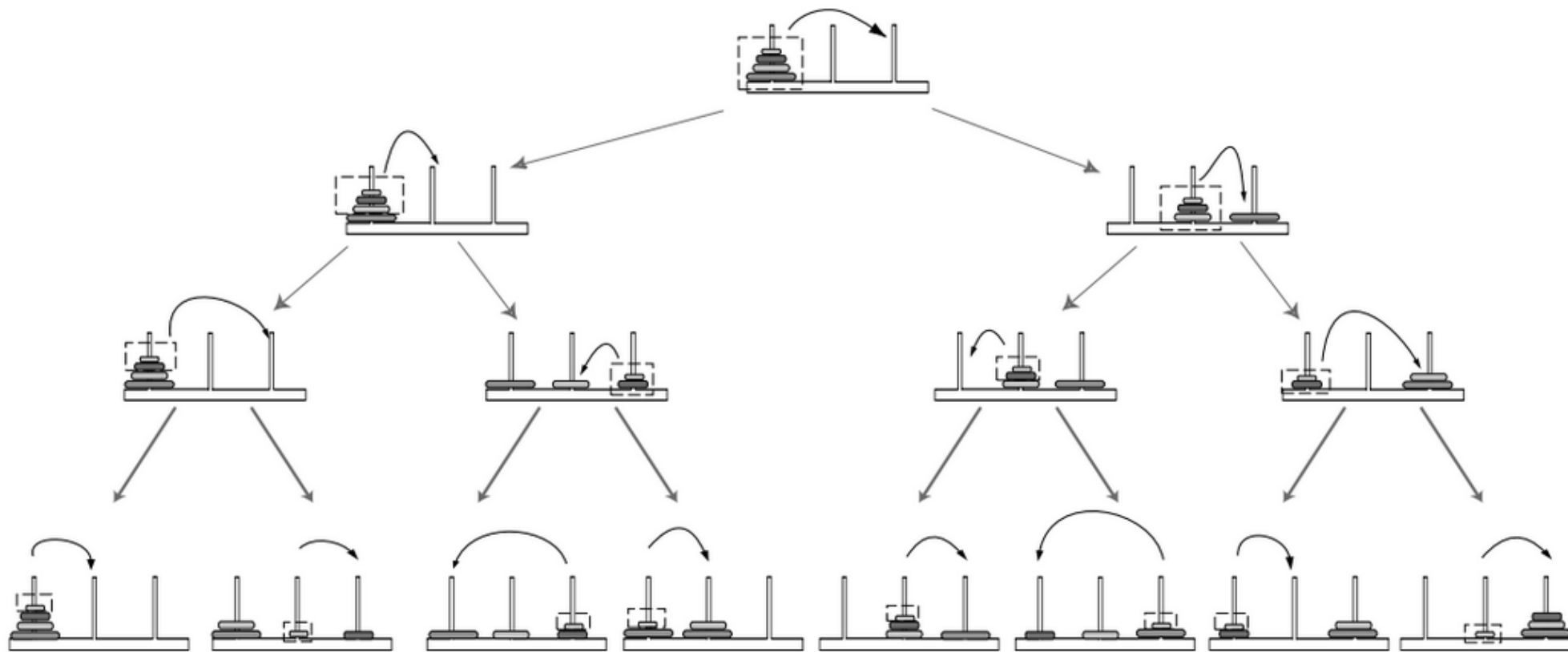
Towers of Hanoi: 4 disks

```
HANOITOWERS(n, fromPeg, toPeg)  
1  if n = 1  
2      output "Move disk from fromPeg to toPeg"  
3      return  
4  unusedPeg ← 6 - fromPeg - toPeg  
5  HANOITOWERS(n - 1, fromPeg, unusedPeg)  
6  output "Move disk from fromPeg to toPeg"  
7  HANOITOWERS(n - 1, unusedPeg, toPeg)  
8  return
```



Towers of Hanoi: 4 disks

```
HANOITOWERS( $n$ ,  $fromPeg$ ,  $toPeg$ )  
1 if  $n = 1$   
2   output "Move disk from  $fromPeg$  to  $toPeg$ "  
3   return  
4  $unusedPeg \leftarrow 6 - fromPeg - toPeg$   
5 HANOITOWERS( $n - 1$ ,  $fromPeg$ ,  $unusedPeg$ )  
6 output "Move disk from  $fromPeg$  to  $toPeg$ "  
7 HANOITOWERS( $n - 1$ ,  $unusedPeg$ ,  $toPeg$ )  
8 return
```



Iterative Algorithms – Fibonacci Series



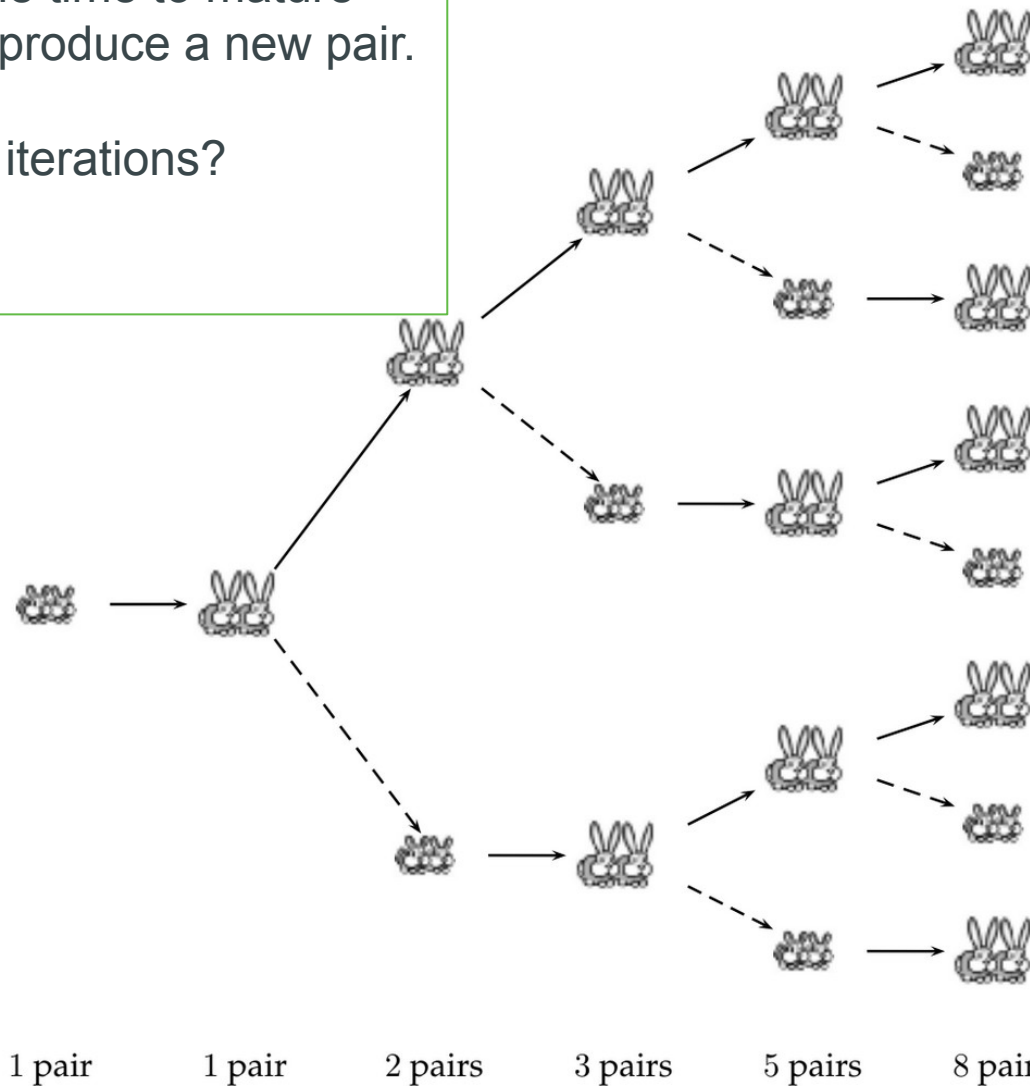
$$\frac{a+b}{a} = \frac{a}{b} = \phi$$

Iterative Algorithms – Immortal Rabbits

A baby pair of rabbits takes the same time to mature as a mature pair of rabbits takes to produce a new pair.

How many rabbits are there after N iterations?

PS: rabbits cannot die!



Iterative Algorithms vs Recursive Algorithms

RECURSIVEFIBONACCI(n)

```
1  if  $n = 1$  or  $n = 2$ 
2      return 1
3  else
4       $a \leftarrow$  RECURSIVEFIBONACCI( $n - 1$ )
5       $b \leftarrow$  RECURSIVEFIBONACCI( $n - 2$ )
6      return  $a + b$ 
```

Recursive: Slow (exponential)

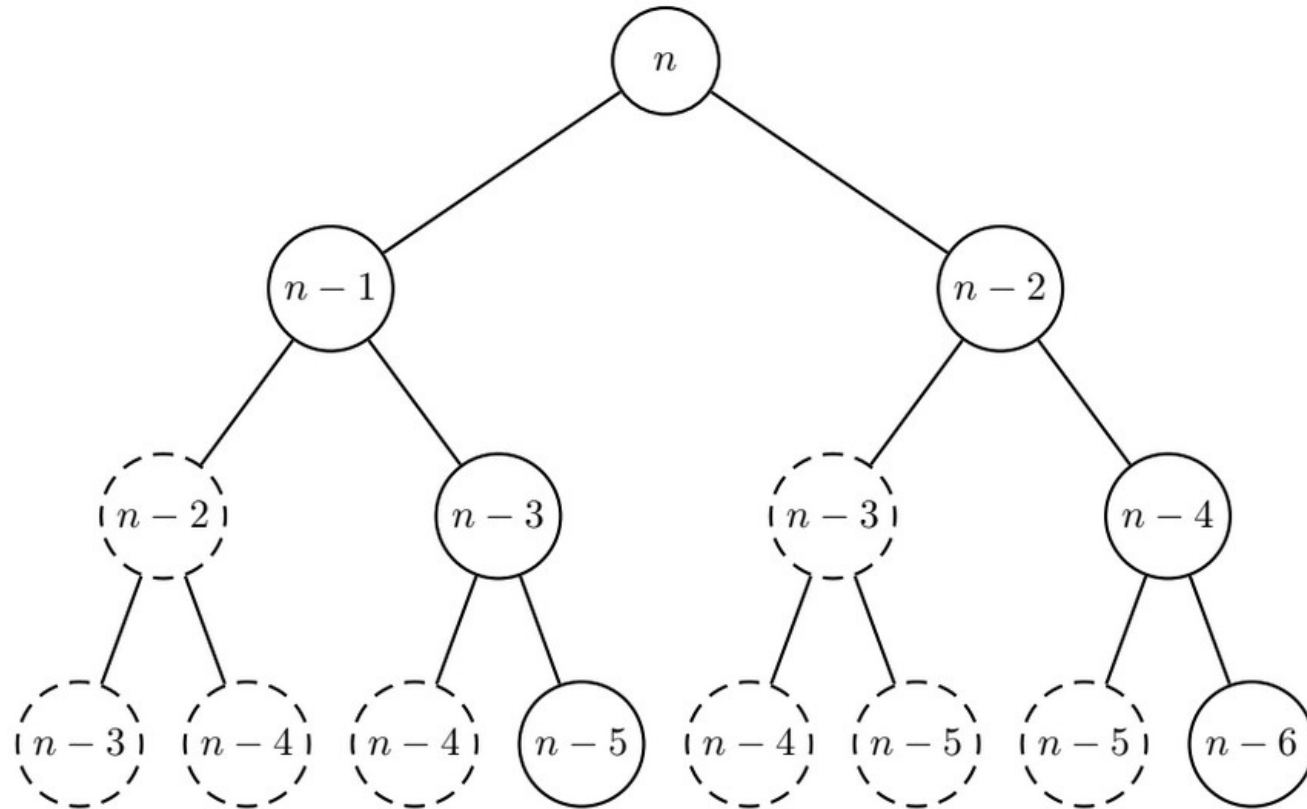
FIBONACCI(n)

```
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  $F_n$ 
```

Iterative: Fast (linear)

RECURSIVEFIBONACCI(n)

```
1  if  $n = 1$  or  $n = 2$   
2      return 1  
3  else  
4       $a \leftarrow$  RECURSIVEFIBONACCI( $n - 1$ )  
5       $b \leftarrow$  RECURSIVEFIBONACCI( $n - 2$ )  
6      return  $a + b$ 
```



Recursive: Slow
(exponential)

Algorithms

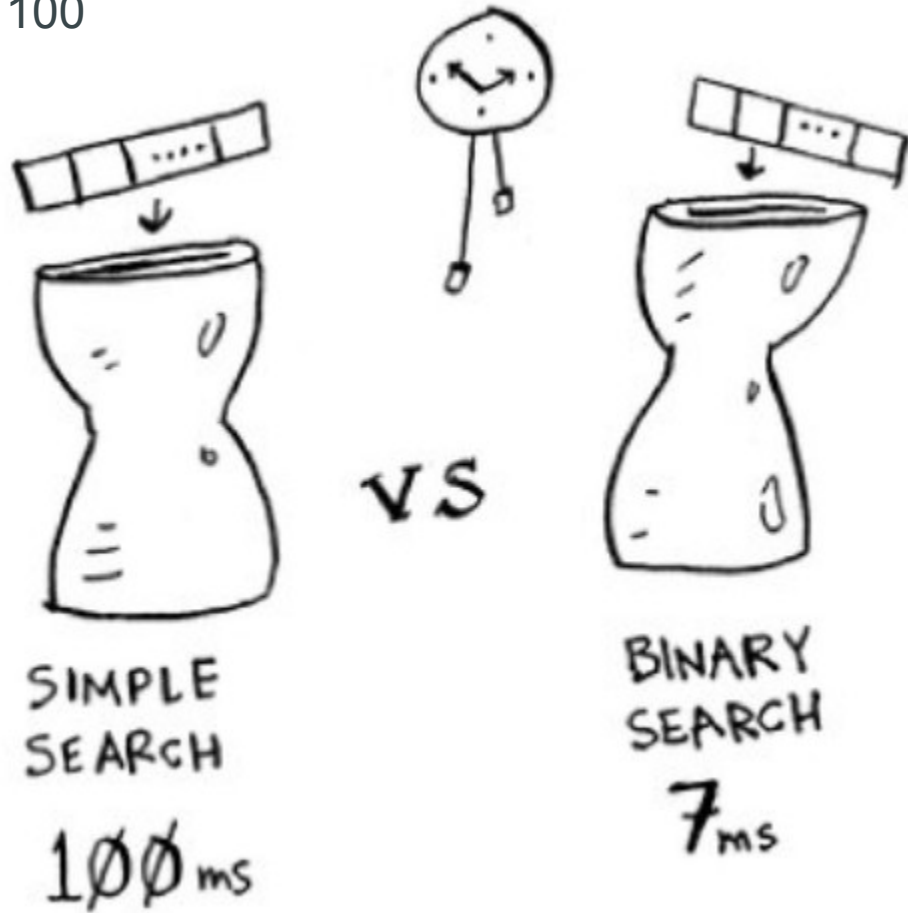
- Brute force : Try Everything, slow but always correct
- Recursive : To Solve for n , first solve for $n-1$
- Iterative : Loop on something, can be faster

Fast vs Slow algorithms

- How many operations does an algorithm take as N increases?
- Is the relationship linear? Quadratic? Exponential?
- What is the upper limit of the running time of an algorithm as N increases?

Guess random number (up/down)

1ms / check
N = 100



Simple search:

```
For i in 1 to N  
If i == the number  
return i
```

Binary search:

```
Range-min = 1  
Range-max = N  
While ()  
i = middle number of range  
if i == the number; return I  
elseif i < number; Range-max=i;  
elseif i > number; Range-min=i;
```

Guess random number (up/down)

	SIMPLE SEARCH	BINARY SEARCH	
100 ELEMENTS	100ms	7ms	~15 times faster
10,000 ELEMENTS			
1,000,000,000 ELEMENTS			

??? Guess ???

Guess random number (up/down)

	SIMPLE SEARCH	BINARY SEARCH	
100 ELEMENTS	100ms	7ms	~15 times faster
10,000 ELEMENTS			
1,000,000,000 ELEMENTS	~450ms ?	32ms	~15 times faster ?

Guess random number (up/down)

	SIMPLE SEARCH	BINARY SEARCH	
100 ELEMENTS	100ms	7ms	~15 times faster
10,000 ELEMENTS			
1,000,000,000 ELEMENTS	11 days	32ms	~15 times faster doesn't make sense!

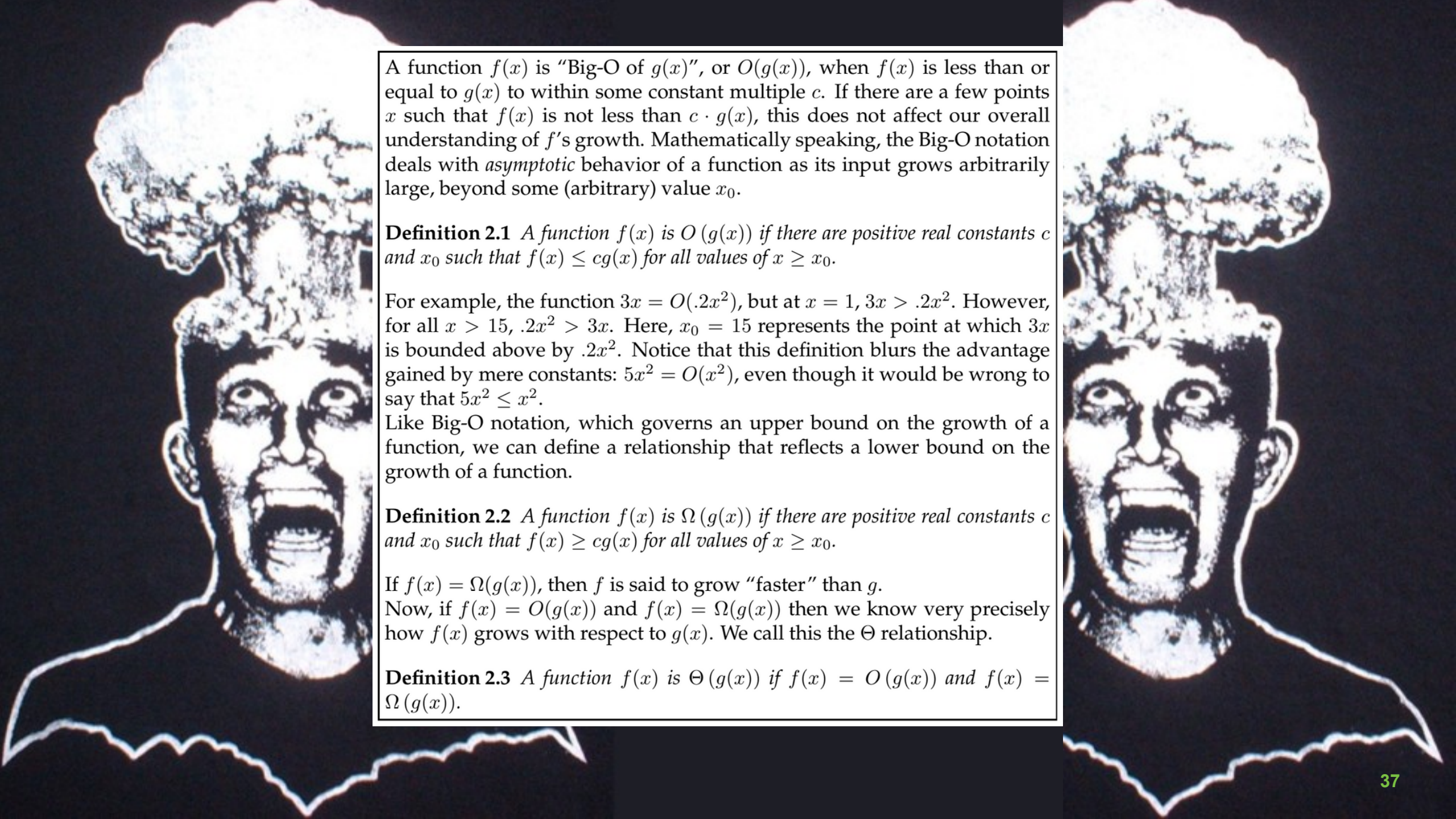
Guess random number (up/down)

	SIMPLE SEARCH	BINARY SEARCH
100 ELEMENTS	100ms	7ms
10,000 ELEMENTS	10 seconds	14ms
1,000,000,000 ELEMENTS	11 days	32ms

Linear
1 ms/element
 $O(n)$

Logarithmic
1 ms/ $\log_2(\text{element})$
 $O(\log n)$

"BIG O" → $O(n)$ ← NUMBER OF OPERATIONS (Worst case scenario)



A function $f(x)$ is “Big-O of $g(x)$ ”, or $O(g(x))$, when $f(x)$ is less than or equal to $g(x)$ to within some constant multiple c . If there are a few points x such that $f(x)$ is not less than $c \cdot g(x)$, this does not affect our overall understanding of f 's growth. Mathematically speaking, the Big-O notation deals with *asymptotic* behavior of a function as its input grows arbitrarily large, beyond some (arbitrary) value x_0 .

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 $x \geq x_0$.

For example, the function $3x = O(.2x^2)$, but at $x = 1$, $3x > .2x^2$. However, for all $x > 15$, $.2x^2 > 3x$. Here, $x_0 = 15$ represents the point at which $3x$ is bounded above by $.2x^2$. Notice that this definition blurs the advantage gained by mere constants: $5x^2 = O(x^2)$, even though it would be wrong to say that $5x^2 \leq x^2$.

Like Big-O notation, which governs an upper bound on the growth of a function, we can define a relationship that reflects a lower bound on the growth of a function.

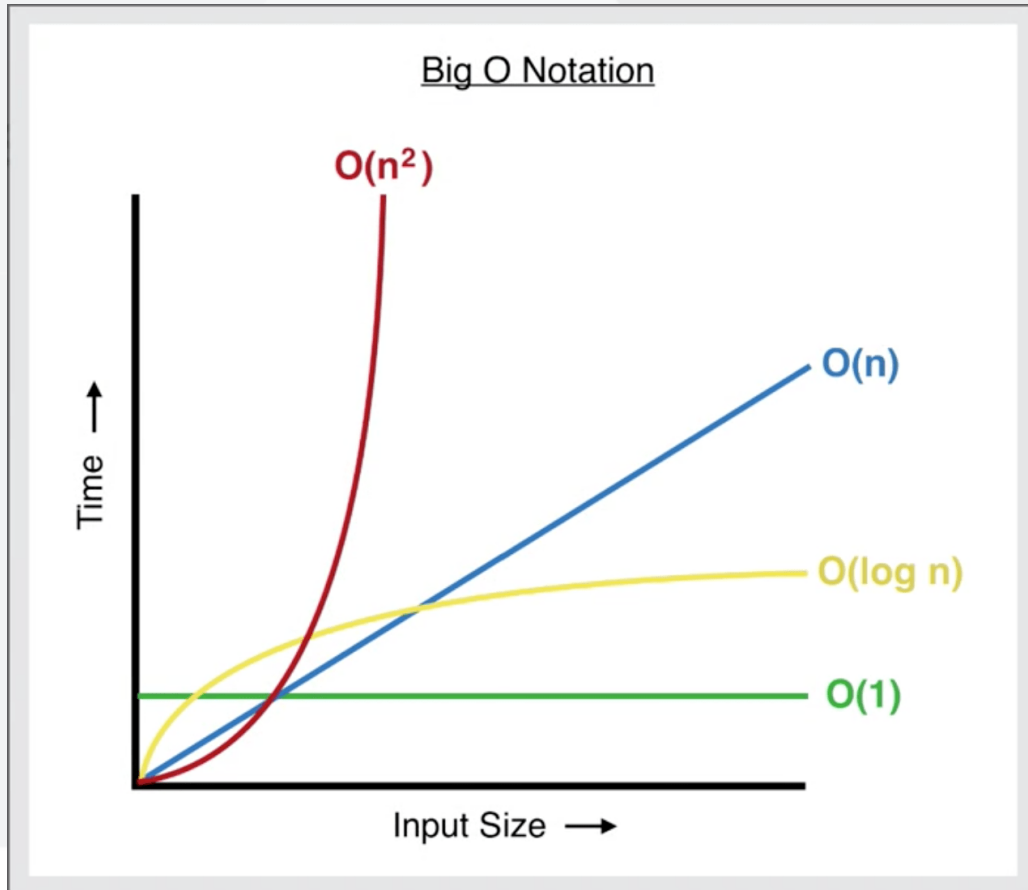
Definition 2.2 A function $f(x)$ is $\Omega(g(x))$ if there are positive real constants c and x_0 such that $f(x) \geq cg(x)$ for all values of $x \geq x_0$.

If $f(x) = \Omega(g(x))$, then f is said to grow “faster” than g .

Now, if $f(x) = O(g(x))$ and $f(x) = \Omega(g(x))$ then we know very precisely how $f(x)$ grows with respect to $g(x)$. We call this the Θ relationship.

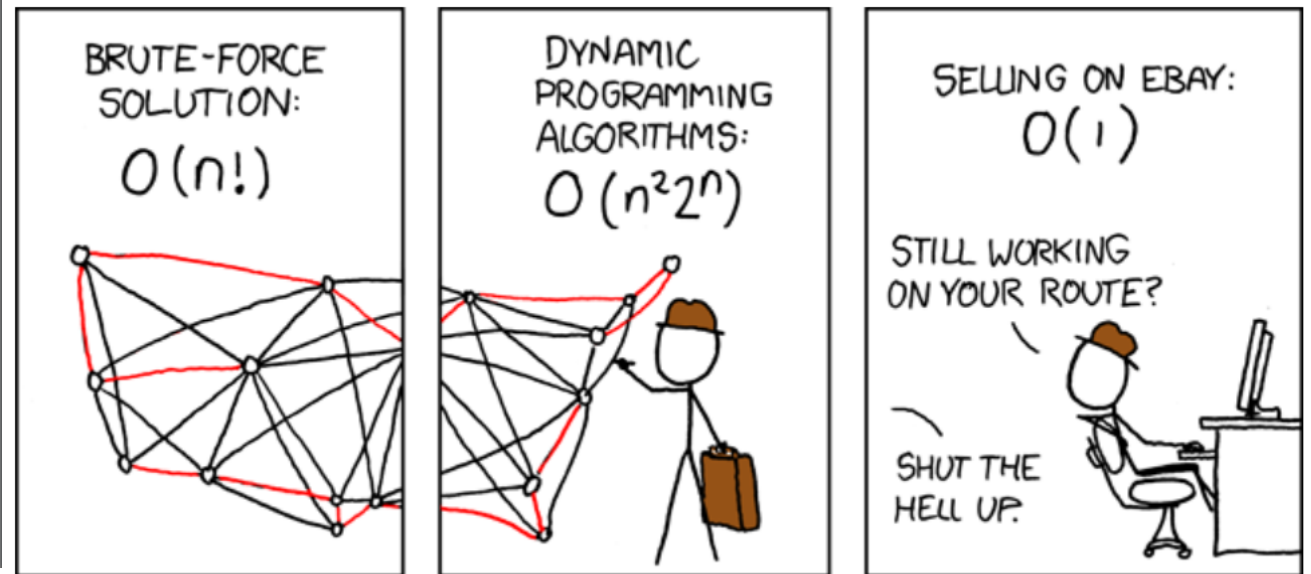
Definition 2.3 A function $f(x)$ is $\Theta(g(x))$ if $f(x) = O(g(x))$ and $f(x) = \Omega(g(x))$.

Common Big-Os



- $O(\log n)$, also known as *log time*. Example: Binary search.
- $O(n)$, also known as *linear time*. Example: Simple search.
- $O(n * \log n)$. Example: A fast sorting algorithm, like quicksort.
- $O(n^2)$. Example: A slow sorting algorithm, like selection sort.
- $O(n!)$. Example: A really slow algorithm, like the traveling salesperson.

"Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city and returns to the origin city?"



<https://www.freecodecamp.org/news/big-o-notation-simply-explained-with-illustrations-and-video-87d5a71c0174/>



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Thank you for your attention!
60 minutes lunch break.



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