Introduction to Computation

ESR Programming Workshop - IGNITE

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Winter 2018-19

Introduction

- This is meant as a quick and interactive overview of data structures and algorithms.
- If you see something you are interested in we can spend more time on it.
- Feel free to interrupt if you have questions or comments. We have lots of time.

Algorithms

The step-by-step procedure of solving a problem. Roughly speaking, they follow one of the following patterns:

- Divide and Conquer (inductive)
- Greedy (optimal subproblems)
- Dynamic (recurrence relations)
- Brute Force / Heuristic / Statistical

Measuring Performance

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- Asymptotic Complexity
  - Limit as size of input n approaches ∞
  - Time or Space

Asymptotic Complexity

We care about the number of steps taken given an arbitrary input(s).

- $O(f) \rightarrow$ function f is an *upper* bound
- $\Theta(f) \rightarrow$ function f is an *exact* bound
- $\Omega(f) \rightarrow$ function f is a *lower* bound

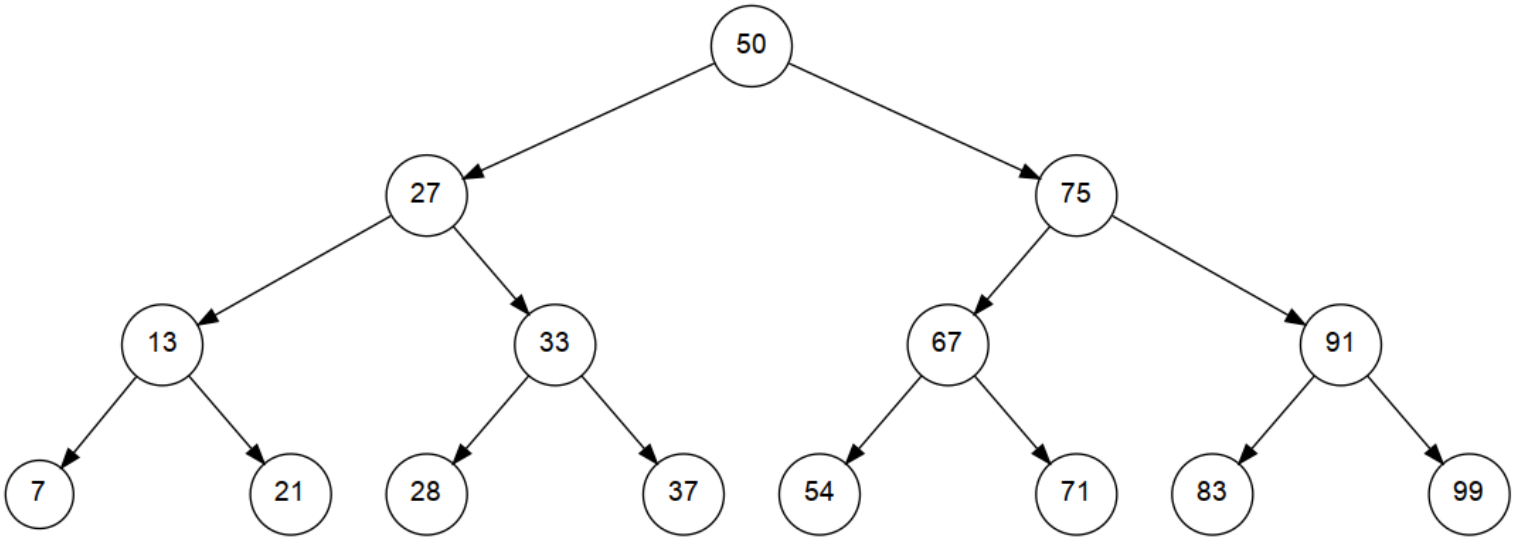
List Example

Given a list of n elements in $\mathbb{Z}$, how many steps are needed to compute the sum?

- Initialize our algorithm with a sum of 0 as an accumulator.
- Add the x_0 element to the accumulator
  - Then add the x_1 element to accumulator
  - Then add the x_2 element to the accumulator
  - ...
- This repeats **exactly** n times: therefore this algorithm is $\Theta(n)$.
  - We can also call this a *linear* algorithm.

BST Example

Given a *Binary Search Tree* of n elements in $\mathbb{Z}$, how many steps are needed to search for a given $x \in \mathbb{Z}$? Assume that the tree is perfectly balanced.



BST Example (cont)

- Start at the root node that contains element k.
  - If $x = k$, return *true*.
  - If $x < k$, go to the left child.
  - If $x > k$, go to the right child.
- Repeat until x is found or *empty* tree is reached.

BST Example (cont)

How many steps is this compared to the tree size of n?

Consider when the worst case occurs.

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- When we travel the whole *height* of the tree.
  - A tree of height 1 can have 1 element
  - A tree of height 2 can have 3 elements
  - A tree of height 3 can have 7 elements

Which means...

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Which means...

- A tree of height h can have $2^h - 1$ elements

BST Example (cont)

- Rewrite in terms of n.

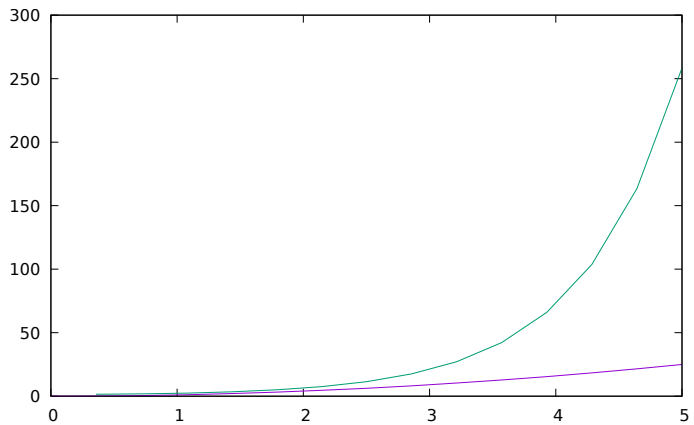
$$
\begin{aligned}
2^h - 1 &= n \\
2^h &= n + 1 \\
h &= log_2(n+1) \\
h &= log(n) \qquad \leftarrow \text{what happened here?}
\end{aligned}
$$

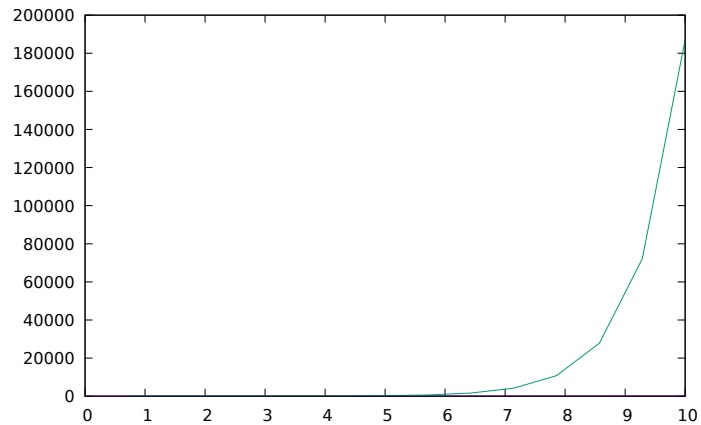
- This is the *worst case* for a *balanced* tree, so we would say the complexity is $O(log(n))$, or has a logarithmic running time.
- What happens if the tree is not balanced?

Importance of Complexity Analysis

String Alignment

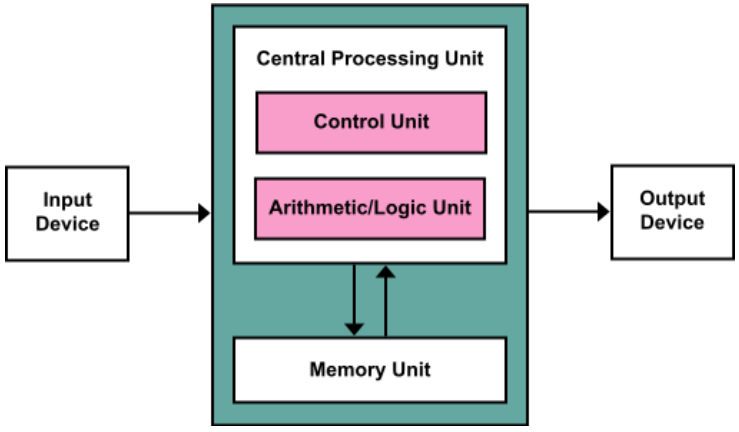
- Brute Force $\in NP := \binom{m+n}{n} = O(\frac{(m+n)!}{(n!)^2})$
- Dynamic (Needleman-Wunsh) $\in P := O(mn)$





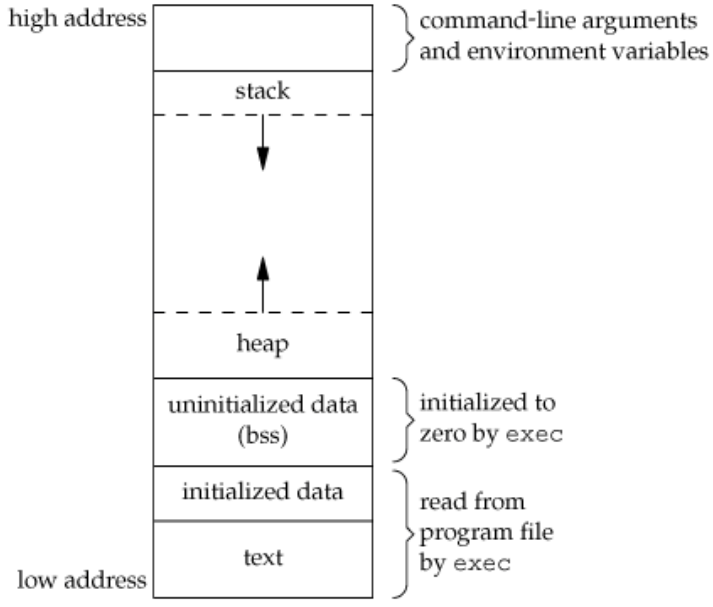
Machine

Hardware



Source : Kapooht - CC BY-SA 3.0

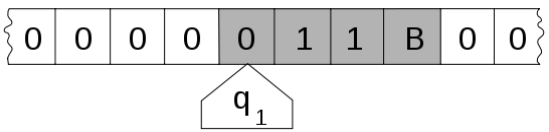
Memory



Source : Holberton School

What is Computable?

Turing Machine



Source : wikipedia.org

Lambda Calculus

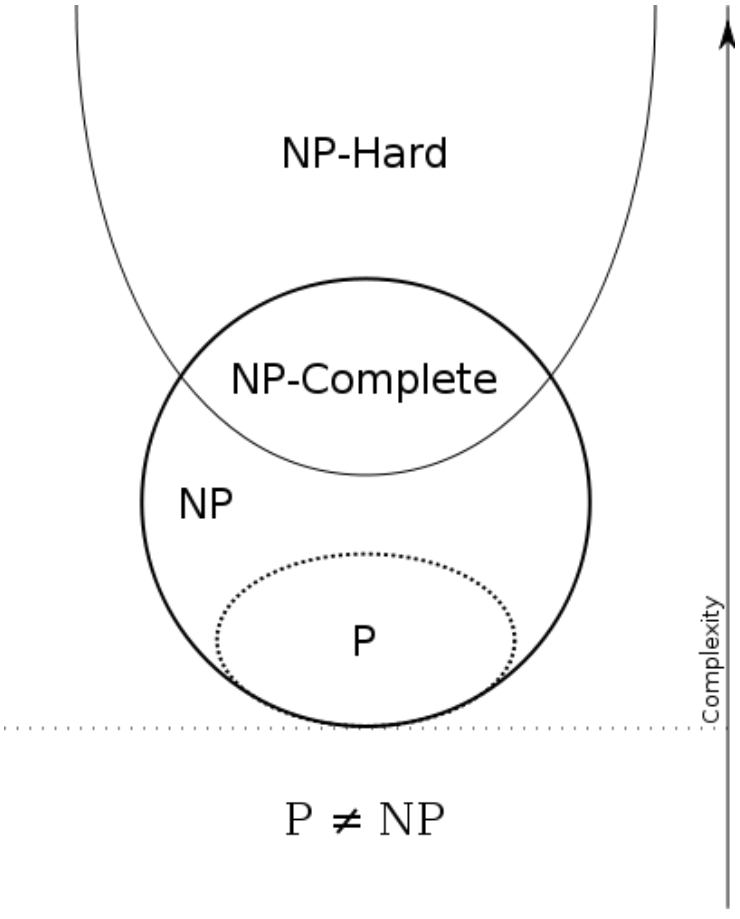
$$0 := \lambda f.\lambda x.x$$

$$1 := \lambda f.\lambda x.fx$$

$$2 := \lambda f.\lambda x.f(fx)$$

$$3 := \lambda f.\lambda x.f(f(fx))$$

What is Computable? (cont)

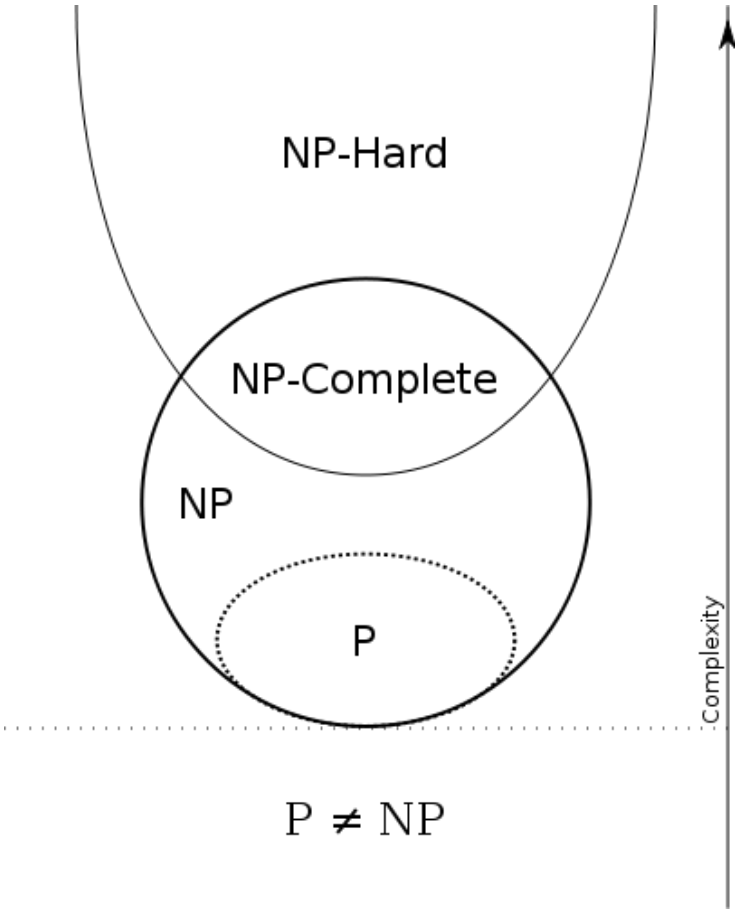


Source : wikipedia.org

Problems in P

- Polynomial time *computable*
- Solvable by a deterministic Turing machine or primitive recursion
- Max element, sorting....

What is Computable? (cont)

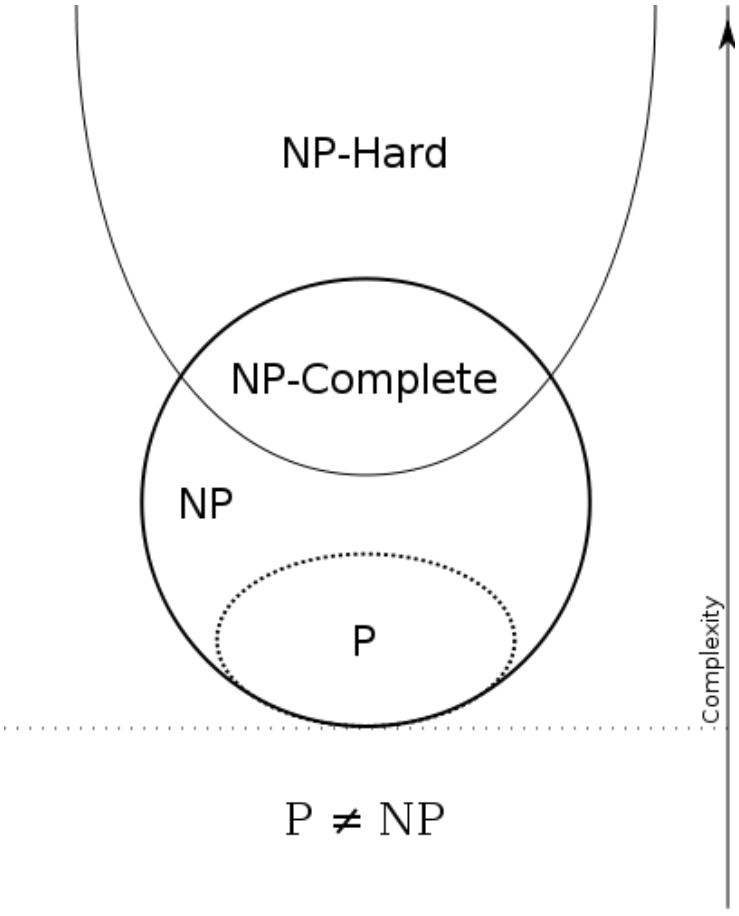


Source : wikipedia.org

Problems in *NP*

- Polynomial time *verifiable*
- Solvable by a non-deterministic Turing machine or general recursion
- 3-SAT, traveling salesman...

What is Computable? (cont)



Source : wikipedia.org

Problems in *NP-Hard*

- At least as hard as NP-Complete.
- Halting Problem, Max Clique...

Computability in Bioinformatics

Problems $\in P$

- Relative Amino Abundance
- String Alignment
- String Search

Problems $\notin P$

- Sequence Assembly
- Breakpoint Distance
- Topology of Pangenomes

Data Types / Data Structures

Computer memory is *linear* and cells are *fixed* size. Real world data needs to be parsed into a format that a machine can operate over. Data can be constructed with:

- Unboxed raw values (machine words)
- Boxed values with a type (pointer to data)
- Product of datum (**and**)
- Coproduct of datum (**or**)

Data Types / Data Structures (cont)

There are 2 special types:

- Empty Type (0) - No inhabitants
- Unit Type (1) - Single inhabitant

We can also leave "holes" in data to fill in later. This is called *polymorphism*.

Linked List

We define a list inductively: it can either be empty or some element and the rest of the list. Mathematically, we could write

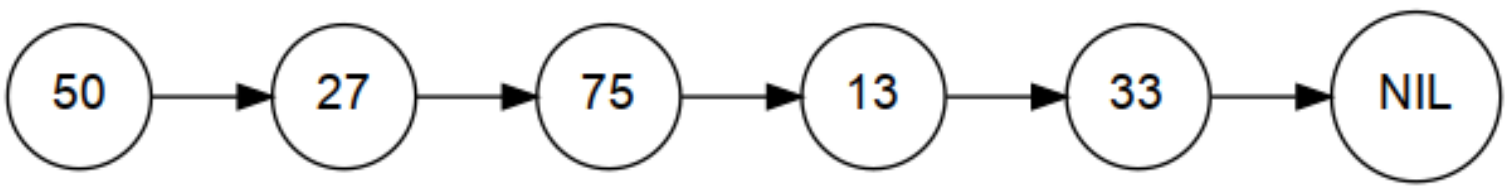
$$L_a = 1 + a * L_a$$

where a is the placeholder for the type of data that will eventually be in the list (i.e.- polymorphism).

Linked List (cont)

To decompose to a machine representation, determine what the building blocks of the structure are. In this case:

- We can make a unit type (the *Nil* or empty list).
- Or we can make a pair of a value $x \in a$ and another list structure (which is a pointer)



Control

Data Types mean nothing without proper control structures for manipulation. Machines have many variations of *JMP*. This is bad for actual software!

Control (cont)

Imperative remedy this with:

- Conditional Branching (if-then-else, switch)
- Semi-Structured Looping (while, do-while, for-loop)

Declarative remedy this with:

- Conditional Branching (if-then-else)
- Pattern Matching
- Recursion

Exercises (1)

Max Element in Linked List

- Algorithm
- Complexity

Exercises (2)

Max Element in a BST

- Algorithm
- Complexity

Exercises (3)

Sorting a List

- Bubble/Insertion Sort
- Merge Sort
- Compare

Exercises (3)

Fractional Knapsack Problem

Given a bag that can hold W kilograms, and piles of spices $S_1, S_2 ... S_n$, which have a price value of $V_1, V_2 ... V_n$, find an algorithm to maximize the value of the spices contained in the bag.

- Algorithm
- Complexity

End

Questions or Comments?