

# Scientific Programming: Algorithms (part B)

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Programming paradigms

# Problems and solutions

Given a problem:

- There are no "general recipes" to solve it
- Nevertheless, we can identify four phases:
  - Problem classification
  - Solution characterization
  - Selection of the algorithmic technique
  - Selection of the data structure
- These phases are not strictly sequential

# Classification of problems

## Decisional problems

- Does the input satisfy a given property?
- Output: the answer is yes/no
- Example: is the graph connected?

## Search problems

- Research space: a set of possible "solutions"
- Admissible solution: a solution that does satisfy some conditions
- Example: position of a substring in the string

# Classification of problems

## Optimization problems

- Each solution is associated with a cost function
- We want to identify the solution with minimum cost
- Example: the shortest path between nodes in a graph

## Approximation problems

- Sometimes, obtaining the optimal solution is computationally infeasible
- We may be satisfied by an approximate solution: low cost, but we are not sure that the cost is the smallest possible
- Example: the traveling salesman problem

# Mathematical characterization

It is important to mathematically define the relationship between input and output

- Very often the mathematical characterization is trivial...
- ... but it could provide a first idea of the solution
- Example: given a sequence of  $n$  elements, a sorted permutation is given by the minimum followed by a sorted permutation of the remaining  $n - 1$  elements (Selection Sort)

The mathematical characterization can suggest a possible technique

- Optimal substructure  $\rightarrow$  Dynamic programming
- Greedy choice  $\rightarrow$  Greedy technique

# Mathematical characterization

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# Algorithmic techniques

## Divide-et-impera

- The problem is subdivided in **independent** subproblems, that are solved recursively (in a **top-down** approach)
- Area of application: decision problems, search

## Dynamic programming

- The solution is built in a **bottom-up** way from the solution of smaller problems (**potentially repeated**)
- Area of application: optimization problems

## Memoization

- Top-down version of dynamic programming

# Algorithmic techniques

## Greedy

- Greedy approach: select the choice which appears "locally optimal"
- Area of application: optimization problems

## Backtrack

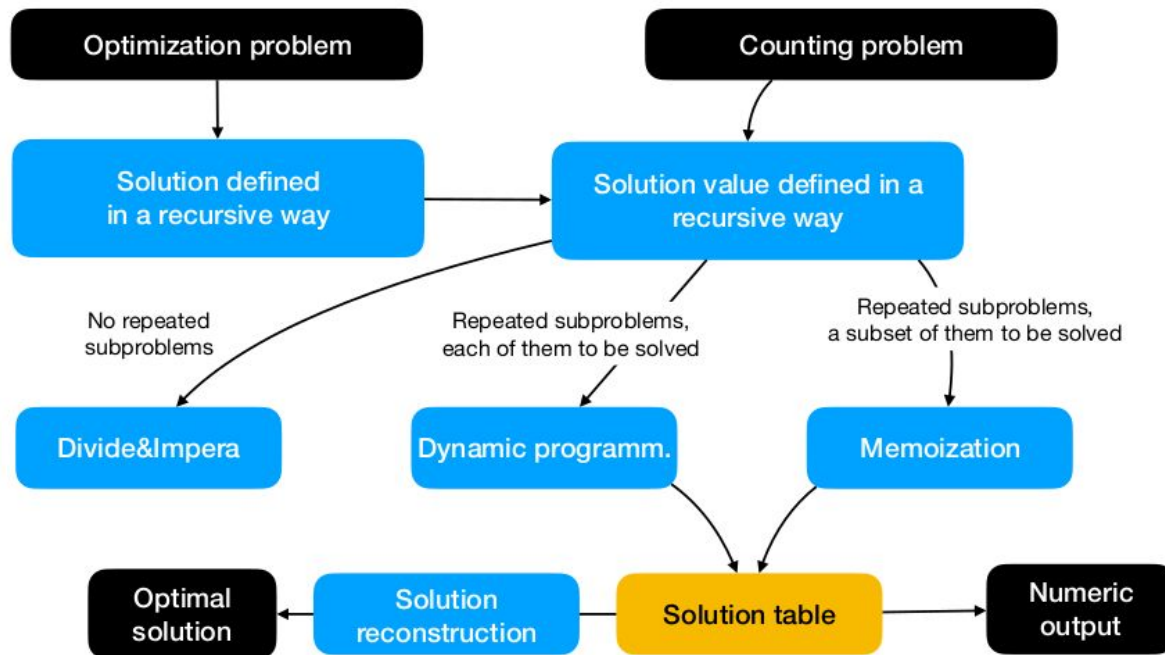
- Try something, and if does not work, try something else
- Area of application: search problems, optimization problems

## Local search

- The optimal solution can be obtained by continuously improving sub-optimal solutions



# General approach



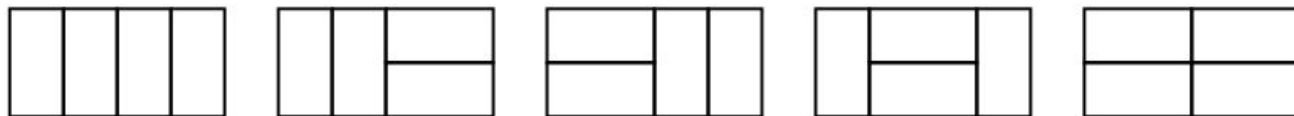
# Dominoes

## Definition

The dominoes game consists of tiles with size  $2 \times 1$ . Let us consider the arrangements of  $n$  tiles inside a rectangle  $2 \times n$ . Write an efficient algorithm that computes the number of possible arrangements and discuss its correctness. Compute an upper bound to its complexity.

## Example

The cases below represent the five possible arrangements in a rectangle  $2 \times 4$ .



Any ideas on how to solve this problem?

# Dominoes

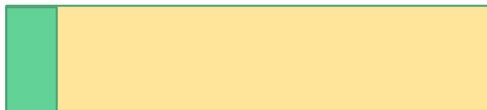
## Recursive definition

Let's define a recursive formula that computes the number of possible arrangements.

- If a vertical tile is placed, the problem of size  $n - 1$  must be solved.
- If an horizontal tile is placed, then another horizontal tile must be placed as well; the problem of size  $n - 2$  must be solved.

$$D(n) = \begin{cases} 1 \\ ? \end{cases}$$

$2 \times n$

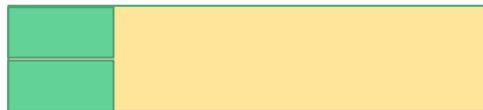


$$n \leq 1$$

$$n > 1$$



$2 \times n$



$n = 0$ , only one possibility: **no tiles**.  
 $n = 1$ , only 1 possibility,  
**vertical tile**

# Dominoes

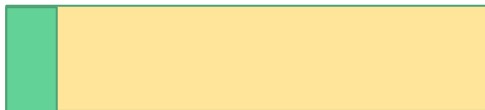
## Recursive definition

Let's define a recursive formula that computes the number of possible arrangements.

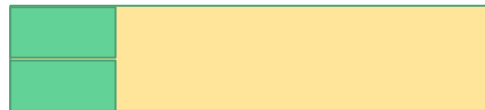
- If a vertical tile is placed, the problem of size  $n - 1$  must be solved.
- If an horizontal tile is placed, then another horizontal tile must be placed as well; the problem of size  $n - 2$  must be solved.

$$D(n) = \begin{cases} 1 & n \leq 1 \\ D(n-2) + D(n-1) & n > 1 \end{cases} \quad \leftarrow$$

2xn



2xn



We sum because the two cases originate different solutions

# Dominoes

$$D(n) = \begin{cases} 1 & n \leq 1 \\ D(n-2) + D(n-1) & n > 1 \end{cases}$$

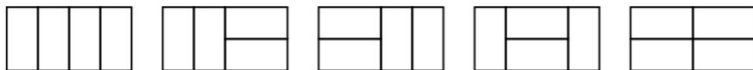
The generated mathematical series is the following:

1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, ...

Does it sound familiar?

Fibonacci's numbers!

$N = 4$  (i.e.  $2 \times 4$ )  $\rightarrow$  5 possible dispositions



# Dominoes: recursive algorithm

$$D(n) = \begin{cases} 1 & n \leq 1 \\ D(n-2) + D(n-1) & n > 1 \end{cases}$$

Write a recursive algorithm that solves the problem

```
def dominoes(n):  
    if n <= 1:  
        return 1  
    else:  
        return dominoes(n-2) + dominoes(n-1)  
  
for i in range(10):  
    print(dominoes(i), end = " ")
```

1 1 2 3 5 8 13 21 34 55

# Complexity

What is the complexity of dominoes?

```
def dominoes(n):  
    if n <= 1:  
        return 1  
    else:  
        return dominoes(n-2) + dominoes(n-1)  
  
for i in range(10):  
    print(dominoes(i), end = " ")  
  
1 1 2 3 5 8 13 21 34 55
```

$$T(n) = \begin{cases} 1 & n \leq 1 \\ T(n-1) + T(n-2) + 1 & n > 1 \end{cases}$$

Theorem not seen:

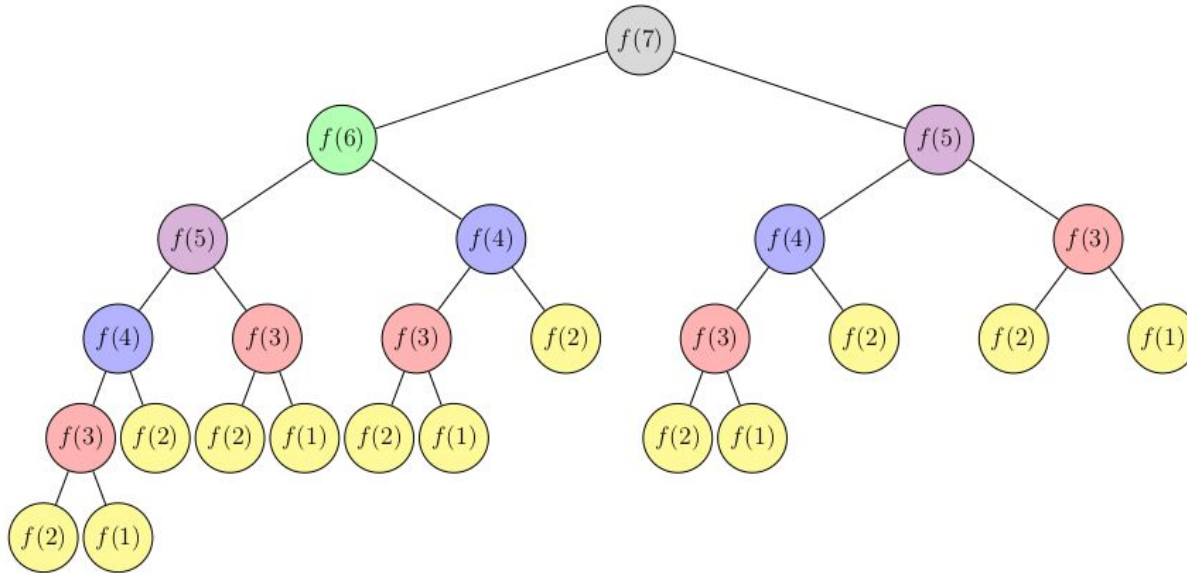
Linear recurrences with constant order:

- $a_1 = 1, a_2 = 1, a = 2, \beta = 0$
- Complexity:  $\Theta(a^n \cdot n^\beta)$

$$T(n) = \Theta(2^n)$$

# Recursive tree

```
def dominoes(n):  
    if n <= 1:  
        return 1  
    else:  
        return dominoes(n-2) + dominoes(n-1)  
  
for i in range(10):  
    print(dominoes(i), end = " ")  
  
1 1 2 3 5 8 13 21 34 55
```



Several sub-problems are repeated!



# How to avoid computing the same thing over and over again

## DP Table

- We use a *DP table* (list, matrix, dictionary, etc.) to store results of sub-problems already solved
- The table contains an entry for each subproblem to be solved
- The table is indexed by a description of the input (e.g., size)
- When the same subproblem has to be solved again, we use the result stored in the table

# How to avoid computing the same thing over and over again

## Base cases

- The base cases do not need to be computed, they can be stored immediately

## Bottom-up iteration

- We start from problems that can be solved using only base cases
- We go up to larger and larger problems...
- ... up to the final goal

$n$	0	1	2	3	4	5	6	7
$DP[]$	1	1	2	3	5	8	13	21

# An iterative solution

$$D(n) = \begin{cases} 1 & n \leq 1 \\ D(n-2) + D(n-1) & n > 1 \end{cases}$$

Write an iterative algorithm that solves the Dominoes problem

```
def dominoes2(n):  
    res = [0]*(n+1)  
    res[0] = 1  
    res[1] = 1  
    for i in range(2,n+1):  
        res[i] = res[i-1] + res[i-2]  
    return res[n]
```

What is the computational complexity of domino2(n)?

$$T(n) = \Theta(n)$$

How about the space complexity?

What is the size of res?

$$S(n) = \Theta(n)$$

**Ideas on how to improve this?**

## Another iterative solution

$$D(n) = \begin{cases} 1 & n \leq 1 \\ D(n-2) + D(n-1) & n > 1 \end{cases}$$

```
def dominoes3(n):  
    dp0 = 1  
    dp1 = 1  
    dp2 = 1  
    for i in range(2, n+1):  
        dp0 = dp1  
        dp1 = dp2  
        dp2 = dp0 + dp1  
    return dp2
```

What is the space complexity of domino3(n)?

$$S(n) = \Theta(1)$$

$n$	0	1	2	3	4	5	6	7
$DP[]$	1	1	2	3	5	8	13	21

# Uniform vs Logarithmic cost model

$$D(n) = \begin{cases} 1 & n \leq 1 \\ D(n-2) + D(n-1) & n > 1 \end{cases}$$

Are you sure that our complexity formulas are correct?

## Binet's Formula for Fibonacci's number

$$D(n-1) = F(n) = \frac{\phi^n}{\sqrt{5}} - \frac{(1-\phi)^n}{\sqrt{5}} = \frac{\phi^n - (-\phi)^{-n}}{\sqrt{5}}$$

where

$$\phi = \frac{1 + \sqrt{5}}{2} = 1,6180339887 \dots \quad \text{golden ratio}$$

Watch out: the Fibonacci's number grows exponentially!

How many bits are needed to store  $F(n)$ ?

# Uniform vs Logarithmic cost model

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where

$$\phi = \frac{1 + \sqrt{5}}{2} = 1,6180339887 \dots$$

How many bits are needed to store  $F(n)$ ?

$$\log F(n) = \Theta(n)$$



complexity seen before needs to be multiplied by  $n$

# Uniform vs Logarithmic cost model

$$D(n) = \begin{cases} 1 & n \leq 1 \\ D(n-2) + D(n-1) & n > 1 \end{cases}$$

Under the logarithmic cost model, the three versions have the following complexities:

Function	Time complexity	Space complexity
domino1()	$O(n2^n)$	$O(n^2)$
domino2()	$O(n^2)$	$O(n^2)$
domino3()	$O(n^2)$	$O(n)$

```
s = time.time()
for i in range(1,45):
    print(dominoes(i), end = " ")
e = time.time()
print("Elapsed time: {}s".format(e-s))
s = time.time()
for i in range(1,45):
    print(dominoes2(i), end = " ")
e = time.time()
print("Elapsed time: {}s".format(e-s))

s = time.time()
for i in range(1,45):
    print(dominoes3(i), end = " ")
e = time.time()
print("Elapsed time: {}s".format(e-s))
```

1 2 3 5 8 ... 1134903170  
Elapsed time: 659.3645467758179s

1 2 3 5 8 ... 1134903170  
Elapsed time: 0.0007071495056152344s

1 2 3 5 8 ... 1134903170  
Elapsed time: 0.0011742115020751953s

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$$D(n) = \begin{cases} 1 & n \leq 1 \\ D(n-2) + D(n-1) & n > 1 \end{cases}$$

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# Hateville

- Hateville is a strange village, composed of  $n$  houses, numbered  $1$ - $n$  and placed along a single road
- In Hateville, everybody hates his next-door neighbors, on both sides: thus a person living in house  $i$  hates the neighbors living in houses  $i - 1$  and  $i + 1$  (if they exist)
- Hateville wants to organize a festival; your task is to collect money to organize it.
- Each inhabitant  $i$  wants to donate a quantity  $D[i]$  of money, but he will give nothing if any of his neighbors is donating.



# Hateville



Consider the following problems:

- Write an algorithm that returns the largest amount of money that can be collected
- Write an algorithm that returns a subset of indexes  $S \subseteq \{1, \dots, n\}$  such that the total amount  $T = \sum_{i \in S} D[i]$  is maximal.



remember the  
additional constraint  
that indexes must not  
be consecutive

Examples:

- |                                     |                                       |
|-------------------------------------|---------------------------------------|
| • Donation list: $D = [4, 3, 6, 5]$ | • Donation list: $D = [10, 5, 5, 10]$ |
| • Maximum amount: 10                | • Maximum amount: 20                  |
| • Index set: $\{1, 3\}$             | • Index set: $\{1, 4\}$               |

# Hateville

- Donation list:  $D = [4, 3, 6, 5]$
- Maximum amount: 10
- Index set:  $\{1, 3\}$
- Donation list:  $D = [10, 5, 5, 10]$
- Maximum amount: 20
- Index set:  $\{1, 4\}$

How would you solve the problem?

We re-define the problem

- Let  $HV(i)$  be the set of numbers to be selected to obtain the maximum amount of donations from the first  $i$  houses, numbered  $1 \dots n$
- $HV(n)$  is the solution to the original problem

# Hateville

- Donation list:  $D = [4, 3, 6, 5]$
- Maximum amount: 10
- Index set:  $\{1, 3\}$
- Donation list:  $D = [10, 5, 5, 10]$
- Maximum amount: 20
- Index set:  $\{1, 4\}$

Let's compute  $HV(i)$  based on  $HV(0) \dots HV(n-1)$  values

- What happens if I don't accept its donation?

$$HV(i) =$$

# Hateville

- Donation list:  $D = [4, 3, 6, 5]$
- Maximum amount: 10
- Index set:  $\{1, 3\}$
- Donation list:  $D = [10, 5, 5, 10]$
- Maximum amount: 20
- Index set:  $\{1, 4\}$

Let's compute  $HV(i)$  based on  $HV(0) \dots HV(n-1)$  values

- What happens if I don't accept its donation?

$$HV(i) = HV(i-1)$$

# Hateville

- Donation list:  $D = [4, 3, 6, 5]$
- Maximum amount: 10
- Index set:  $\{1, 3\}$
- Donation list:  $D = [10, 5, 5, 10]$
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- What happens if I accept its donation?

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- Donation list:  $D = [4, 3, 6, 5]$
- Maximum amount: 10
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- Maximum amount: 20
- Index set:  $\{1, 4\}$

Let's compute  $HV(i)$  based on  $HV(0) \dots HV(n-1)$  values

- What happens if I don't accept its donation?

$$HV(i) = HV(i-1)$$

- What happens if I accept its donation?

$$HV(i) = HV(i-2) + D[i]$$

- How can I choose between the two cases?

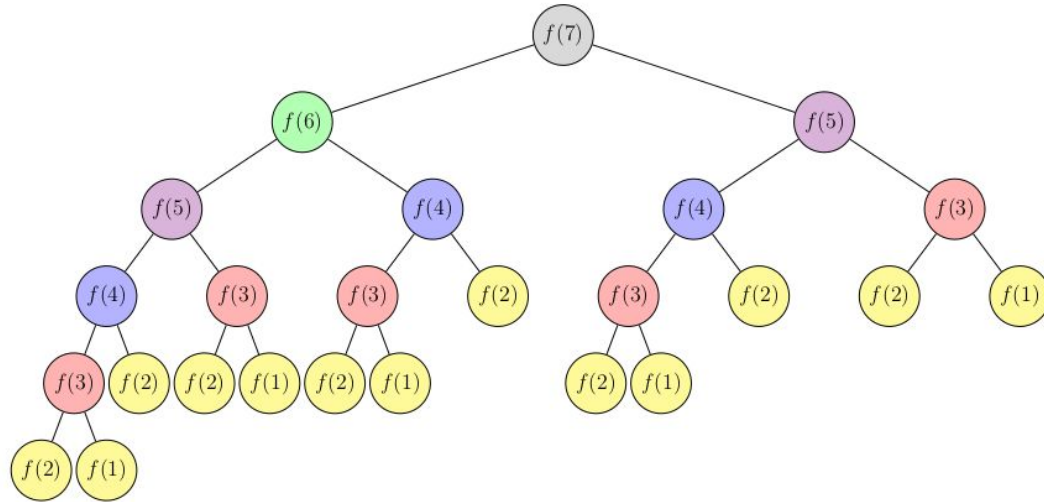
$$\max(HV(i-1), HV(i-2) + D[i])$$

## Hateville: recursive algorithm?

$$\max(HV(i-1), HV(i-2) + D[i])$$

Write a recursive algorithm that solves Hateville?

Would it be a good idea?





# DP Table

$$\max(HV(i-1), HV(i-2) + D[i])$$

## Value of the optimal solution

- Let  $DP(i)$  be the **value** of the maximum amount of donation that we can obtain from the first  $i$  houses of Hateville
- $DP(n)$  is the value of the optimal solution

$$DP(i) = \begin{cases} 0 & \text{if } i = 0 \\ D[1] & \text{if } i = 1 \\ \max(DP(i-1), DP(i-2) + D[i]) & \text{if } n \geq 2 \end{cases}$$

# Iterative solution

$$DP(i) = \begin{cases} 0 & \text{if } i = 0 \\ D[1] & \text{if } i = 1 \\ \max(DP(i-1), DP(i-2) + D[i]) & \text{if } i \geq 2 \end{cases}$$

Write an algorithm that solves the Hateville problem

```
def hateville(D, n):
    dp = [0]*(n+1)
    if n > 0:
        dp[1] = D[0]
    for i in range(2, n+1):
        dp[i] = max(dp[i-1], dp[i-2] + D[i-1])

    return dp[n]
```

```
D = [10,5,5,8,4,7,12]

print("Donations: {}".format(D))
for i in range(len(D)+1):
    print("Solution for {}: {}".format(D[0:i],hateville(D, i)))
```

```
Donations: [10, 5, 5, 8, 4, 7, 12]
Solution for []: 0
Solution for [10]: 10
Solution for [10, 5]: 10
Solution for [10, 5, 5]: 15
Solution for [10, 5, 5, 8]: 18
Solution for [10, 5, 5, 8, 4]: 19
Solution for [10, 5, 5, 8, 4, 7]: 25
Solution for [10, 5, 5, 8, 4, 7, 12]: 31
```

```
D1 = [10,1,1,10,1,1,10]

print("Donations: {}".format(D1))
for i in range(len(D1)+1):
    print("Solution for {}: {}".format(D1[0:i],hateville(D1, i)))
```

```
Donations: [10, 1, 1, 10, 1, 1, 10]
Solution for []: 0
Solution for [10]: 10
Solution for [10, 1]: 10
Solution for [10, 1, 1]: 11
Solution for [10, 1, 1, 10]: 20
Solution for [10, 1, 1, 10, 1]: 20
Solution for [10, 1, 1, 10, 1, 1]: 21
Solution for [10, 1, 1, 10, 1, 1, 10]: 30
```

# Iterative solution

$$DP(i) = \begin{cases} 0 & \text{if } i = 0 \\ D[1] & \text{if } i = 1 \\ \max(DP(i-1), DP(i-2) + D[i]) & \text{if } n \geq 2 \end{cases}$$

<i>i</i>	0	1	2	3	4	5	6	7
<i>D</i>		10	5	5	8	4	7	12
<i>DP</i>	0	10	10	15	18	19	25	31

<i>i</i>	0	1	2	3	4	5	6	7
<i>D</i>		10	1	1	10	1	1	10
<i>DP</i>	0	10	10	11	20	20	21	30

## Problem

- We have the **value** of the optimal solution, but we don't have the solution!
- Look in position  $DP[i]$ . From which cells this value has been computed?
  - If  $DP[i] = DP[i-1]$ , the house  $i$  has not been selected
  - If  $DP[i] = DP[i-2] + D[i-1]$ , house  $i$  has been selected

**Build solution(i) recursively as:**

```
solution(i-2) + index i  
or  
solution(i-1)
```

# Iterative solution

```
def hateville(D, n):
    dp = [0]*(n+1)
    if n > 0:
        dp[1] = D[0]
    for i in range(2, n+1):
        dp[i] = max(dp[i-1], dp[i-2] + D[i-1])

    return build_solution(D, dp, n)

def build_solution(D, dp, i):
    if i == 0:
        return []
    elif i == 1:
        return [0]
    else:
        if dp[i] == dp[i-1]:
            sol = build_solution(D, dp, i-1)
        else:
            sol = build_solution(D, dp, i-2)
            sol.append(i-1)
    return sol
```

```
D = [10,5,5,8,4,7,12]
print("Donations: {}".format(D))
for i in range(len(D)+1):
    HV = hateville(D, i)
    print("Donors for {}: {}. Donations: {}".format(D[0:i], HV, sum([D[x] for x in HV])))
print("\n\n")

D1 = [10,1,1,10,1,1,10]
print("Donations: {}".format(D1))
for i in range(len(D1)+1):
    HV = hateville(D1, i)
    print("Donors for {}: {}. Donations: {}".format(D1[0:i], HV, sum([D1[x] for x in HV])))
```

```
Donations: [10, 5, 5, 8, 4, 7, 12]
Donors for []: []. Donations: 0
Donors for [10]: [0]. Donations: 10
Donors for [10, 5]: [0]. Donations: 10
Donors for [10, 5, 5]: [0, 2]. Donations: 15
Donors for [10, 5, 5, 8]: [0, 3]. Donations: 18
Donors for [10, 5, 5, 8, 4]: [0, 2, 4]. Donations: 19
Donors for [10, 5, 5, 8, 4, 7]: [0, 3, 5]. Donations: 25
Donors for [10, 5, 5, 8, 4, 7, 12]: [0, 2, 4, 6]. Donations: 31
```

```
Donations: [10, 1, 1, 10, 1, 1, 10]
Donors for []: []. Donations: 0
Donors for [10]: [0]. Donations: 10
Donors for [10, 1]: [0]. Donations: 10
Donors for [10, 1, 1]: [0, 2]. Donations: 11
Donors for [10, 1, 1, 10]: [0, 3]. Donations: 20
Donors for [10, 1, 1, 10, 1]: [0, 3, 5]. Donations: 20
Donors for [10, 1, 1, 10, 1, 1]: [0, 3, 5]. Donations: 21
Donors for [10, 1, 1, 10, 1, 1, 10]: [0, 3, 6]. Donations: 30
```

# Complexity

```
def hateville(D, n):
    dp = [0]*(n+1)
    if n > 0:
        dp[1] = D[0]
    for i in range(2, n+1):
        dp[i] = max(dp[i-1], dp[i-2] + D[i-1])

    return build_solution(D, dp, n)

def build_solution(D, dp, i):
    if i == 0:
        return []
    elif i == 1:
        return [0]
    else:
        if dp[i] == dp[i-1]:
            sol = build_solution(D, dp, i-1)
        else:
            sol = build_solution(D, dp, i-2)
            sol.append(i-1)
    return sol
```

What is the complexity of build\_solution?

$$T(n) = O(n)$$

What is the complexity of hate\_ville?

$$T(n) = O(n)$$

**Exercise:**

write hateville with  $S(n) = O(1)$

# Knapsack

## Problem

Given a set of items, each of them characterized by a **weight** and a **value**, determine which items to include in a collection so that the total weight of the collection is less than or equal to a given "knapsack" **capacity** and the total value (or profit) is as large as possible.

## Input

- List  $w$ , where  $w[i]$  is the weight of the  $i$ -th item
- List  $p$ , where  $p[i]$  is the value (or profit) of the  $i$ -th item
- The capacity  $C$  of the knapsack

## Output

A collection  $S \subseteq \{1, \dots, n\}$  such that:

- Total volume should be smaller or equal than the capacity:  
$$w(S) = \sum_{i \in S} w[i] \leq C$$
- Total profit is maximized:  $p(S) = \sum_{i \in S} p[i]$  is maximal



# Knapsack

## Problem

Given a set of items, each of them characterized by a **weight** and a **value**, determine which items to include in a collection so that the total weight of the collection is less than or equal to a given "knapsack" **capacity** and the total value (or profit) is as large as possible.

Which are the best items for this example?

Item id	1	2	3
Weight	10	4	8
Profit	20	6	12

$$C = 12$$



$$S = \{1\}$$

Item id	1	2	3
Weight	10	4	8
Profit	20	7	15

$$C = 12$$



$$S = \{2,3\}$$

Design an algorithm to solve the Knapsack problem

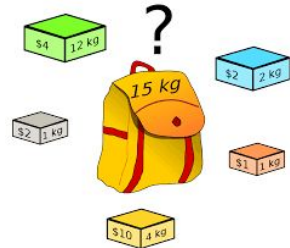
# Knapsack

## Definition: Sub-problem $DP(i, c)$

Given a knapsack with capacity  $C$  and  $n$  items characterized by weights  $w$  and profits  $p$ , we define  $DP(i, c)$  as the maximal profit we can obtain from the first  $i$  items in a knapsack of capacity  $c$ .

Original problem

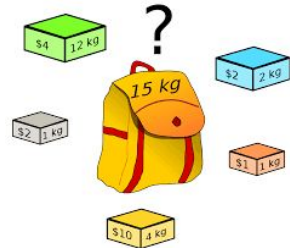
The maximal profit of the original problem corresponds to  $DP(n, C)$ .



$$\begin{aligned} i &\leq n \\ c &\leq C \end{aligned}$$



# Knapsack



Let us consider the last item of problem  $DP(i, c)$

- What happens if you don't take it?

$$DP(i, c) =$$

The capacity and profit do not change

- What happens if you take it?

$$DP(i, c) =$$

The capacity and profit do not change

# Exercises

# DNA sequence comparison

## Problem

Given two DNA sequences, find how "similar" they are.

## Examples

- One **substring** of the other?  
 $\text{CCTT} \subseteq \text{AGACCCTTAA}$
- **Edit distance**:  
AGACCCTTAA can be changed into AGACTCTTAA by substituting a T with a C
- **Longest common subsequence**:  
the longest common subsequence of TCGCA and TTGCCA is TGA

# Longest common subsequence

## Problem

Given two DNA sequences, find how "similar" they are.

## Examples

- One **substring** of the other?  
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