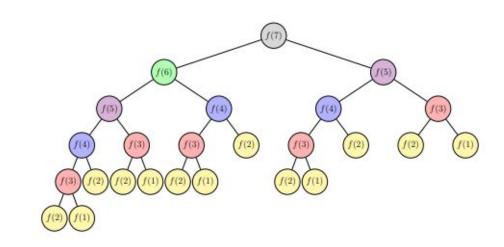
Scientific Programming Practical 20

Introduction

Dynamic Programming

Dynamic programming is a way to **optimize** recursive algorithms.

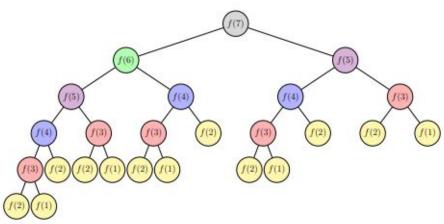
Every time we find an algorithm with repetitive recursive calls to smaller subproblems to solve a bigger problem, we can optimize it by using **dynamic programming**.



Dynamic Programming

Two approaches

- Top-down: solve the problem breaking it down in smaller subproblems. If the subproblem has already been solved. then the answer has already been saved somewhere. If i has not already been solved, compute a solution and sto it. This method is called memoization;
- 2. **Bottom-up:** solve the problem starting from the most triv subproblems going up until the complete problem has be solved. Smaller subproblems are guaranteed to be solve before bigger ones. This method is called **dynamic programming**.



Consider the classic example of the computation of Fibonacci numbers:

which can be computed with the following recursive formula:

$$F(n) = \begin{cases} n & \text{if } n == 0 \text{ or } n == 1 \\ F(n-1) + F(n-2) & \text{if } n > 1 \end{cases}$$

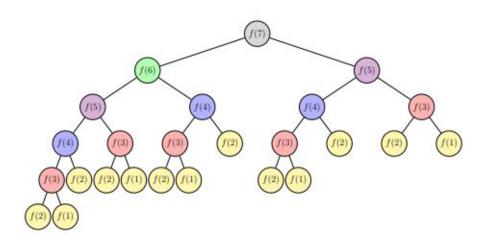
Recursive code

```
import time
def fib(n):
    if n <= 1:
        return n
    else:
        return fib(n - 1) + fib(n - 2)
for i in range(20):
    print("Fib({})= {}".format(i, fib(i)))
for i in range(35,38):
    start t = time.time()
    print("\nFib({})= {}".format(i, fib(i)))
    end t = time.time()
    print("It took {:.2f}s".format(end t-start t))
```

```
F(n) = \begin{cases} n & \text{if } n == 0 \text{ or } n == 1 \\ F(n-1) + F(n-2) & \text{if } n > 1 \end{cases}
```

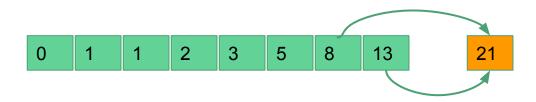
```
Fib(0) = 0
Fib(1) = 1
Fib(2) = 1
Fib(3)=2
Fib(4) = 3
Fib(5) = 5
Fib(6) = 8
Fib(7) = 13
Fib(8) = 21
Fib(9) = 34
Fib(10) = 55
Fib(11) = 89
Fib(12)= 144
Fib(13) = 233
Fib(14) = 377
Fib(15) = 610
Fib(16) = 987
Fib(17)= 1597
Fib(18) = 2584
Fib(19)= 4181
Fib(35)= 9227465
It took 4.39s
Fib(36)= 14930352
It took 6.88s
Fib(37)= 24157817
It took 10.58s
```

$$F(n) = \begin{cases} n & \text{if } n == 0 \text{ or } n == 1 \\ F(n-1) + F(n-2) & \text{if } n > 1 \end{cases}$$



$$F(n) = \begin{cases} n & \text{if } n == 0 \text{ or } n == 1 \\ F(n-1) + F(n-2) & \text{if } n > 1 \end{cases}$$

We can use dynamic programming to avoid computing over and over again the same values:



$$F(n) = \begin{cases} n & \text{if } n == 0 \text{ or } n == 1 \\ F(n-1) + F(n-2) & \text{if } n > 1 \end{cases}$$

We can use dynamic programming to avoid computing over and over again the same values:

```
import time
def fib dp(n):
   fib = [0]* (n+1)
   if n > 1:
        fib[1] = 1
   for i in range(2, n + 1):
        fib[i] = fib[i-2] + fib[i-1]
    return fib[n]
for i in range(20):
   print("Fib({})= {}".format(i, fib dp(i)))
for i in range(35,38):
    start t = time.time()
   print("\nFib({})={}".format(i, fib dp(i)))
    end t = time.time()
   print("It took {:.2f}s".format(end t-start t))
#we can even do:
for i in range(1000,1003):
    start t = time.time()
   print("\nFib({})={})".format(i, fib dp(i)))
   end t = time.time()
   print("It took {:.2f}s".format(end t-start t))
```

$$F(n) = \begin{cases} n & \text{if } n == 0 \text{ or } n == 1 \\ F(n-1) + F(n-2) & \text{if } n > 1 \end{cases}$$

We can use dynamic programming to avoid computing over and over again the same values:

```
Fib(1000)= 43466557686937456435688527675...49228875
It took 0.00s
Fib(1001)= 70330367711422815821835254877...23403501
It took 0.00s
Fib(1002)= 11379692539836027225752378255...72632376
It took 0.00s
```

```
import time
def fib dp(n):
   fib = [0]* (n+1)
   if n > 1:
        fib[1] = 1
    for i in range(2, n + 1):
        fib[i] = fib[i-2] + fib[i-1]
    return fib[n]
for i in range(20):
   print("Fib({})= {}".format(i, fib dp(i)))
for i in range(35,38):
    start t = time.time()
    print("\nFib({})={}".format(i, fib dp(i)))
    end t = time.time()
   print("It took {:.2f}s".format(end t-start t))
#we can even do:
for i in range(1000,1003):
    start t = time.time()
    print("\nFib({})={}".format(i, fib dp(i)))
   end t = time.time()
    print("It took {:.2f}s".format(end t-start t))
```

```
Fib(0) = 0
Fib(1) = 0
Fib(2) = 1
Fib(3) = 2
Fib(4) = 3
Fib(5) = 5
Fib(6) = 8
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Fib(36)= 14930352
It took 0.00s
Fib(37)= 24157817
It took 0.00s
```

Greedy paradigm

In the **greedy programming** paradigm, at each step of the computation the choice that seems the best **at the time** is always taken. In other words, greedy algorithms build a solution by choosing the **local best value** in the hope that this would lead to a **global best solution**. As we will see later, this is not always guaranteed.



Greedy paradigm: example

Example: Let's write a method that a coffee selling machine can use to give change using the least amount of coins of 50,20,10, 5 and 1 cents.

```
def giveChange(amount):
    #res counts the used coins
    #having value 50,20,10,5,1
    print("Computing change of {} cents".format(amount))
    coins = [50, 20, 10, 5, 1]
    res = [0,0,0,0,0]
    while amount > 0:
        nextCoin = 0
        #order makes greedy choice! First 50, then 20, 10...
        if amount > 50:
            res[0] += 1
            nextCoin = 50
        elif amount > 20:
            res[1] += 1
            nextCoin = 20
        elif amount > 10:
            res[2] += 1
            nextCoin = 10
        elif amount > 5:
            res[3] +=1
            nextCoin = 5
        else:
            res[4] += 1
            nextCoin = 1
        amount -= nextCoin
    for i in range(len(coins)):
        if res[i] > 0:
            print("{} x {} cent coins".format(res[i],coins[i]))
```

GREEDY CHOICE: always pick the biggest coin

Greedy paradigm: example

Example: Let's write a method that a coffee selling machine can use to give change using the least amount of coins of 50,20,10, 5 and 1 cents.

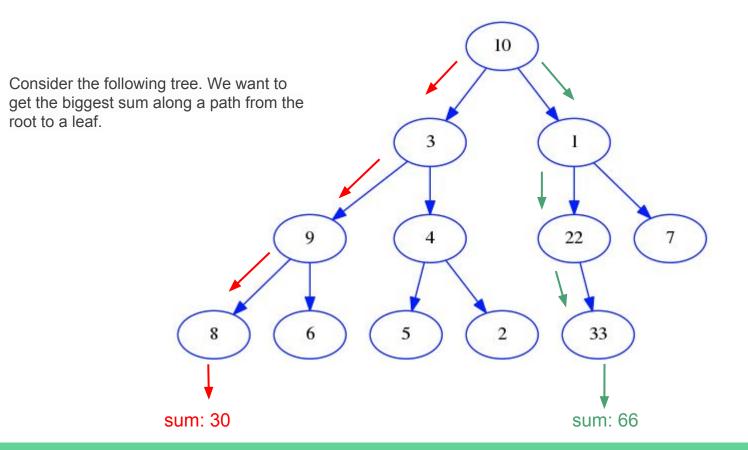
```
def giveChange(amount):
    #res counts the used coins
    #having value 50,20,10,5,1
   print("Computing change of {} cents".format(amount))
    coins = [50, 20, 10, 5, 1]
    res = [0,0,0,0,0]
    while amount > 0:
        nextCoin = 0
        #order makes greedy choice! First 50, then 20, 10...
       if amount > 50:
            res[0] += 1
            nextCoin = 50
        elif amount > 20:
            res[1] += 1
            nextCoin = 20
        elif amount > 10:
            res[2] += 1
            nextCoin = 10
        elif amount > 5:
            res[3] +=1
            nextCoin = 5
        else:
            res[4] += 1
            nextCoin = 1
        amount -= nextCoin
    for i in range(len(coins)):
       if res[i] > 0:
            print("{} x {} cent coins".format(res[i],coins[i]))
```

GREEDY CHOICE: always pick the biggest coin

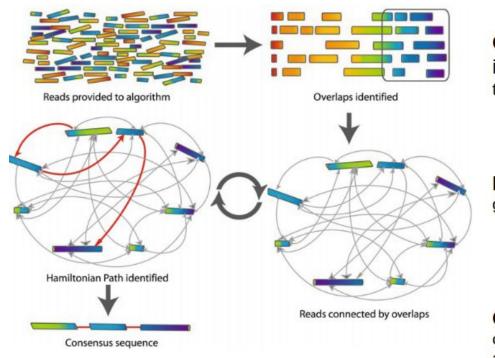
```
giveChange(72)
giveChange(232)
Computing change of 36 cents
1 x 20 cent coins
1 x 10 cent coins
1 x 5 cent coins
1 x 1 cent coins
Computing change of 72 cents
1 x 50 cent coins
1 x 20 cent coins
2 x 1 cent coins
Computing change of 232 cents
4 x 50 cent coins
1 x 20 cent coins
1 x 10 cent coins
2 x 1 cent coins
```

giveChange(36)

Greedy algos: not always finding the right solution



Motivation: long read (PacBio, Oxford Nanopore) genome assembly



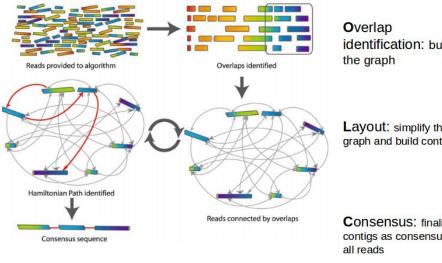
Overlap identification: build the graph

O(N²) overlaps

Layout: simplify the graph and build contigs

Consensus: finalize contigs as consensus of all reads

Motivation: long read (PacBio, Oxford Nanopore) genome assembly



identification: build

Layout: simplify the graph and build contigs

Consensus: finalize contigs as consensus of Assembly: consensus of overlapping reads

TAGATTACACAGATTACTGA TTGATGGCGTAA CTA TAGATTACACAGATTACTGACTTGATGGCGTAAACTA TAG TTACACAGATTATTGACTTCATGGCGTAA CTA TAGATTACACAGATTACTGACTTGATGGCGTAA CTA TAGATTACACAGATTACTGACTTGATGGCGTAA CTA

TAGATTACACAGATTACTGACTTGATGGCGTAA CTA

Given two reads X and Y the optimal overlap among them is the longest suffix of X that matches (possibly with some mismatches) a prefix of Y.

X = ATCGGTTCGGTGAAGTAA

Y = CGGTGACGTTACCATATCCAG

overlap:

ATCGGTTCGGTGAAGTAA

CGGTGACGTTACCATATCCAG

Given two reads X and Y the optimal overlap among them is the longest suffix of X that matches (possibly with some mismatches) a prefix of Y.

X = ATCGGTTCGGTGAAGTAA

Y = CGGTGACGTTACCATATCCAG

overlap:

ATCGGTTCGGTGAAGTAA

CGGTGACGTTACCATATCCAG

Alignment score

	Α	С	G	T	-
Α	0	4	2	4	8
C	4	0	4	2	8
G	2	4	0	4	8
Т	4	2	4	0	8
	8	8	8	8	8

Given the two reads X and Y

The global alignment recurrence:

$$A[i,j] = min \begin{cases} A[i-1,j] + score(x[i-1], "-") \\ A[i,j-1] + score("-", y[j-1]) \\ A[i-1,j-1] + score(x[i-1], y[j-1]) \end{cases}$$

This provides a N+1 x M+1 matrix (where N and M are the lengths of X and Y)

The first row of the matrix corresponds to "-" in XX and all elements are initialized to ∞ , while the first column corresponds to a "-" in YY and all elements are initialized to 0.

$$A[i,j] = min \begin{cases} A[i-1,j] + score(x[i-1], "-") \\ A[i,j-1] + score("-", y[j-1]) \\ A[i-1,j-1] + score(x[i-1], y[j-1]) \end{cases}$$

7.		C	G	G	Т	G	Α	С	G	Т	Т	Α	С	С	Α	Т	Α	Т	С	С	Α	G
-	0	inf																				
Α	0	4	12	20	28	36	44	52	60	68	76	84	92	100	108	116	124	132	140	148	156	164
T	0	2	8	16	20	28	36	44	52	60	68	76	84	92	100	108	116	124	132	140	148	156
C	0	0	6	12	18	24	32	36	44	52	60	68	76	84	92	100	108	116	124	132	140	148
G	0	4	0	6	14	18	26	34	36	44	52	60	68	76	84	92	100	108	116	124	132	140
G	0	4	4	0	8	14	20	28	34	40	48	54	62	70	78	86	94	102	110	118	126	132
T	0	2	8	8	0	8	16	22	30	34	40	48	56	64	72	78	86	94	102	110	118	126
T	0	2	6	12	8	4	12	18	26	30	34	42	50	58	66	72	80	86	94	102	110	118
C	0	0	6	10	14	12	8	12	20	28	32	38	42	50	58	66	74	82	86	94	102	110
G	0	4	0	6	14	14	14	12	12	20	28	34	42	46	52	60	68	76	84	90	96	102
G	0	4	4	0	8	14	16	18	12	16	24	30	38	46	48	56	62	70	78	86	92	96
T	0	2	8	8	0	8	16	18	20	12	16	24	32	40	48	48	56	62	70	78	86	94
G	0	4	2	8	8	0	8	16	18	20	16	18	26	34	42	50	50	58	66	74	80	86
A	0	4	6	4	12	8	0	8	16	22	24	16	22	30	34	42	50	54	62	70	74	82
Α	0	4	6	8	8	14	8	4	10	18	26	24	20	26	30	38	42	50	58	66	70	76
G	0	4	4	6	12	8	16	12	4	12	20	28	28	24	28	34	40	46	54	62	68	70
T	inf	2	8	8	6	14	12	18	12	4	12	20	28	30	28	28	36	40	48	56	64	72
A	inf	10	4	10	12	8	14	16	20	12	8	12	20	28	30	32	28	36	44	52	56	64
Α	inf	inf	inf	inf	14	14	8	16	18	20	16	8	16	24	28	34	32	32	40	48	52	58

X = ATCGGTTCGGTGAAGTAA

Y = CGGTGACGTTACCATATCCAG

overlap:

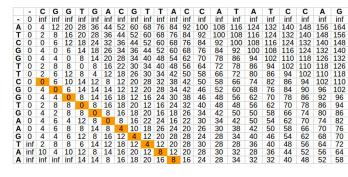
travel back from minimum value to min value to find overlap

ATCGGTTCGGTGAAGTAA
CGGTGACGTTACCATATCCAG

set to infinity to force overlap len > 3

Finding overlaps: build the matrix

```
def score(a,b):
    mat = \{\}
   mat["A"] = {"A" : 0, "C" : 4, "G" : 2, "T" : 4, "-" : 8}
   mat["C"] = {"A" : 4, "C" : 0, "G" : 4, "T" : 2, "-" : 8}
   mat["G"] = {"A" : 2, "C" : 4, "G" : 0, "T" : 4, "-" : 8}
   mat["T"] = {"A" : 4, "C" : 2, "G" : 4, "T" : 0, "-" : 8}
   mat["-"] = {"A" : 8, "C" : 8, "G" : 8, "T" : 8, "-" : 8}
    return mat[a][b]
def computeMatrix(X.Y. minLen = 0):
    # + 1 is for leading "-"
   x len = len(X) + 1
   y len = len(Y) + 1
    print(X)
   print(Y)
    A = []
    #initialize first column to 0 and first row to infinite
   for i in range(x len - minLen + 1):
        A.append([0])
    for i in range(minLen -1):
        A.append([math.inf])
    for i in range(y len -1):
        A[0].append(math.inf)
    for i in range(1,x len):
        for j in range(1, y len):
            c1 = A[i-1][j] + score(X[i-1], "-")
            c2 = A[i][j-1] + score("-", Y[j-1])
            c3 = A[i-1][j-1] + score(X[i-1],Y[j-1])
            #print("i, i: {}, {}".format(i, i))
            A[i].append(min([c1,c2,c3]))
   if minLen != 0:
        for i in range(0, minLen):
            A[-1][i] = math.inf
    return A
```





$$A[i,j] = min \begin{cases} A[i-1,j] + score(x[i-1], "-") \\ A[i,j-1] + score("-", y[j-1]) \\ A[i-1,j-1] + score(x[i-1], y[j-1]) \end{cases}$$

Finding overlaps: build the matrix

```
A[i,j] = min \begin{cases} A[i-1,j] + score(x[i-1], "-") \\ A[i,j-1] + score("-", y[j-1]) \\ A[i-1,j-1] + score(x[i-1], y[j-1]) \end{cases}
def plotMatrix(Mat, X,Y):
     X = "-" + X
     outStr = "\t-" +"\t"+ "\t".join(list(Y))
    for i in range(len(X)):
          outStr+="\n" + X[i] +"\t"+ "\t".join([str(x) for x in Mat[i]])
     print(outStr)
    "CTCGGCCCTAGG"
     "GGCTCTAGGCCC"
    computeMatrix(X,Y,minLen = 5)
                                               CTCGGCCCTAGG
print("The overlap matrix:")
                                               GGCTCTAGGCCC
plotMatrix(A,X,Y)
                                               The overlap matrix:
                                                                                                                                                                 C
                                                                inf
                                                                         inf
                                                                                  inf
                                                                                           inf
                                                                                                    inf
                                                                                                            inf
                                                                                                                     inf
                                                                                                                                                        inf
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                                                                                                                                                                  92
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                                                                                                                                                                 68
                                                                                                                                                                 60
                                                                                                                                                                  52
                                                                                                                                                                  36
                                                       inf
                                                       inf
                                                                12
                                                       inf
                                                                20
                                                                         12
                                                                                  10
                                                                                           16
                                                                                                                                                                  34
                                                       inf
                                                                inf
                                                                         inf
                                                                                  inf
                                                                                           inf
                                                                                                    20
                                                                                                            22
                                                                                                                     18
                                                                                                                                                                  26
```

http://qcbprolab.readthedocs.io/en/latest/practical20.html

Exercises

1. Catalan numbers (info here) are defined by the following recurrence equation:

$$C(n) = \begin{cases} 1 & \text{if } n = 0\\ \sum_{i=0}^{n-1} C_i \dot{C}_{n-1-i} & \text{if } n > 1 \end{cases}$$

the first few values are reported below:

```
1, 1, 2, 5, 14, 42, 132, 429, 1430, 4862, 16796, 58786, 208012, 742900, 2674440, 9694845, 35357670, 129644790, 477638700, 1767263190, 6564120420, 24466267020, 91482563640, . . .
```

- a. Write a recursive function recCatalan(n) to compute the n-th catalan number;
- b. Write a dynamic programming function dpCatalan(n) to compute the n-th catalan number.

Test your code with:

```
catN = []
for i in range(0,15):
    catN.append(recCatalan(i))
print("First 15 catalan numbers:")
print(catN)
```

Finally, check how long it takes to compute the 20th catalan number with the recursive algorithm and with the dynamic programming one.

Show/Hide Solution

2. Recall the code that computes the overlap matrix given two DNA reads (strings). The code is