

Algorithmics and Complexity Cours 5/7 : Dynamic Programming

CentraleSupélec – Gif

ST2 - Gif

Change making Dynamic programming Shortest Path Conclusion Sequ Problem Algorithms Dynamic programming

Sequence alignment

Plan

Change making

- Problem
- Algorithms
- Dynamic programming

Dynamic programming

3 Shortest Path

4 Conclusion







Change making

Give back 3,57 EUR with coins worth 1 and 2 euros and 1, 2, 5, 10, 20 and 50 cents.



Shortest Path

Conclusion

Sequence alignment

Change making



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Give back 3,57 EUR with coins worth 1 and 2 euros and 1, 2, 5, 10, 20 and 50 cents.

Solutions

A set of coins:

→ $2 \in +1 \in +50 \notin +5 \notin +2 \notin$





Change making

Give back 3,57 EUR with coins worth 1 and 2 euros and 1, 2, 5, 10, 20 and 50 cents.

Solutions

A set of coins:

- ✓ $2 \in +1 \in +50 \notin +5 \notin +2 \notin$
- → $1 \in + 1 \in + 50$ ¢ + 4×20¢ + 2×10¢ + 3×2¢ + 1¢





Change making

Give back 3,57 EUR with coins worth 1 and 2 euros and 1, 2, 5, 10, 20 and 50 cents.

Solutions

A set of coins:

- ✓ $2 \in +1 \in +50 \notin +5 \notin +2 \notin$
- $\checkmark 1 \in +1 \in +50 \notin +4 \times 20 \notin +2 \times 10 \# +3 \times 2 \# +1 \#$





Change making

Give back 3,57 EUR with coins worth 1 and 2 euros and 1, 2, 5, 10, 20 and 50 cents.

Solutions

A set of coins:

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- $\checkmark 1 \in +1 \in +50 \notin +4 \times 20 \notin +2 \times 10 \# +3 \times 2 \# +1 \#$

✓ 357×1¢





Change making

Give back 3,57 EUR with coins worth 1 and 2 euros and 1, 2, 5, 10, 20 and 50 cents.

Solutions

A set of coins:

- ✓ $2 \in +1 \in +50 \notin +5 \notin +2 \notin$
- $\checkmark 1 \in +1 \in +50 \notin +4 \times 20 \notin +2 \times 10 \# +3 \times 2 \# +1 \#$
- ✓ 357×1¢

→ With how many minimum number of coins can we return 3,57€?



• $total \in \mathbb{N}$ the amount to give back: total = 357

Output data

c the number of coins used to obtain the value *total*, as it exists $L \in \mathbb{N}^n$ a n-tuple, checking:

• total = $\sum_{i=0}^{n-1} L_i \times S_i$ L indicates the number of each piece



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• $total = \sum_{i=0}^{n-1} L_i \times S_i$ L indicates the number of each piece • $c = \sum_{i=0}^{n-1} L_i$ c is the cost of the solution L



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- $total = \sum_{i=0}^{n-1} L_i \times S_i$ L indicates the number of each piece • $c = \sum_{i=0}^{n-1} L_i$ c is the cost of the solution L
- and *c* is minimal!

Example

$$L=(0,2,1,4,2,0,3,1)
ightarrow c=13$$
 $ightarrow$ not minimal!



Shortest Path

Some observations...

Solution

Coins of unit value \rightarrow at least one solution $\forall \textit{total} \in \mathbf{N}$

We assume an infinity of coins for each of the values. . .

Problem size ?



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Problem size

- *n* (the number of different coin values)
- → The sum to be returned is a **parameter** of the problem



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Goal

- ✓ Return the sum → a solution
- \checkmark With a minimum number of coins $\ \rightarrow$ the optimal solution!



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Goal

- ✓ Return the sum → a solution
- \checkmark With a minimum number of coins $\ \rightarrow$ the optimal solution!

Optimal solution

We are looking for the cost of the optimal solution!



- one coin of $2 \in$ then 1,57;
- one coin of $1 \in$ then 2,57;
- one coin of 50 ¢ then 3,07;
- etc. for every possible coin value



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- \rightarrow The best solution is then:

 $1 + min(given_back(2, 57), given_back(1, 57), \ldots)$



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Recursive calculation of the cost of the optimal solution

Denote by C(s) the minimum number of coins to obtain s.



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Recursive calculation of the cost of the optimal solution

Denote by C(s) the minimum number of coins to obtain s.

- Base case: C(0) = 0
- General case: $C(s) = 1 + \min_{i \in [0, n-1], S_i \leq s} C(s S_i)$



$$\begin{vmatrix} C(0) = 0 \\ C(s) = 1 + \min_{i \in [0, n-1], S_i \le s} C(s - S_i) \end{vmatrix}$$



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357: (0, 0, 0, 0, 0, 0, 0, 0)



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357: (0, 0, 0, 0, 0, 0, 0, 0) **157:** (1, 0, 0, 0, 0, 0, 0, 0)



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$$\begin{vmatrix} C(0) = 0 \\ C(s) = 1 + \min_{i \in [0, n-1], S_i \le s} C(s - S_i) \end{vmatrix}$$







Exponential complexity!

• Unbalanced *n*-ary exploration tree of depth within $\left[\frac{total}{S_0}, \frac{total}{S_{n-1}}\right]$

• Complexity higher than
$$n^k$$
 where $k = \frac{total}{S_0}$.

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Exponential complexity!

- Unbalanced *n*-ary exploration tree of depth within $\left[\frac{total}{S_0}, \frac{total}{S_{n-1}}\right]$
- Complexity higher than n^k where $k = \frac{total}{S_0}$.
- Redundant computation!



Idea

- ✓ Solve optimization problems
- \checkmark Where there is a recursive construction of the solution



Idea

- ✓ Solve optimization problems
- \checkmark Where there is a recursive construction of the solution
- Dynamic programming

Principle

- Store the intermediate solutions so as not to recalculate them
- Invented by Bellman in the 1950s
- Applies when the optimal solution of the problem is composed of the optimal solutions of its subproblems



Plan



- Dynamic programming
 - Principle
 - Comparison with the recursive approach
 - Change making

3 Shortest Path

4 Conclusion





Principle

• Recursively, start by solving the smallest sub-problems, then solve bigger and bigger sub-problems until the solution to the global problem is obtained.



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- As we know how to make change for all s' < s:
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- We memorize the result in the array
 - ightarrow needed later to compute the min cost of $s+S_i$


Dynamic programming

Optimal sub-structure

- Divide the problem in sub-problems
- Onstruct the optimal solution from optimal solutions of sub-problems
- Oeduce a recurrence formula



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Examples of applications

- Sequence alignment
- Change making
- Shortest path
- Knapsack





- If the sub-problems are independents (all the sub-problems are different)
 - Dynamic programming is useless
 - classic example: $fact(n + 1) = (n + 1) \times fact(n)$



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 - Dynamic programming is useless
 - classic example: $fact(n + 1) = (n + 1) \times fact(n)$
- Otherwise
 - Dynamic programming is more efficient in time (in return, we pay in space because nothing is free!)
 - classic example: fib(n+2) = fib(n+1) + fib(n)



• Divide and conquer (recursive approach)

```
def fib(n):
    if n==1 or n==2:
        return 1
    return fib(n-1)+fib(n-2)
```

• exponential complexity $\mathcal{O}(\phi^n)$ (ϕ the golden ratio)



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```

- exponential complexity $\mathcal{O}(\phi^n)$ (ϕ the golden ratio)
- Dynamic programming

```
table = {0:0, 1:1}
def fib(n):
    if not n in table:
        table[n] = fib(n-1) + fib(n-2)
    return table[n]
```

```
• linear complexity \mathcal{O}(n)
```

Resolution with dynamic programming (Algorithm 1)

• We reuse the previous recurrence formula while saving the intermediate results:

$$\left\{ \begin{array}{ll} C(s)=1 & \text{si } \exists i \in [0,n-1] \text{ tel que } s=S_i \\ C(s)=1+\min_{i\in [0,n-1],S_i\leq s} C(s-S_i) \end{array} \right.$$

• Let S = (10, 5, 2, 1) and total = 14



Resolution with dynamic programming (Algorithm 1)

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• Let
$$S = (10, 5, 2, 1)$$
 and $total = 14$



• computation time $n \times total$



Algorithm 1, recursive version

```
import math
S = (200, 100, 50, 20, 10, 5, 2, 1); n = len(S)
total = 357;
C = [math.inf for i in range(total+1)]
def given_back(sum):
    if C[sum] == math.inf:
        if sum in S:
            C[sum] = 1
        else:
            best = math.inf
            for i in range(n):
                 if S[i]<sum:
                     best = min(best,given_back(sum-S[i]))
            C[sum] = best+1
    return C[sum]
print("Number_of_coins:", given_back(total))
```



Algorithm 1, iterative version

```
import math
S = (200, 100, 50, 20, 10, 5, 2, 1); n=len(S)
total = 357;
C = [0]
for i in range(1,total+1):
    C.append(math.inf)
    for j in range(n):
        if i>=S[j] and 1+C[i-S[j]]<C[i]:
            C[i] = 1+C[i-S[j]]
print("Number_of_coins:", str(C[total]))</pre>
```



Algorithm 1, iterative version

```
import math
S = (200, 100, 50, 20, 10, 5, 2, 1); n = len(S)
total = 357:
C = [0]
for i in range(1,total+1):
    C.append(math.inf)
    for j in range(n):
        if i>=S[j] and 1+C[i-S[j]]<C[i]:</pre>
             C[i] = 1 + C[i - S[j]]
print("Number_of_coins:", str(C[total]))
```

→ In both cases, we do not have the solution, only its cost C(total).



Plan

3





Shortest Path

- Shortest Paths algorithm
- Bellman-Ford
- Algorithm
- Negative weight cycles detection
- Application: routing

4 Conclusion





Node	Distance	Parent
S 0	0	•
s 1	∞	•
<i>s</i> ₂	∞	•
s 3	∞	•

Frontier =	$\{s_0\}$
x =	



Node	Distance	Parent
S 0	0	•
S 1	5	S 0
s ₂	3	s 0
s 3	3	s 0

Frontier =	$\{s_1, s_2, s_3\}$	
x =	S 0	



Node	Distance	Parent
S 0	0	•
S 1	5	S 0
s ₂	3	s 0
s 3	3	s 0

Frontier =	$\{s_1, s_3\}$
x =	s 2



Node	Distance	Parent
S 0	0	•
s 1	5	S 0
s ₂	3	s 0
s 3	3	s 0

Frontier =	$\{s_1\}$
x =	S 3

The Shortest Paths algorithm does not work with negative weights



Node	Distance	Parent
S 0	0	•
S 1	5	S 0
s ₂	1	s 1
s 3	3	s 0

Frontier =

$$x = s_1$$

The Shortest Paths algorithm does not work with negative weights



Node	Distance	Parent
S 0	0	•
s 1	5	S 0
s ₂	1	s 1
s 3	3	<i>s</i> ₀

Frontier = x =

The Shortest Paths algorithm gives a wrong answer for s_3 !

The Shortest Paths algorithm does not work with negative weights



Node	Distance	Parent
S 0	0	•
s 1	5	S 0
s ₂	1	s 1
s 3	3	s 0

Frontier = x =

The Shortest Paths algorithm gives a wrong answer for s_3 !

Why would someone want to calculate a shortest path on a graph with negative weights?

→ answer to TD 4, exercise 1 (placement problem)



Change making Dynamic programming Shortest Path Conclusion Sequence alignment Shortest Paths algorithm Bellman-Ford Algorithm Negative weight cycles detection Application: routing

Bellman-Ford algorithm (1956, 1958)

Principle

- Based on the principle of the dynamic programming
- Calculate the cost of the shortest path

but we can recover the path from the memoization table...



Change making Dynamic programming Shortest Path Conclusion Sequence alignment Shortest Paths algorithm Bellman-Ford Algorithm Negative weight cycles detection Application: routing

Bellman-Ford algorithm (1956, 1958)

Principle

- Based on the principle of the dynamic programming
- Calculate the cost of the shortest path
 - but we can recover the path from the memoization table...

Reminder: problem data

An arbitrary weighted and directed graph G, two vertices s and t including negative weights...

→ What is the length of the shortest path from s to t?

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Attention to the negative weight cycles!

Definition: negative weight cycle



The cycle *c* in this example is a *negative weight cycle*, because $\sum_{e=(v,u)\in c} \omega(e) < 0.$

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Attention to the negative weight cycles!

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Shortest path with negative weights

Need a more precise formulation:

→ We are looking for the shortest path without cycle!



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Bellman-Ford algorithm (1956, 1958)

Principle

- Based on the principle of the dynamic programming
- Calculate the cost of the shortest path
 - but we can recover the path from the memoization table...

Properties

- ✓ Supports negative weights (unlike Dijkstra)
- ✓ Detects if there is a negative weight cycle

6

Change making Dynamic programming Shortest Path Conclusion Sequence alignment Shortest Paths algorithm Bellman-Ford Algorithm Negative weight cycles detection Application: routing

Principles of the Bellman-Ford algorithm

Divide into subproblems

Let OPT(i, v) be the length of the shortest path to the target node t from a node $v, v \neq t$, which contains at most i arcs.



6

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OPT(2,s1)=?
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OPT(2,s1)=?

the length of the shortest path in 2 arcs from s1 to t (s5) (in this case, it is 0 through s4)

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OPT(|V| - 1,s1) = ?

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OPT(|V| - 1,s1) = ?

the length of the shortest path from s1 to t (s5) (in this case, it is -2)



Principles of the Bellman-Ford algorithm

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Recursive construction of a solution

•
$$OPT(i, v) = \min_{(v,u)\in E}(OPT(i-1, u) + \omega((v, u)))$$

 \rightarrow To reach t, first go to u by taking the shortest path in i-1 steps.



Principles of the Bellman-Ford algorithm

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Recursive construction of a solution

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$$OPT(i, v) = \min_{(v,u) \in E} (OPT(i-1, u) + \omega((v, u)))$$

 \rightarrow To reach t, first go to u by taking the shortest path in i-1 steps.

• Unless there is already a path in i - 1 steps from v which is shorter than all the rest!

 \rightarrow In which case OPT(i, v) = OPT(i - 1, v)



Principles of the Bellman-Ford algorithm

Divide into subproblems

Let OPT(i, v) be the length of the shortest path to the target node t from a node $v, v \neq t$, which contains at most i arcs.

Recursive construction of a solution

$$\mathsf{OPT}(i, v) = \min\left(\mathsf{OPT}(i-1, v), \min_{u \in V}(\mathsf{OPT}(i-1, u) + \omega((v, u)))\right)$$

Store the OPT $(i, v) \rightarrow 2$ -dimensional array.

Example

6



Example

6



	S 0	S 1	s 2	S 3	S 4	S 5
0	∞	∞	∞	∞	∞	0

Example



Example



Example



 $\textit{s}_2 = \textit{min}(\infty,\textit{min}(8+\infty,3+0))$

Example



	50	51	52	53	54	35
0	∞	∞	∞	∞	∞	0
1	-3	∞	3	4	2	0

we end the line on the same principle

Example

6



	s 0	s 1	s 2	S 3	S 4	s 5
0	∞	∞	∞	∞	∞	0
1	-3	∞	3	4	2	0
2	-3	0	3	3	0	0

then we do the next line

Example

6



	s 0	s 1	s ₂	s 3	S 4	S 5
0	∞	∞	∞	∞	∞	0
1	-3	∞	3	4	2	0
2	-3	0	3	3	0	0
3	-4	-2	3	3	0	0

and so on. . .

Example





When to stop?

Proprerty

- In an acyclic graph, the shortest path contains at most |V|-1 arcs
- → This is also true in every graph without negative weight cycle





When to stop?

Proprerty

- In an acyclic graph, the shortest path contains at most |V|-1 arcs
- → This is also true in every graph without negative weight cycle



→ Stop as soon as you have computed the paths with |V| - 1 arcs.



One implementation of Bellman-Ford

```
(adjacency matrix)
```

```
import math
```

```
# graph is an adjacency matrix
n = len(graph)
# initialization of OPT table
OPT = [[math.inf for _ in range(n)] for _ in range(n)]
OPT[0][5] = 0
# filling the table
for i in range(1,n):
    for v in range(n):
        OPT[i][v] = OPT[i-1][v]
        for u in range(n):
            if graph[v][u] != None and \
                    OPT[i][v] > OPT[i-1][u] + graph[v][u]:
                OPT[i][v] = OPT[i-1][u] + graph[v][u]
```



Complexity

adjacency matrix

- 3 nested loops of |V| iterations each
- an access in $\mathcal{O}(1)$ to $\omega((v, u))$ at each turn of the inner loop!



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adjacency list

- do it home.
- 2 loops: for each of the |V| lines, we iterate over the |E| edges



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Complexity

adjacency list

- do it home.
- 2 loops: for each of the |V| lines, we iterate over the |E| edges
- → Hence, the total complexity of the algorithm is: $\mathcal{O}(|V| \times |E|)$.



Negative weight cycles detection

Proprerty (reminder)

- In an graph without negative cycle, the shortest path has at most |V| 1 arcs.
- → $\forall v, \mathsf{OPT}(|V| 1, v)$ is the length of the shortest path

 (\Longrightarrow)



Negative weight cycles detection

$$\Longrightarrow$$
)

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Contraposition

If a shortest path holds more than $\left|V\right|-1$ arcs, then G has negative cycles.

Change making Dynamic programming Shortest Path Conclusion Sequence alignment Shortest Paths algorithm Bellman-Ford Algorithm Negative weight cycles detection Application: routing

Negative weight cycles detection

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Contraposition

If a shortest path holds more than $\left|V\right|-1$ arcs, then G has negative cycles.

Corollary 1

If one value in the row |V| is smaller than the one of the previous row:

$$\exists v. \ OPT(|V|, v) < OPT(|V| - 1, v)$$

then there is a negative cycle in the graph.

 (\Longrightarrow)

 (\Longrightarrow)





Properties

- - **1** If G contains a negative cycle, then for any node v from that cycle, we can always improve its distance.
 - → $\exists v. \forall n. \exists m > n \ OPT(m, v) < OPT(n, v)$



(=)

Properties

 If G contains a negative cycle, then for any node v from that cycle, we can always improve its distance.

→ $\exists v. \forall n. \exists m > n \ OPT(m, v) < OPT(n, v)$

- If a row of the table is equal to the next one, then all the following rows are equal to it as well
 - consequence of the recurrence formula



Properties



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- If a row of the table is equal to the next one, then all the following rows are equal to it as well
 - consequence of the recurrence formula

Corollary 2

If G contains a negative cycle, **then**:

$$\exists v. \ OPT(|V|, v) < OPT(|V| - 1, v)$$

(=)

(==)



Theorem

G contains a negative cycle iff

$\exists v. \ OPT(|V|, v) < OPT(|V| - 1, v)$



Theorem

 ${\it G}$ contains a negative cycle iff

```
\exists v. \ OPT(|V|, v) < OPT(|V| - 1, v)
```

```
# filling the table
for i in range(1,n+1): # filling one more line
    for v in range(n):
        OPT[i][v] = OPT[i-1][v]
        for u in range(n):
            if graph[v][u] != None and \
                    OPT[i][v] > OPT[i-1][u] + graph[v][u]:
                OPT[i][v] = OPT[i-1][u] + graph[v][u]
# Detection of cycles
for v in range(n):
    if OPT[n-1][v] > OPT[n][v]:
      print("Found:_negative_cycle!\n")
      break;
```

Example

6.



Example





Example

Be careful

As soon as there is a negative weight cycle, the calculated cost for s
ightarrow t may be wrong !

... even if OPT(|V| - 1, s) = OPT(|V|, s)



	S	1	2	t
0	∞	∞	∞	0
1	1	∞	∞	0
2	1	0	∞	0
3	0	0	∞	0
4	0	-1	∞	0



Demo



Distributed Bellman-Ford

Property

To compute the cost OPT(i, v) for node v at step i, we only need:

- OPT(i 1, v) the value at the previous step for v;
- OPT(i 1, u) the value at the previous step for all the neighbours u of v.
- \rightarrow Each node can compute its cost independently, only by communicating with its neighbours

... without being aware of the whole graph!



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Application in telecommunication networks

Routing problem


Problem

Find the best path to route packets up to their destinations.



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Criteria (weights)

Shortest routes w.r.t number of links, minimal latency,



Problem

Find the best path to route packets up to their destinations.

Criteria (weights)

Shortest routes w.r.t number of links, minimal latency, ...

Routing specifics

- Each router holds a table (destination, next_router (Next_Hop)).
- Computations done locally in routers (without knowing the configuration of the network)



Data model (network)

- routers are modeled by graph nodes
- links between routers are modeled by graph arcs
- distances (links numbers, latency) are modeled by arc weights

Routing in packet-switched communication networks

Data model (network)

- routers are modeled by graph nodes
- links between routers are modeled by graph arcs
- distances (links numbers, latency) are modeled by arc weights

Communication

As soon as a router changes its routing table, it warns its neighbours so that they can update their own tables also.





Each router runs a loop:

Wait for a change notification of routing from one of its neighbours



- Wait for a change notification of routing from one of its neighbours
- **2** recompute its own routing table (Final destination $p \rightarrow Next_Hop$)



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Each router runs a loop:

- Wait for a change notification of routing from one of its neighbours
- **2** recompute its own routing table (Final destination $p \rightarrow Next_Hop$)
- Send its new distances to its neighbours
- 🕘 goto 1

Each router v keeps locally:

- an array M_v with $M_v[p]$ being the distance of the shortest path between v and p
- an array Next_Hop, where Next_Hop, [p] is the identifier of the next router for any dispatch towards p

```
Dynamic programming Shortest Path
     Change making
                                              Conclusion
                                                        Sequence alignment
     Shortest Paths algorithm Bellman-Ford Algorithm Negative weight cycles detection Application: routing
Algorithm for each node v
    Nv = ... # the list of neighbours of v
    def process(u, Mu) :
         At each notification received from a neighbour u
         :param Mu: routing table of u
         # update the local routing table
         update = False
         for p in V:
              if Mu[p] + Timings[v][u] < Mv[p]:</pre>
                   Mv[p] = Mu[p] + Timings[v][u]
                   NextHop_v[p] = u
                   update = True
         # notifying neighbours
         if update:
              for u in Nv:
                   send_update(u,Mv)
```



Bellman-Ford algorithm as protocol

Distance Vector Protocol

This protocol is used in computer networks (e.g. on Internet)

 \rightarrow Routing Information Protocol (RIP)





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Plan

Change making



Conclusion





Main points to remember

- « General » resolution method
- Recurrence formula (sub-optimal structure)
- The subproblems are not independent
- Memoization technique: *decrease the execution time by memorizing the calculated values*
 - → Classic compromise in computer science: time vs memory
- Generally efficient but not always applicable
- Shortest paths
 - X Be careful with negative weights!
 - X Be careful with negative cycles!
 - ➔ Bellman-Ford algorithm: circumvents these two difficulties
 - Polynomial complexity ($\mathcal{O}(|V|^3)$ or $\mathcal{O}(|V| \times |E|)$)
 - Principle also used for packet routing



Plan



Dynamic programming

3 Shortest Path

4 Conclusion

- Sequence alignment
 - Problem
 - Exhaustive approach
 - Dynamic programming
 - Algorithm



Going further

Concret problem

In bioinformatics (computer science dedicated to biology), sequence alignment allows two biological sequences (DNA, RNA or proteins) to be closer, so as to explain the similar regions.



• Given 2 sequences of any size: the first of size n and the second of size m



G – A G C A T C A T C G



match



match substitution







• to each elementary operation we associate a score:

•	match :	1
•	substitution :	-1
•	insert/delete :	-2

Change making Dynamic programming Shortest Path Conclusion Sequence alignm Problem Exhaustive approach Dynamic programming Algorithm	nent		
Which alignment to chose?			
• to each elementary operation we associate a score:			
• match :	1		
• substitution :	-1		
• insert/delete :	-2		
·			
The score of an alignment is the sum of the elementary scores			



The score of an alignment is the sum of the elementary scores

● first alignment: -3





Conclusion

Sequence alignment

Optimization problem

Sequence alignment

Given :

- 2 sequences
- 3 scores associated to the 3 elementary operations (match, subst, ins/del)



Optimization problem

Sequence alignment

Given :

- 2 sequences
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Problem : find the alignment with the maximal score


Optimization problem

Sequence alignment

Given :

- 2 sequences
- 3 scores associated to the 3 elementary operations (match, subst, ins/del)

Problem : find the alignment with the maximal score

Exponential Complexity!

Number of alignments:
$$\sum_{i=0}^{n} C_{m+i}^{i} \times C_{m}^{n-i} = \mathcal{O}(2^{n+m})$$



Recursive Approach

Align([],[]) = 0 $Align(S[0:n],[]) = n \times score['ins/del']$ $Align([],T[0:m]) = m \times score['ins/del']$ Align(S[0:n],T[0:m]) = max



Recursive Approach





Recursive Approach

$$Align([],[]) = 0$$

$$Align(S[0:n],[]) = n \times score['ins/del']$$

$$Align([],T[0:m]) = m \times score['ins/del']$$

$$Align(S[0:n],T[0:m]) = max \begin{cases} Align(S[0:n],T[0:m-1]) + score['ins/del' \\ Align(S[0:n-1],T[0:m]) + score['ins/del' \\ \end{bmatrix}$$

$$S: C T A G C A G T C A T C G$$

$$C T A G C A G T C A T C G$$

$$C T A G C A G T C A T C G$$

$$C T A G C A G T C A T C G$$





Recursive approach

Exponential complexity!

- Ternary search tree of depth n + m
- Complexity in $\mathcal{O}(3^{n+m})$





Recursive approach

Exponential complexity!

- Ternary search tree of depth n + m
- Complexity in $\mathcal{O}(3^{n+m})$
- Redundant computation!





Recurrence formula

Sequence alignment

Let OPT(M, N) be the maximal score of the alignment of the **M** first nucleotides of the first sequence with the **N** first nucleotides of the second sequence

•
$$OPT(0,0) = 0$$



Conclusion

Sequence alignment

Needleman and Wunsch algorithm (1970)

s ^T	G	A	G	С	Α	Т	С	Α	Т	С	G
С											
Т											
Α											
G											
С											
A											
G											
Т											
С											
A											



 $C \ T \ A \ G \ C \ A \ G \ - \ - \ T \ C \ A$

$$G - A G C A T C A T C G$$



Conclusion

Sequence alignment







Conclusion

Sequence alignment







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Sequence alignment







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Sequence alignment







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Conclusion

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Change making Dynamic programming Shortest Path Problem Exhaustive approach Dynamic programming Algorithm

h Conclusion

Sequence alignment



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Nee	dle	ma	n a	nd	W	uns	sch	alg	gori	thr	n (197	70)		
	s T		G	Α	G	С	A	Т	С	A	Т	С	G	** skip	
		0													
	С														
	Т														
	A														
	G														
	С														
	Α														
	G														
	т														
	С														
	Α														
	~		<i>c</i> .												

Goal: to find the alignment with the maximal score

Ś	Cha Pro	inge r blem	nakin Exha	g austiv	Dy e app	namio roach	prog Dyr	ramn namic	ning prog	ramm	Short ing	est Pa Algori	ath ithm	Conclusion	Sequence alignment	
Nee	Needleman and Wunsch algorithm (1970)															
	s T		G	A	G	С	A	Т	С	A	Т	С	G	✤ skip		
		0	,−2_	→-4	, _ 6_	→ ⁻⁸ -	\rightarrow^{-10}	\rightarrow^{-12}	\rightarrow^{-14}	\rightarrow^{-16}	\rightarrow^{-18}	_20 →	\rightarrow^{-22}			
	С	-2														
	Т	-4														
	Α	-6														
	G	-8														
	С	-10														
	A	-12														
	G	-14														
	т	-16														
	С	-18														
	A	-20														
	Ste	n 1	·	- fil	l th	e fi	rst I	ine	and	ł th	e fi	rst	colu	ımn		
	010	м т.			. [2]	• III		1		/ .ii	۰ III ۱		0010			
	•	he he	ere	scol	re[]	ns/	ael] =	-2	$(\rightarrow$)					



 $\bullet~$ here score['match'] = 1 ($\rightarrow)$ and score['subst'] = -1 ($\rightarrow)$



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Conclusion

Sequence alignment

Needleman and Wunsch algorithm (1970)

s T		G	A	G	С	Α	Т	С	A	Т	С	G
	0	-2	-4	-6	-8	-10	-12	-14	-16	-18	-20	-22
С	-2	-1	-3	-5	-5	-7	-9	-11	-13	-15	-17	-19
Т	-4	-3	-2	-4	-6	-6	-6	-8	-10	-12	-14	-16
Α	-6	-5	-2	-3	-5	-5	-7	-7	-7	-9	-11	-13
G	-8	-5	-4	-1	-3	-6	-6	-8	-8	-8	-10	-10
С	-10	-7	-6	-3	0	-2	-4	-5	-7	-9	-7	-9
Α	-12	-9	-6	-5	-2	1	-1	-3	-4	-6	-8	-8
G	-14	-11	-8	-5	-4	-1	0	-2	-4	-5	-7	-7
Т	-16	-13	-10	-7	-6	-3	0	-1	-3	-3	-5	-7
С	-18	-15	-12	-9	-6	-5	-2	1	-1	-3	-2	-4
Α	-20	-17	-14	-11	-8	-5	-4	-1	2	0	-2	

>> skip

Step 2: we fill every cells by maximizing on the 3 axes

• here score['match'] = 1 (\rightarrow) and score['subst'] = -1 (\rightarrow)

Conclusion

>> skip

Sequence alignment

Needleman and Wunsch algorithm (1970)

T S		G	A	G	С	A	Т	С	A	Т	С	G
	0	-2	-4	-6	-8	-10	-12	-14	-16	-18	-20	-22
С	-2	-1	-3	-5	-5	-7	-9	-11	-13	-15	-17	-19
т	-4	-3	-2	-4	-6	-6	-6	-8	-10	-12	-14	-16
Α	-6	-5	-2	-3	-5	-5	-7	-7	-7	-9	-11	-13
G	-8	-5	-4	-1	-3	-6	-6	-8	-8	-8	-10	-10
С	-10	-7	-6	-3	0	-2	-4	-5	-7	-9	-7	-9
Α	-12	-9	-6	-5	-2	1	-1	-3	-4	-6	-8	-8
G	-14	-11	-8	-5	-4	-1	0	-2	-4	-5	-7	-7
Т	-16	-13	-10	-7	-6	-3	0	-1	-3	-3	-5	-7
С	-18	-15	-12	-9	-6	-5	-2	1	-1	-3	-2	-4
Α	-20	-17	-14	-11	-8	-5	-4	-1	2	0	-2	-3

Step 3: at the end of the table, we get the maximal score and the optimal alignments



Conclusion

Sequence alignment

Needleman and Wunsch algorithm (1970)

s T		G	Α	G	С	A	Т	С	A	Т	С	G
	0	-2	-4	-6	-8	-10	-12	-14	-16	-18	-20	-22
С	-2	Y	-3	-5	-5	-7	-9	-11	-13	-15	-17	-19
Т	-4	-2	-2	-4	-6	-6	-6	-8	-10	-12	-14	-16
Α	-6	-5	-2	-3	-5	-5	-7	-7	-7	-9	-11	-13
G	-8	-5	-4	-1	-3	-6	-6	-8	-8	-8	-10	-10
С	-10	-7	-6	-3	R	-2	-4	-5	-7	-9	-7	-9
Α	-12	-9	-6	-5	-2	×	-1	-3	-4	-6	-8	-8
G	-14	-11	-8	-5	-4	-1	8	-2	×	-5	-7	-7
Т	-16	-13	-10	-7	-6	-3	0	-1	-3	-2	-5	-7
С	-18	-15	-12	-9	-6	-5	-2	1	-1	-3	-2	-4
A	-20	-17	-14	-11	-8	-5	-4	-1	2	0	-2	-2

Step 3: at the end of the table, we get the maximal score and the optimal alignments



Conclusion

Sequence alignment

Needleman and Wunsch algorithm (1970)

• Among the 3^{n+m} possible paths in the matrix, we found the optimal alignment in $n \times m$ steps



Conclusion

Sequence alignment

Needleman and Wunsch algorithm (1970)

Among the 3^{n+m} possible paths in the matrix, we found the optimal alignment in n × m steps

Algorithm complexity

- $\mathcal{O}(n \times m)$ in time: size of the matrix
- O(min(n, m)) in space: instead of keeping the complete matrix, we keep only the current and precedent line