CS 577 - Dynamic Programming

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Summer 2023
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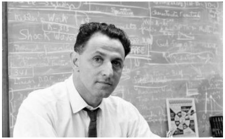
Dynamic Programming

DYNAMIC PROGRAMMING



Richard Bellman

It is "programming" that is "dynamic"!

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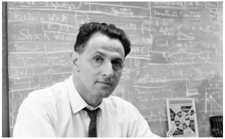

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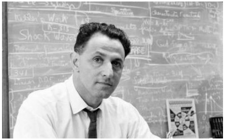
Why "Dynamic Programming"?

Reasons for the name:

- In the 1950s, "programming" was about "planning" rather than coding.
- "Dynamic" is exciting – Air Force director didn't like research and wanted pizzazz.
- "Dynamic" sounds better than "linear" (Re: rival Dantzig).

Dynamic Programming



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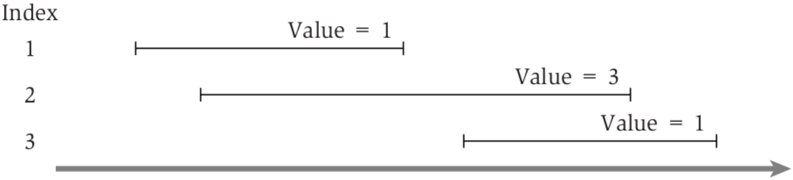
It is "programming" that is "dynamic"!

What is it?

- Your new favourite algorithmic technique.
- Extreme Divide and Conquer
- Many sub-problems, but not quite brute-force.
- Dynamic in that it calculates a bunch of solutions from the "smallest" to the "largest".

Weighted Interval Scheduling

WEIGHTED INTERVAL SCHEDULING



Problem Definition

- Requests: $\sigma = \{r_1, \cdots, r_n\}$

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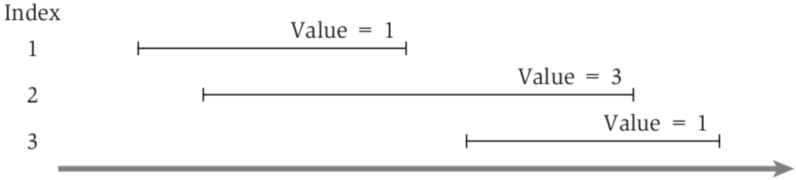

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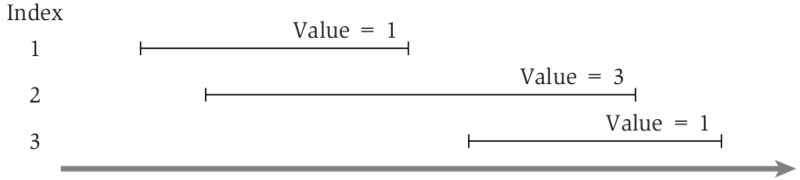

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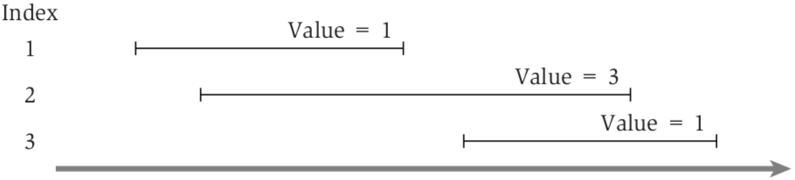

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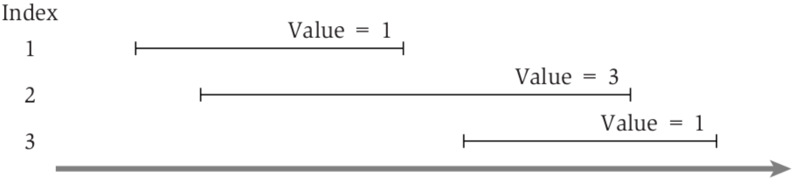

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TH1: What is the value of the FF heuristic?

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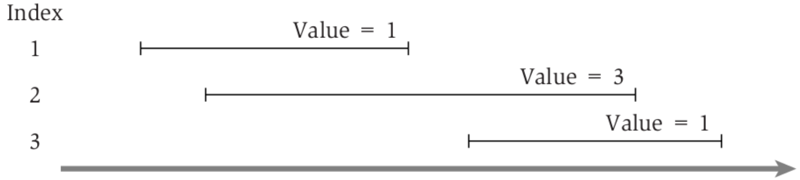

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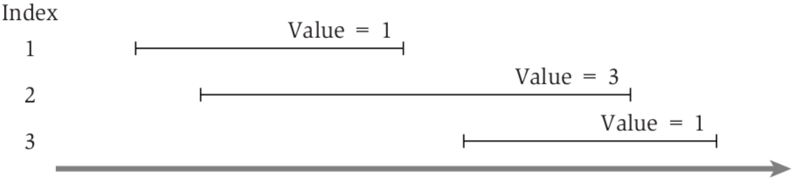

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TH2: What is the optimal value?

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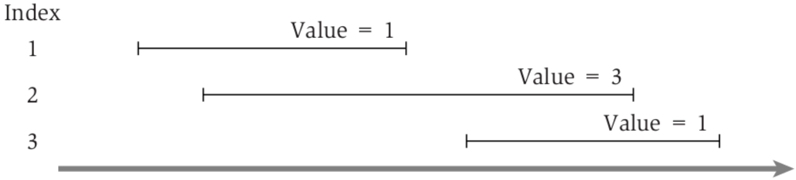

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Recursive Solution

Recursive Procedure

1. Assume σ ordered by finish time (asc).

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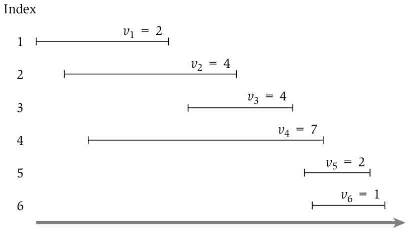
Proof of optimality.

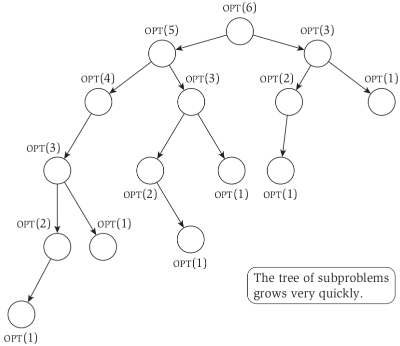
By strong induction on j.
Base cases: $j = 0$ or $j = 1$: Only 1 possible optimal solution.
Inductive step:

- By ind hyp, we have opt for $j-1$ and opt for i.
- FF assures the dichotomy that the last interval is either in the solution or not.
- Take the max of whether or not a given interval is included. □

CONSIDER THE RECURSION

$$\text{OPT}(j) = \max(\text{OPT}(j-1), \text{OPT}(i) + v_j)$$





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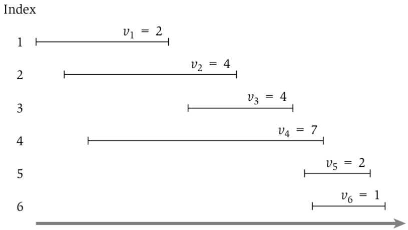

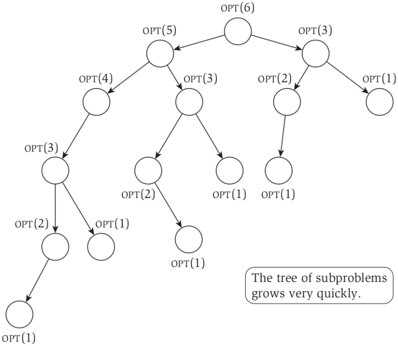

TH3: What is the asymptotic number of recursive calls with n jobs?

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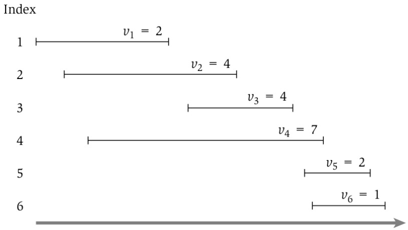

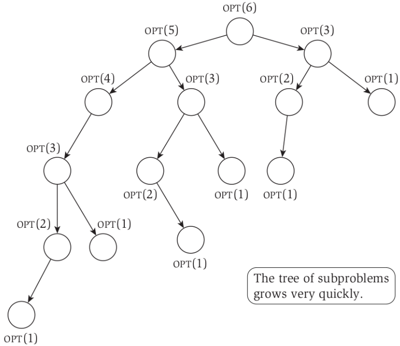

TH3: What is the asymptotic number of recursive calls with n jobs? $O(2^n)$

Memoizing the Recursion

Memoization

- Not a typo.
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Basic Technique

- Calculate once: store the value in array and retrieve for future calls.
- Can be implemented recursively, but tends to be more natural as an iterative process.

Dynamic Program Solution

Algorithm: WeightIntDP

Sort σ by finish time
$m[0] := 0$
for $j = 1$ *to* n **do**
  Find index i
  $m[j] = \max(m[j-1], m[i] + v_j)$
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- DP algorithms are formulaic.
- We understand how loops work.
- NO Pseudocode.

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We want:

- Definitions required for algorithm to work
- Description of matrix
- Bellman Equation
- Location of solution, order to populate the matrix

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- 1D array M, where $M[j]$ is the maximum value of a compatible schedule for the first j items in sorted σ. Initialize $M[1] = v_1$.

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Solution, order to populate

- The maximum value of a compatible schedule for the n jobs is found at $M[n]$. Populate from 2 to n.

Analyze the Algorithm

DP Solution

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- Preprocessing:

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- Preprocessing:
  - Sorting jobs: $O(n \log n)$.

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  - Number of cells: TopHat 4

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Runtime

- Preprocessing:
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- Populate the matrix:
  - Number of cells: $O(n)$
  - Cost per cell: TopHat 5

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Runtime

- Preprocessing:
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Overall: TopHat 6

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Overall: $O(n^2)$ linear search, $O(n \log n)$ binary search

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ANALYZE THE ALGORITHM

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What about the schedule S?

Trace back from the optimal value:

- Job j is part of the optimal schedule from 1 to j iff $v_j + \textsc{opt}(i) \geq \textsc{opt}(j-1)$

Basic DP Outline

Algorithm Template

- Preprocessing of data
- Populate the matrix:
  - Iterate over the cells in the correct order.
  - Understand the work done per cell.

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1. There are only a polynomial number of subproblems.

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2. The solution to the larger problem can be efficiently calculated from the subproblems.

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Algorithm Guidelines

1. There are only a polynomial number of subproblems.
2. The solution to the larger problem can be efficiently calculated from the subproblems.
3. Natural ordering of the subproblems from “smallest” to “largest”.

Longest Increasing Subsequence

Longest Increasing Subsequence

Problem

- Given an integer array $A[1..n]$.
- Find the longest increasing subsequence. That is, let i be a sequence of indexes, we have $A[i_k] < A[i_{k+1}]$ for all k.

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Recursive Approach

Algorithm: LIS

Input : Integer k, and array of integers $A[1..n]$.
Output: Return length of LIS where every value $> k$.
Exo: Complete the algorithm

RECURSIVE APPROACH

Algorithm: LIS

Input : Integer k, and array of integers $A[1..n]$.
Output: Return length of LIS where every value $> k$.

if $n = 0$ **then** **return** 0
else if $A[1] \leq k$ **then**
  return LIS$(k, A[2..n])$
else
  skip :=LIS$(k, A[2..n])$
  take :=LIS$(A[1], A[2..n]) + 1$
  return $\max\{skip, take\}$
end

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else if $A[1] \leq k$ **then**
  return LIS$(k, A[2..n])$
else
  skip :=LIS$(k, A[2..n])$
  take :=LIS$(A[1], A[2..n]) + 1$
  return $\max\{skip, take\}$
end

TH2: For an array $A[1..n]$, how would you find the length of the LIS using the LIS$(\cdot)$ algorithm?

RECURSIVE APPROACH

Algorithm: LIS

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TH2: For an array $A[1..n]$, how would you find the length of the LIS using the LIS$(\cdot)$ algorithm? LIS$(-\infty, A[1..n])$

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TH3: Run time of the algorithm for a length n array?

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TH3: Run time of the algorithm for a length n array? $O(2^n)$

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TH3: Run time of the algorithm for a length n array? $O(2^n)$
TH4: How many distinct recursive calls for a length n array? $O(n^2)$

DYNAMIC PROGRAM FOR LIS

Description of matrix

TH5: Number of dimensions of array?

Dynamic Program for LIS

Description of matrix

TH5: Number of dimensions of array? 2

Dynamic Program for LIS

Description of matrix

2D array L, where $L[i, j]$ is the maximum LIS of $A[j..n]$ with every item $> A[i], i < j$.

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$$L[i,j] = \begin{cases} 0, \text{if } j > n \\ L[i,j+1], \text{if } A[i] \geq A[j] \\ \max\{L[i,j+1], L[j,j+1]+1\}, \text{otherwise} \end{cases}$$

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Solution and populating L

- Solution in $L[0][1]$; add $A[0] = -\infty$.
- Populate j from n to 1; i from 0 to $j-1$ or $j-1$ to 0.

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- TH6: Run time:

Dynamic Program for LIS

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Solution and populating L

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- Run time: $O(n^2)$

Dynamic Programming for Games

Dynamic Programming for Games

Games

- Some number of players (1 to many).
- Set of rules with some objective.
- Huge domain, started by Von Neumann, that spans many fields such as Economics, Math, Biology, and Computer Science.

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DP for Games

In many games, DP is a natural paradigm for an optimal strategy.

Coins in a Line

Players

Two players:

Alice
(Player A)

Bob
(Player B)

Coins in a Line

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- n (even) coins in a line; each coin has a value.
- Starting with Alice, each player will pick a coin from the head or the tail.

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- Starting with Alice, each player will pick a coin from the head or the tail.
- Winner: Player with the max value at the end; winning player keeps the coins.

Greedy Approaches

Largest Coin

TopHat D1: Give a counter-example.

Greedy Approaches

Largest Coin

```
[1,3,6,3]
A: 3; [1,3,6]
B: 6; [1,3]
A: 6; [1]
B: 7; []
```

Greedy Approaches

Largest Coin

Even or Odd

```
[1,3,6,3,1,3]
A: 3; [1,3,6,3,1]
B: 1; [1,3,6,3]
A: 6; [1,3,6]
B: 7; [1,3]
A: 9; [1]
B: 8; []
```

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Largest Coin

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- Alice can always win.

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- But are we optimal?

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B: 7; [1,3]
A: 9; [1]
B: 8; []
```

```
[1,3,6,3,1,3]
A: 3; [1,3,6,3,1]
B: 1; [3,6,3,1]
A: 4; [3,6,3]
B: 4; [6,3]
A: 10; [3]
B: 7; []
```

- Alice can always win.
- But are we optimal? No

Natural Dichotomy

TH D2: What is the natural dichotomy?

NATURAL DICHOTOMY

Head or Tail?

- Two players: Assume that Bob will play optimally.

Natural Dichotomy

Head or Tail?

- Two players: Assume that Bob will play optimally.
- For Alice's kth turn:
  - Coin array: $C[i..j]$
  - $\max\{c[i] + \text{BobOpt}(c[i+1..j]), c[j] + \text{BobOpt}(c[i..j-1])\}$

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TH1: How many dimensions for DP array?

Natural Dichotomy

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TH1: How many dimensions for DP array? 2

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DP Description

- 2D array M:
  - $M[i, j]$ is the maximum value possible for Alice when choosing from $c[i..j]$, assuming Bob plays optimally.

Head or Tail DP

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  TopHat 2

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$$M[i,j] = \max\{c[i] + \min\{M[i+2,j], M[i+1,j-1]\},\\ c[j] + \min\{M[i+1,j-1], M[i,j-2]\}\}$$

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- Solution: TH3

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- Runtime: TH4

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- Runtime: $O(n^2)$

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- Proof of correctness:

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- Solution: $M[1,n]$
- Runtime: $O(n^2)$
- Proof of correctness: Strong induction on the cell population order.

Max Subarray

MAX SUBARRAY

Problem

Given an array A of integers, find the (non-empty) contiguous subarray of A of maximum sum.

MAX SUBARRAY

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Given an array A of integers, find the (non-empty) contiguous subarray of A of maximum sum.

Exercise – Teams of 3 or so

- Solve the problem in $\Theta(n^2)$.
- Solve the problem in $O(n \log n)$.
- Prove correctness and complexity.

PART 1: GIVE A $\Theta(n^2)$ SOLUTION.

Algorithm: CHECKALLSUBARRAYS

Input : Array A of n ints.
Output: Max subarray in A.

```
Let M be an empty array
for i := 1 to len(A) do
    for j := i to len(A) do
        if sum(A[i..j]) > sum(M) then
            M := A[i..j]
        end
    end
end
return M
```

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Analysis

- Correct: Checks all possible contiguous subarrays.

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    end
  end
end
return M

Analysis

- Correct: Checks all possible contiguous subarrays.
- Complexity:
  - Re-calculating the sum will make it $O(n^3)$. Key is to calculate the sum as you iterate.
  - For each i, check $n - i + 1$ ends. Overall:

$$\sum_{i=1}^{n} i = \frac{n(n+1)}{2} = \Theta(n^2).$$

PART 2: GIVE AN $O(n \log n)$ SOLUTION.

Algorithm: MAXSUBARRAY

Input : Array A of n ints.
Output: Max subarray in A.
if $|A| = 1$ **then return** $A[1]$
$A_1 :=$ MAXSUBARRAY(Front-half of A)
$A_2 :=$ MAXSUBARRAY(Back-half of A)
$M :=$MIDMAXSUBARRAY(A)
return *Array with max sum of* $\{A_1, A_2, M\}$

Part 2: Give an $O(n \log n)$ solution.

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$M :=$MidMaxSubarray(A)
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Algorithm: MidMaxSubarray

Input : Array A of n ints.
Output: Max subarray that crosses midpoint A.
$m :=$ mid-point of A
$L :=$ max subarray in $A[i, m-1]$ for $i = m-1 \to 1$
$R :=$ max subarray in $A[m, j]$ for $j = m \to n$
return $L \cup R$ `// subarray formed by combining` L `and` R.

Part 2: Give an $O(n \log n)$ solution.

Algorithm: MaxSubarray

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return *Array with max sum of* $\{A_1, A_2, M\}$

Analysis

- Correctness: By induction, A_1 and A_2 are max for subarray and M is max mid-crossing array.
- Complexity: Same recurrence as MergeSort.

Max Subarray

Problem

Given an array A of integers, find the (non-empty) contiguous subarray of A of maximum sum.

Exercise – Teams of 3 or so

- Solve the problem in $\Theta(n^2)$.
- Solve the problem in $O(n \log n)$.
- Prove correctness and complexity.
- **With dynamic programming, solve the problem in $O(n)$!**

PART 3: GIVE AN $O(n)$ SOLUTION.

DP Solution

- 1D array s, where $s[i]$ contains the value of the max subarray ending at i. ($O(n)$ cells)
- Bellman equation: $s[i] = \max(s[i-1] + A[i], A[i])$. ($O(1)$ time)
- Solutions is: $\max_j\{s[j]\}$. ($O(n)$ time)

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But we need the subarray not the value!

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- Use a parallel array that memoizes the starting index of the subarray ending at i:

$$\text{start}[i] = \begin{cases} \text{start}[i-1] & \text{if } s[i-1] + a[i] > a[i] \\ i & \text{, otherwise} \end{cases}$$

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- Or, trace back from max value at index j until $s[i] = A[i]$.

Subset and Knapsack

Subset Problem

Problem Definition

- A single machine that we can use for time W.

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Greedy Heuristics

- Decreasing weights: TopHat D1

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- Decreasing weights: $\{W/2 + 1, W/2, W/2\}$

Subset Problem

Problem Definition

- A single machine that we can use for time W.
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Dynamic Programming Approach

1D Approach

- if $n \notin S$, then $v[n] = v[n-1]$

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Need to consider more

To solve $v[n]$, we need to consider:

- the best solution with $n-1$ previous items restricted by W, and
- the best solution with $n-1$ previous items restricted by $W - w_n$

Dynamic Programming Approach

2D Approach

Dynamic Programming Approach

2D Approach

- 2D Matrix v:
  - i: Item indices from 0 to n.
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Dynamic Programming Approach

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TH8: Is this polynomial?

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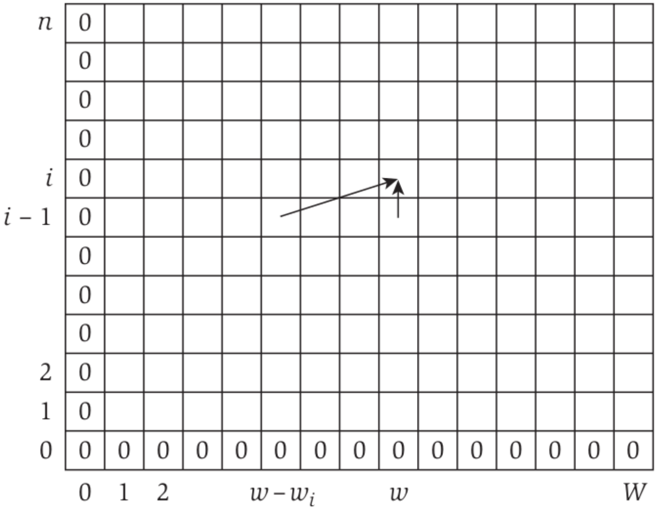
TH7: Running time to populate the matrix: $O(nW)$
TH8: Is this polynomial? No, *pseudo-polynomial* because of W which is unbounded.

Subset Visualization

Matrix Visualization:



Subset Visualization

Example Run:

$W = 6$, items $w_1 = 2$, $w_2 = 2$, $w_3 = 3$

3							
2							
1							
0	0	0	0	0	0	0	0
	0	1	2	3	4	5	6

Initial values

Subset Visualization

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3							
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Initial values

3							
2							
1	0	0	2	2	2	2	2
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Filling in values for $i = 1$

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3							
2	0	0	2	2	4	4	4
1	0	0	2	2	2	2	2
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	0	1	2	3	4	5	6

Filling in values for $i = 2$

Subset Visualization

Example Run:

$W = 6$, items $w_1 = 2$, $w_2 = 2$, $w_3 = 3$

	0	1	2	3	4	5	6
3							
2							
1							
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Initial values

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3							
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1	0	0	2	2	2	2	2
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Filling in values for $i = 1$

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3							
2	0	0	2	2	4	4	4
1	0	0	2	2	2	2	2
0	0	0	0	0	0	0	0

Filling in values for $i = 2$

	0	1	2	3	4	5	6
3	0	0	2	3	4	5	5
2	0	0	2	2	4	4	4
1	0	0	2	2	2	2	2
0	0	0	0	0	0	0	0

Filling in values for $i = 3$

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TH9: Running time of recovery of subset: $O(n)$

KNAPSACK EXTENSION

Problem Definition

- You are a thief with a knapsack that can carry W weight of goods.

Knapsack Extension

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- Each item has a weight: $w_1, w_2, \ldots, w_n$.
- Each item has a value: $v_1, v_2, \ldots, v_n$.
- What is the subset S of items to steal that maximizes $\sum_{i \in S} v_i$ with the constraint that $\sum_{i \in S} w_i \leq W$?

Exercise: Solve this with DP in $O(nW)$.

EXERCISE: SOLVE THIS WITH DP IN $O(nW)$.

DP Solution

- 2D Matrix:
  - i: Item indices from 0 to n.
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Edit Distance

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Problem

Minimum number of letter

- insertions: adding a letter,
- deletions: removing a letter,
- substitutions: replacing a letter

to change string $A[1..m]$ to string $B[1..n]$.

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Ex: TUESDAY $\rightarrow$ THUESDAY $\rightarrow$ THURSDAY

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to change string $A[1..m]$ to string $B[1..n]$.

Ex: TUESDAY → THUESDAY → THURSDAY

Or, align and count mismatched letters

```
T UESDAY
THURSDAY
```

Recursive Approach

Smaller Subproblems

- Let $A[1..m]$ and $B[1..n]$ be the 2 input strings.
- What is the edit distance for $A[1..i]$ and $B[1..j]$:

RECURSIVE APPROACH

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  - $j = 0$: $\text{Edit}(i, j) = i$.

Dynamic Program for Edit Distance

Description of matrix

TH4: Number of dimensions of array?

Dynamic Program for Edit Distance

Description of matrix

TH4: Number of dimensions of array? 2

Dynamic Program for Edit Distance

Description of matrix

2D array E, where $E[i,j]$ is the edit distance for $A[1..i]$ and $B[1..j]$.

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Bellman Equation

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Solution and populating L

- Solution in TopHat 5
- Set $E[0,j] = j$; $E[i,0] = i$; populate from 1 to n, 1 to m.

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Solution and populating L

- Solution in $E[m,n]$
- Set $E[0,j] = j$; $E[i,0] = i$; populate from 1 to n, 1 to m.
- TH6: Run time:

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$$E[i,j] = \begin{cases} i, \text{ if } j = 0 \\ j, \text{ if } i = 0 \\ \min\{E[i,j-1]+1, E[i-1,j]+1, \\ \qquad E[i-1,j-1] + A[i] \neq B[j]\}, \text{ otherwise} \end{cases}$$

Solution and populating L

- Solution in $E[m,n]$
- Set $E[0,j] = j$; $E[i,0] = i$; populate from 1 to n, 1 to m.
- Run time: $O(mn)$

Space Savings

Bellman Equation

$$E[i,j] = \begin{cases} i, \text{if } j = 0 \\ j, \text{if } i = 0 \\ \min\{E[i,j-1]+1, E[i-1,j]+1, \\ \qquad E[i-1,j-1] + A[i] \neq B[j]\}, \text{otherwise} \end{cases}$$

How much space do we need?

- Notice that $E[i][j]$ depends on $E[i,j-1]$, $E[i-1,j]$, and $E[i-1,j-1]$.
- We only need previous and current row of matrix for calculations.

Shortest Path

Shortest Path

Going Negative

Problem Definition

We have a directed graph $G = (V, E)$, where $|V| = n$ and $|E| = m$ and a node s that has a path to every other node in V. For each edge $e = (i, j)$, c_{ij} is the weight of the edge, and the are no cycles with negative weight.

- What is the shortest path from s to each other node?

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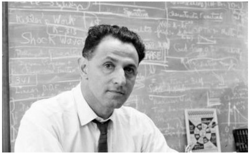
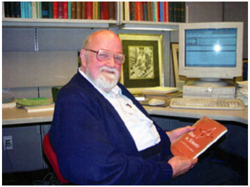


Richard Bellman



L R Ford Jr.

Shortest Path

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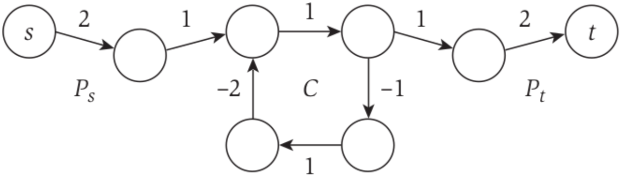
Why no negative cycles?



Dijkstra's

Algorithm: *Dijkstra's*

Let S be the set of explored nodes.
For each $u \in S$, we store a distance value $d(u)$.
Initialize $S = \{s\}$ and $d(s) = 0$
while $S \neq V$ **do**
  Choose $v \notin S$ with at least one incoming edge originating from a node in S with the smallest

$$d'(v) = \min_{e=(u,v):u\in S} d(u) + \ell_e$$

  Append v to S and define $d(v) = d'(v)$.
end
return S

Dijkstra's

Negative Problem

Dijkstra's

Negative Problem

- Lose guarantee that minimum edge between S and $V \setminus S$ is part of minimum path.

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- A path with x edges: Cost increases $x \cdot \beta$.

Dijkstra's

Negative Problem

- Lose guarantee that minimum edge between S and $V \setminus S$ is part of minimum path.

Why not just boost all edges by max negative value plus a bit (β)?

- A path with x edges: Cost increases $x \cdot \beta$.
- Solution in new graph is not guaranteed to be optimal in original graph.

Bellman-Ford

Observation 1

If G has no negative cycles, then there exists a shortest path from s to t that is simple, and has at most $n - 1$ edges.

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- 2D matrix M of # edges in path $\times$ vertices.

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- 2D matrix M of # edges in path $\times$ vertices.
  - $M[i][v]$ is the shortest path from v to t using $\leq i$ edges.

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  - TH23: Where is the solution?

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- 2D matrix M of # edges in path $\times$ vertices.
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  - Solution: $M[n-1][s]$

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TH24: Build the Bellman equation.

Bellman-Ford

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  - Use $\leq i$ edges.

$$M[i][v] = \min\{M[i-1][v], \min_{w \in V}\{M[i-1][w] + c_{vw}\}\},$$

where $c_{vw} = \infty$ if no edge from v to w.

Bellman-Ford Analysis

$$M[i][v] = \min\{M[i-1][v], \min_{w \in V}\{M[i-1][w] + c_{vw}\}\}$$

Worst Case: n nodes

- TH25: # of Cells:

Bellman-Ford Analysis

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Worst Case: n nodes

- # of Cells: $O(n^2)$.

Bellman-Ford Analysis

$$M[i][v] = \min\{M[i-1][v], \min_{w \in V}\{M[i-1][w] + c_{vw}\}\}$$

Worst Case: n nodes

- # of Cells: $O(n^2)$.
- TH26: Cost per cell:

Bellman-Ford Analysis

$$M[i][v] = \min\{M[i-1][v], \min_{w \in V}\{M[i-1][w] + c_{vw}\}\}$$

Worst Case: n nodes

- # of Cells: $O(n^2)$.
- Cost per cell: $O(n)$.

Bellman-Ford Analysis

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Worst Case: n nodes

- # of Cells: $O(n^2)$.
- Cost per cell: $O(n)$.
- Overall: $O(n^3)$.

Bellman-Ford Analysis

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Worst Case: n nodes, m edges

- For each node v, we only need to consider outgoing edges to w (denoted by η_v).
- For every node v, we need to do this calculation for $0 \leq i \leq n-1$ lengths.

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BELLMAN-FORD ANALYSIS

$$M[i][v] = \min\{M[i-1][v], \min_{w \in V}\{M[i-1][w] + c_{vw}\}\}$$

Worst Case: n nodes, m edges

- Overall: $O\left(n \sum_{v \in V} \eta_v\right) = O(mn)$.

Space Saving: $O(n)$.

- To build row i:
  - We only need $i-1$ values for each node.
  - $M[v] = \min\{M[v], \min_{w \in V}\{M[w] + c_{vw}\}\}$ for each i.

Bellman-Ford Analysis

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- To build row i:
  - We only need $i-1$ values for each node.
  - $M[v] = \min\{M[v], \min_{w \in V}\{M[w] + c_{vw}\}\}$ for each i.
- Recovery of actual path: An additional array $\mathit{first}[v]$ that maintains the first hop from v to t.

Negative Cycles

Observation 2

If there is a negative cycle along the path from s to t, then the shortest path is $-\infty$.

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$M[i][v] = M[n-1][v]$ *for all* $i > n-1$ *and all nodes* v *if there are no negative cycles on the paths to* t.

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If there is a negative cycle along the path from s to t, then the shortest path is $-\infty$.

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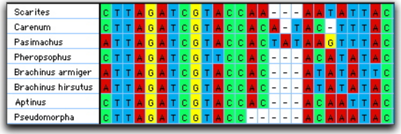
Augmented Graph for Negative Cycle Finding

- Add a node t with an incoming edge from all other nodes with cost 0.
- Run Bellman-Ford from any node s to t until number of edges n.
- If, for some v, $M[n][v] \neq M[n-1][v]$, then there is a negative cycle.

Sequence Alignment

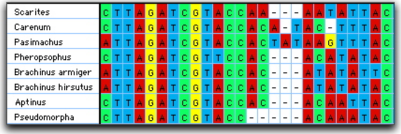
Sequence Alignment



Needleman–Wunsch Problem

- An alphabet S.
- Strings $X = x_1 x_2 \ldots x_m$ and $Y = y_1 y_2 \ldots y_n$ from S.
- A matching $M = \{(i, j)\}$ of pairs without crossings, where $i \in [1, m]$ and $j \in [1, n]$.

SEQUENCE ALIGNMENT



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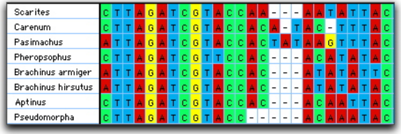
  - Gaps (unmatched indexes) have a cost of δ.
  - For each symbol pair $p, q \in S$, α_{pq} is the matching cost.

SEQUENCE ALIGNMENT



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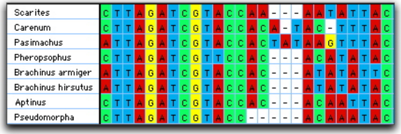

$\delta = 3; \alpha_{pp} = 0; \alpha_{pq} = 1$

TopHat Q16: What is the cost of the matching:

`o-currance`

`occurrence`

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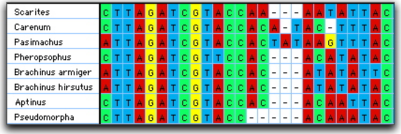

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TopHat Q17: What is the cost of the matching:

```
o-curr-ance
occurre-nce
```

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- Cost:
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SEQUENCE ALIGNMENT

Scarites	CTTAGATCGTACCAA---AATATTAC
Carenum	CTTAGATCGTACCACA-TAC-TTTAC
Pasimachus	ATTAGATCGTACCACTATAAGTTTAC
Pheropsophus	CTTAGATCGTTCCAC---ACATATAC
Brachinus armiger	ATTAGATCGTACCAC---ATATATTC
Brachinus hirsutus	ATTAGATCGTACCAC---ATATATAC
Aptinus	CTTAGATCGTACCAC---ACAATTAC
Pseudomorpha	CTTAGATCGTACC-----ACAAATAC

$\delta = 1; \alpha_{pp} = 0; \alpha_{pq} = 4$

TopHat Q18: What is the cost of the matching:

`o-currance`

`occurrence`

Needleman–Wunsch Problem

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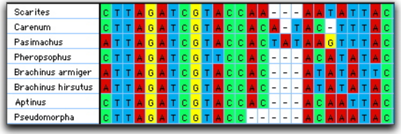
SEQUENCE ALIGNMENT



$\delta = 1; \alpha_{pp} = 0; \alpha_{pq} = 4$

TopHat Q19: What is the cost of the matching:

```
o-curr-ance
occurre-nce
```

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- Cost:
  - Gaps (unmatched indexes) have a cost of δ.
  - For each symbol pair $p, q \in S$, α_{pq} is the matching cost.
- Goal: Find the matching that minimizes the cost.

Designing Needleman–Wunsch Algorithm

Basic Dichotomy

In optimal alignment M, either $(m, n) \in M$ or $(m, n) \notin M$.

DESIGNING NEEDLEMAN–WUNSCH ALGORITHM

Basic Dichotomy

In optimal alignment M, either $(m, n) \in M$ or $(m, n) \notin M$.

Lemma 1

Let M be any alignment of X and Y. If $(m, n) \notin M$, then either the mth position of X, or the nth position of Y is not matched in M.

Designing Needleman–Wunsch Algorithm

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Proof.

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- By way of contradiction, assume that $(m, n) \notin M$, and $(m, j), (i, n) \in M$ for $i < m$ and $j < n$.

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Proof.

- By way of contradiction, assume that $(m, n) \notin M$, and $(m, j), (i, n) \in M$ for $i < m$ and $j < n$.
- Contradicts the non-crossing requirement.

$\square$

Designing Needleman–Wunsch Algorithm

Key Concepts for Optimality

In an optimal alignment M, at least one of the following is true:

1. $(m, n) \in M$; or
2. the mth position of X is not matched; or
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- TH20: How many dimensions for the matrix?

Designing Needleman–Wunsch Algorithm

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- 2D matrix called A, where $A[i][j]$ is alignment of minimum cost for $x_1 x_2 \ldots x_i$ and $y_1 y_2 \ldots y_j$.

Designing Needleman–Wunsch Algorithm

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- TH21: Build the Bellman equation.

Designing Needleman–Wunsch Algorithm

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- Runtime: TH22

Designing Needleman–Wunsch Algorithm

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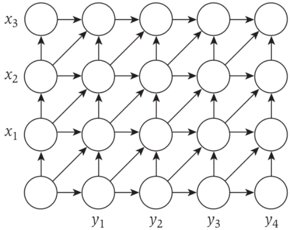
- $A[i][j] = \min\{\alpha_{x_iy_j} + A[i-1][j-1], \delta + A[i-1][j], \delta + A[i][j-1]\}$
- Runtime: $O(mn)$.

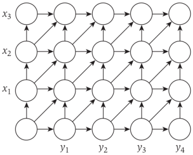
Graphing the Algorithm



Theorem 2

Let $f(i,j)$ denote the minimum cost of a path from $(0,0)$ to (i,j) in G_{XY}. Then, $\forall i,j\; f(i,j) = A[i][j]$.

GRAPHING THE ALGORITHM



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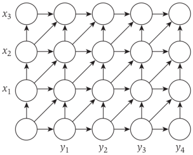
Proof.

Graphing the Algorithm



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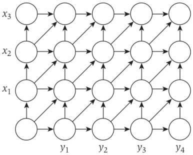

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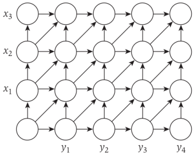

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Proof.

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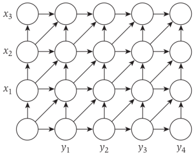
- Base case:

Graphing the Algorithm



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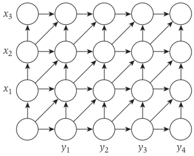

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- Inductive step:

$$\begin{aligned} f(i,j) &= \min\{\alpha_{x_i y_j} + f(i-1,j-1), \delta + f(i-1,j), \delta + f(i,j-1)\} \\ &= \min\{\alpha_{x_i y_j} + A[i-1][j-1], \delta + A[i-1][j], \delta + A[i][j-1]\} \\ &= A[i,j] \end{aligned}$$

□

SEQUENCE ALIGNMENT EXAMPLE

$$A[i][j] = \min\{\alpha_{x_i y_j} + A[i-1][j-1], \delta + A[i-1][j], \delta + A[i][j-1]\}$$

- "mean" vs "name"
- $\delta = 2; \alpha = \begin{cases} 0 & \text{if same letter} \\ 3 & \text{if vowel to consonant} \\ 1 & \text{otherwise} \end{cases}$

n					
a					
e					
m					
-					
	-	n	a	m	e

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n	8	6	5	4	6
a	6	5	3	5	5
e	4	3	2	4	4
m	2	1	3	4	6
-	0	2	4	6	8
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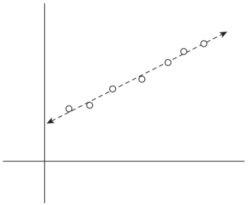
Least Squares

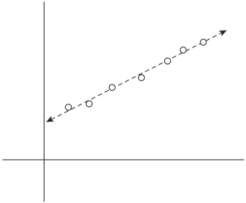
Segmented Least Squares



Problem Setup

- Set of n points: $P := \{(x_1, y1), (x_2, y_2), \ldots, (x_n, y_n)\}$ on the plane.
- Suppose $x_1 < x_2 < \cdots < x_n$.
- Find $L : y = ax + b$ that minimizes: $\text{Error}(L, P) = \sum_{i=1}^{n} (y_i - ax_i - b)^2$.

SEGMENTED LEAST SQUARES



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Problem Formulation

- Partition the points (by x) into contiguous subsets.
- Minimize the sum of $\text{Error}(L, p_i) + C$ for all subsets, where C is a fixed cost per subset.

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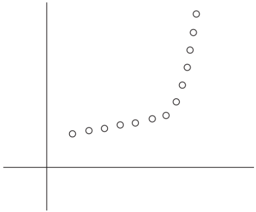

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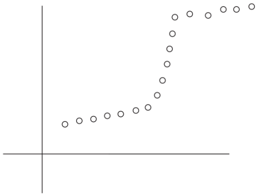

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$$s[j] = \min_{1 \le i \le j} (e_{i,j} + C + s[i-1])$$

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- Number of cells: TH10

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- Number of cells: $O(n)$.
- Work done for cell j: TH11

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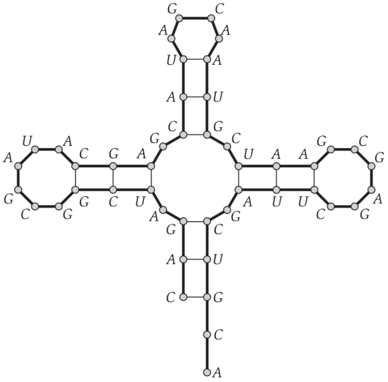
- Number of cells: $O(n)$.
- Work done for cell j: $O(j)$.
- Overall: $O(n^2)$.

RNA Secondary Structure

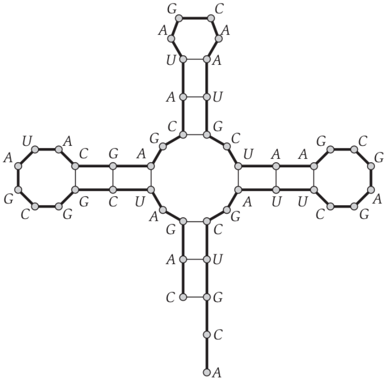
RNA Secondary Structure



Problem Definition

- RNA tends to loop back on itself, forming base pairs.
- RNA alphabet: $\{A, C, G, U\}$.
- Valid pairs: (A, U) or (C, G).

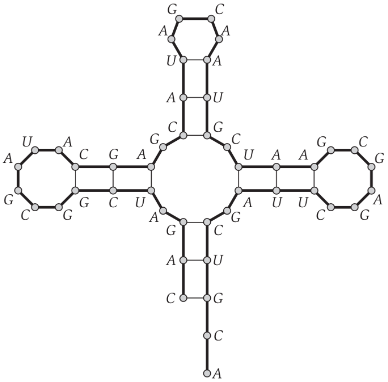
RNA SECONDARY STRUCTURE



Problem Definition

- RNA tends to loop back on itself, forming base pairs.
- RNA alphabet: $\{A, C, G, U\}$.
- Valid pairs: (A, U) or (C, G).
- Input: n length string: $B = b_1 b_2 \ldots b_n$
- Output: Determine a secondary structure with maximum number of base pairs.

RNA Secondary Structure



Secondary Structure

$S = \{(i,j)\}$, where $i < j$ and $i,j \in \{1,\ldots,n\}$, such that:

1. No Sharp turns: $i < j - d$ for some constant d.
2. All pairs are valid.
3. S is a matching: no base appears more than once.
4. Non-crossing: For any $(i,j),(i',j') \in S$, we cannot have $i < i' < j < j'$.

First Dynamic Programming Attempt

1D Approach

- 1D array m, where $m[j]$ is the maximum # of pairs among: $b_1 b_2 \ldots b_j$.

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Recursive Sub-problems

Dichotomy:

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Dichotomy:

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2. j is paired with $t < j - d$:
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     1. Max pairs in $[1, t-1]$: $m[t-1]$.

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     2. Max pairs in $[t+1, j-1]$: Restricted to $b_{t+1} b_{t+2} \dots b_{j-1}$ which current DP does not calculate.

Second Dynamic Programming Attempt

2D Approach

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- Solution: TopHat 12

SECOND DYNAMIC PROGRAMMING ATTEMPT

2D Approach

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- Solution: $m[1][n]$.

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SECOND DYNAMIC PROGRAMMING ATTEMPT

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TopHat 13: What is the Bellman equation?

Second Dynamic Programming Attempt

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$$m[i][j] \;=\; \max\left(m[i][j-1], \max_{i \le t < j-d}\{v_{tj} \cdot (1 + m[i][t-1] + m[t+1][j-1])\}\right)$$

RNA Secondary Structure Example

$$m[i][j] = \max\left(m[i][j-1], \max_{i \le t < j-d}\{v_{tj} \cdot (1 + m[i][t-1] + m[t+1][j-1])\}\right)$$

- $B = ACCGGUAGU$ and $d = 4$

i				
4				
3				
2				
1				
j	6	7	8	9

RNA Secondary Structure Example

$$m[i][j] = \max\left(m[i][j-1], \max_{i \le t < j-d} \{ v_{tj} \cdot (1 + m[i][t-1] + m[t+1][j-1]) \} \right)$$

- $B = ACCGGUAGU$ and $d = 4$

i				
4	0	0	0	
3	0	0		
2	0			
1				
j	6	7	8	9

RNA Secondary Structure Example

$$m[i][j] = \max\left(m[i][j-1], \max_{i \le t < j-d}\{v_{tj} \cdot (1 + m[i][t-1] + m[t+1][j-1])\}\right)$$

- $B = ACCGGUAGU$ and $d = 4$

i				
4	0	0	0	0
3	0	0	1	
2	0	0		
1	1			
j	6	7	8	9

RNA Secondary Structure Example

$$m[i][j] = \max\left(m[i][j-1], \max_{i \leq t < j-d}\{v_{tj} \cdot (1 + m[i][t-1] + m[t+1][j-1])\}\right)$$

- $B = ACCGGUAGU$ and $d = 4$

i				
4	0	0	0	0
3	0	0	1	1
2	0	0	1	
1	1	1		
j	6	7	8	9

RNA Secondary Structure Example

$$m[i][j] = \max\left(m[i][j-1], \max_{i \le t < j-d}\{v_{tj} \cdot (1 + m[i][t-1] + m[t+1][j-1])\}\right)$$

- $B = ACCGGUAGU$ and $d = 4$

i				
4	0	0	0	0
3	0	0	1	1
2	0	0	1	1
1	1	1	1	
j	6	7	8	9

RNA Secondary Structure Example

$$m[i][j] = \max\left(m[i][j-1], \max_{i \le t < j-d}\{v_{tj} \cdot (1 + m[i][t-1] + m[t+1][j-1])\}\right)$$

- $B = ACCGGUAGU$ and $d = 4$

i				
4	0	0	0	0
3	0	0	1	1
2	0	0	1	1
1	1	1	1	2
j	6	7	8	9

RNA SECONDARY STRUCTURE EXAMPLE

$$m[i][j] = \max\left(m[i][j-1], \max_{i \le t < j-d}\{v_{tj} \cdot (1 + m[i][t-1] + m[t+1][j-1])\}\right)$$

- $B = ACCGGUAGU$ and $d = 4$

i				
4	0	0	0	0
3	0	0	1	1
2	0	0	1	1
1	1	1	1	2
j	6	7	8	9

Running Time

- # of cells: TH14
- Work per cell:

RNA Secondary Structure Example

$$m[i][j] = \max\left(m[i][j-1], \max_{i \le t < j-d}\{v_{tj} \cdot (1 + m[i][t-1] + m[t+1][j-1])\}\right)$$

- $B = ACCGGUAGU$ and $d = 4$

i				
4	0	0	0	0
3	0	0	1	1
2	0	0	1	1
1	1	1	1	2
j	6	7	8	9

Running Time

- # of cells: $O(n^2)$.
- Work per cell:

RNA Secondary Structure Example

$$m[i][j] = \max\left(m[i][j-1], \max_{i \le t < j-d}\{v_{tj} \cdot (1 + m[i][t-1] + m[t+1][j-1])\}\right)$$

- $B = ACCGGUAGU$ and $d = 4$

i				
4	0	0	0	0
3	0	0	1	1
2	0	0	1	1
1	1	1	1	2
j	6	7	8	9

Running Time

- # of cells: $O(n^2)$.
- Work per cell: TH15

RNA Secondary Structure Example

$$m[i][j] = \max\left(m[i][j-1], \max_{i \le t < j-d}\{v_{tj} \cdot (1 + m[i][t-1] + m[t+1][j-1])\}\right)$$

- $B = ACCGGUAGU$ and $d = 4$

i				
4	0	0	0	0
3	0	0	1	1
2	0	0	1	1
1	1	1	1	2
j	6	7	8	9

Running Time

- # of cells: $O(n^2)$.
- Work per cell: $O(n)$.

RNA Secondary Structure Example

$$m[i][j] = \max\left(m[i][j-1], \max_{i \le t < j-d}\{v_{tj} \cdot (1 + m[i][t-1] + m[t+1][j-1])\}\right)$$

- $B = ACCGGUAGU$ and $d = 4$

i				
4	0	0	0	0
3	0	0	1	1
2	0	0	1	1
1	1	1	1	2
j	6	7	8	9

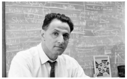
Running Time

- # of cells: $O(n^2)$.
- Work per cell: $O(n)$.
- Overall: $O(n^3)$.

Appendix

References

Image Sources I



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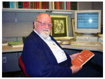

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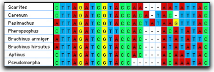

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