

# 6. Dynamic Programming I

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# Algorithmic paradigms

**Greedy.** *Myopically* ordering, making *irrevocable* decisions.

- possibly, *no* natural greedy strategy.

**Divide-and-conquer.** Break up a problem into *independent* sub-problems; solve each subproblem; combine solutions to sub-problems (form solution to original problem).

- Not strong enough: reduce polynomial to faster running time.

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- Not strong enough: reduce polynomial to faster running time.

**Dynamic programming.** Break up a problem into a series of *overlapping* sub-problems; combine solutions to smaller sub-problems (form solution to larger subproblem).

- opposite of greedy: work through all possible global optimal.
  - explores exponentially large space, but not examining explicitly.

# Weighted Interval Scheduling

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Consider  $n$  subjects are sharing a *single* resources.

- job  $j$ : start at  $s_j$  and finish at  $f_j$ 
  - has *weight/value*  $w_j > 0$
- two jobs are **compatible** if they do not overlap

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- two jobs are **compatible** if they do not overlap

**Goal:** find *max-weight* subset of mutually compatible jobs.

	0	1	2	3	4	5	6	7	8	9
9	+	+	+	+	+	+	+			
1	+	+	+	+						
1							+	+	+	+

# Earliest-finish-time-first algorithm

## Earliest-finish-time-first.

- Consider jobs in ascending order of finish time  $f_j$ .
- Add job to subset if it is compatible with previously chosen jobs.

**Recall.** Greedy algorithm is correct if all weights are 1.

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**Recall.** Greedy algorithm is correct if all weights are 1.

**Observation.** Greedy algorithm fails for weighted version.

- goal and progress measure are *unrelated*.
- previous greedy decisions are *irrevocable*.

	0	1	2	3	4	5	6	7	8	9
9	+	+	+	+	+	+	+			
1	+	+	+	+						
1							+	+	+	+



# EFTF extension

**Convention.** Jobs are in ascending order of finish time:  $f_1 \leq f_2 \leq \dots \leq f_n$ .

**Def.**  $p(j)$  = largest index  $i < j$  such that job  $i$  is compatible with  $j$ .

- $i$  is *rightmost* interval that ends before  $j$  begins

	0	1	2	3	4	5	6	7	8	9	$p$
1	+	+	+	+							0
9	+	+	+	+	+	+	+				0
1							+	+	+	+	1

# Dynamic programming: binary choice

**Def.**  $OPT(j)$  = max weight of *any subset* of mutually compatible jobs (for subproblem consisting only of jobs  $1, 2, \dots, j$ ).

**Goal.**  $OPT(n)$  = max weight of *any subset* of mutually compatible jobs.

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**Case 1.**  $OPT(j)$  does not select job  $j$ .

- Optimal solution to *smaller problem*: remaining jobs  $1, 2, \dots, j-1$ .

**Case 2.**  $OPT(j)$  selects job  $j$ .

- Collect profit  $w_j$ .
- Can't use incompatible jobs  $\{p(j) + 1, p(j) + 2, \dots, j-1\}$ .
- Optimal solution to *smaller problem*: remaining compatible jobs  $1, 2, \dots, p(j)$ .

# DP: binary choice (cont.)

**Def.**  $OPT(j)$  = max weight of *any subset* of mutually compatible jobs (for subproblem consisting only of jobs  $1, 2, \dots, j$ ).

**Goal.**  $OPT(n)$  = max weight of *any subset* of mutually compatible jobs.

**Case 1.**  $OPT(j)$  does not select job  $j$ .

**Case 2.**  $OPT(j)$  selects job  $j$ .

**Bellman equation.**

$$OPT(n) = \begin{cases} 0 & \text{if } j = 0 \\ \max\{OPT(j-1), w_j + OPT(p(j))\} & \text{if } j > 0 \end{cases}$$

# Brute-force scheduling

BRUTE-FORCE( $n, s_1, \dots, s_n, f_1, \dots, f_n, w_1, \dots, w_n$ )

1. SORT jobs by finish times and renumber so that  $f_1 \leq f_2 \leq \dots \leq f_n$ ;
2. Compute  $p[1], p[2], \dots, p[n]$  via binary search;
3. RETURN COMPUTE-OPT( $n$ );

COMPUTE-OPT( $j$ )

1. IF ( $j = 0$ ): RETURN 0;
2. ELSE:
  1. RETURN  $\max \{ \text{COMPUTE-OPT}(j-1), w_j + \text{COMPUTE-OPT}(p[j]) \}$ ;

# Quiz: brute-force scheduling

What is running time of `COMPUTE-OPT(n)` in the worst case?

- A.  $\Theta(n \log n)$
- B.  $\Theta(n^2)$
- C.  $\Theta(1.618^n)$
- D.  $\Theta(2^n)$

`COMPUTE-OPT(j)`

1. IF ( $j = 0$ ): RETURN 0;
2. ELSE:
  1. RETURN  $\max \{ \text{COMPUTE-OPT}(j-1), w_j + \text{COMPUTE-OPT}(p[j]) \}$ ;

Discussed next.

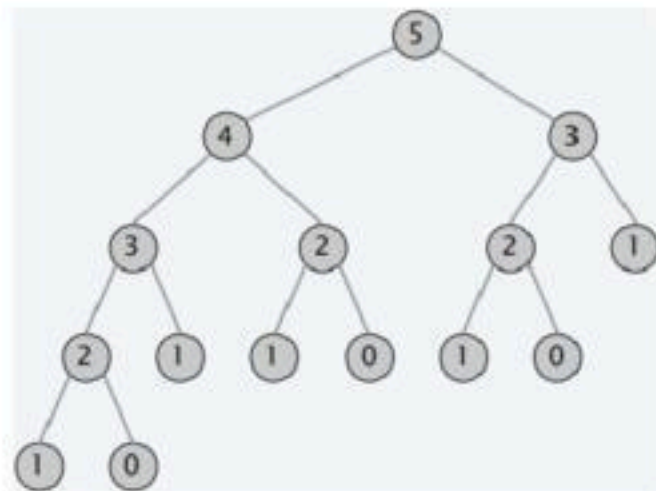


# Brute-force scheduling: analysis

**Observation.** Recursive algorithm is spectacularly slow because of overlapping sub-problems  $\Rightarrow$  *exponential*-time algorithm.

**Ex.** # recursive calls for family of “layered” instances grows like Fibonacci sequence.

0	1	2	3	4	5
+	+	+			
	+	+	+		
		+	+	+	
			+	+	+



**Key insight.** Avoid repeated computations using memory.



# Memoized scheduling

Top-down dynamic programming (memoization).

- Cache result of subproblem  $j$  in  $M[j]$ .
- Use  $M[j]$  to avoid solving subproblem  $j$  more than once.

# Memoized scheduling

## Top-down dynamic programming (memoization).

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TOP-DOWN( $n, s_1, \dots, s_n, f_1, \dots, f_n, w_1, \dots, w_n$ )

1. SORT jobs by finish times and renumber so that  $f_1 \leq f_2 \leq \dots \leq f_n$ ;
2. Compute  $p[1], p[2], \dots, p[n]$  via binary search;
3.  $M[0] = 0$ ;
4. RETURN M-COMPUTE-OPT( $n$ );

M-COMPUTE-OPT( $j$ )

1. IF ( $M[j]$  is uninitialized):
  1.  $M[j] = \max \{ \text{M-COMPUTE-OPT}(j-1), w_j + \text{M-COMPUTE-OPT}(p[j]) \}$ ;
2. RETURN  $M[j]$ ;

# Memoized scheduling: analysis

**Claim.** Memoized version of algorithm takes  $O(n \log n)$  time.

**Pf.**

- Sort by finish time:  $O(n \log n)$ .
- Compute  $p[j]$  for each  $j$ :  $O(n \log n)$  via binary search.
- `M-COMPUTE-OPT`( $j$ ): each invocation takes  $O(1)$  time and either
  - 1. returns an initialized value  $M[j]$
  - 2. initializes  $M[j]$  and makes two recursive calls

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- $M\text{-COMPUTE-OPT}(j)$ : each invocation takes  $O(1)$  time and either
  - 1. returns an initialized value  $M[j]$
  - 2. initializes  $M[j]$  and makes two recursive calls
- Define progress measure  $\Phi$ : # initialized entries among  $M[1..n]$ .
  - initially  $\Phi = 0$ ; throughout  $\Phi \leq n$ .
  - 2. increases  $\Phi$  by 1  $\Rightarrow \leq 2n$  recursive calls.
- Overall running time of  $M\text{-COMPUTE-OPT}(n)$  is  $O(n)$ .

# Memoized scheduling: find a solution

Q. DP algorithm computes optimal *value*. How to find optimal *solution*?

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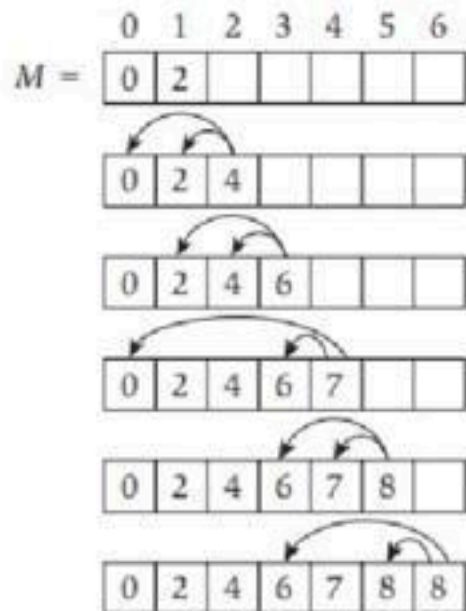
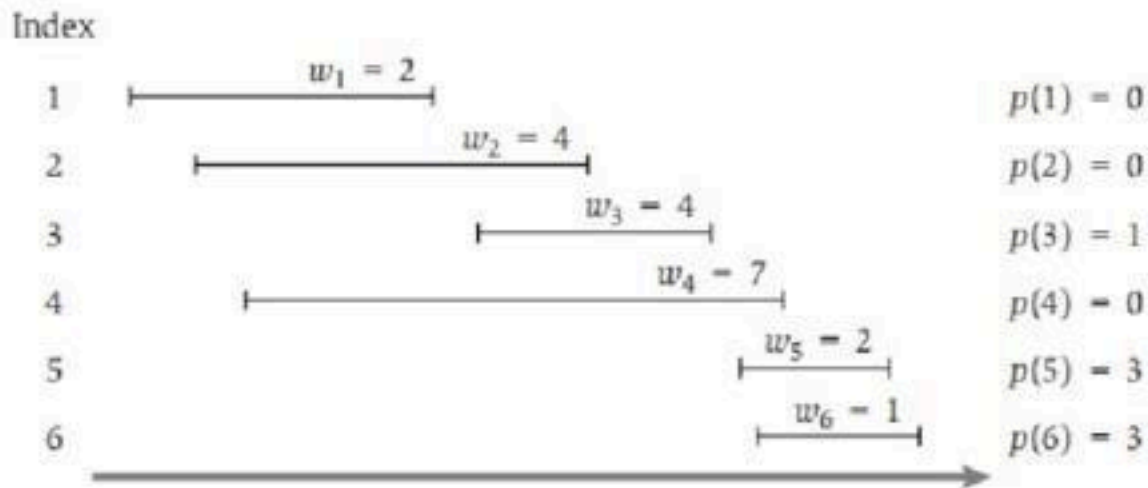
A. Make a second pass, ie., backtrace.

FIND-SOLUTION( $j$ )

1. IF ( $j = 0$ ): RETURN  $\emptyset$ ;
2. ELSE IF ( $w_j + M[p[j]] > M[j-1]$ ):
  1. RETURN  $\{j\} \cup \text{FIND-SOLUTION}(p[j])$ ;
3. ELSE:
  1. RETURN FIND-SOLUTION( $j-1$ );

# Bottom-up DP

Bottom-up dynamic programming. Unwind recursion.



# Bottom-up DP: algorithm

BOTTOM-UP( $n, s_1, \dots, s_n, f_1, \dots, f_n, w_1, \dots, w_n$ )

1. SORT jobs by finish times and renumber so that  $f_1 \leq f_2 \leq \dots \leq f_n$ ;
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4. FOR  $j = 1..n$ :
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# Bottom-up DP: algorithm

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4. FOR  $j = 1..n$ :
  1.  $M[j] = \max\{M[j-1], w_j + M[p[j]]\}$ ;

**Running time.** The bottom-up version takes  $O(n \log n)$  time.

# Maximum Sub-array Problem

**Goal.** Given an array  $x$  of  $n$  integer (positive or negative), find a contiguous sub-array whose sum is maximum.

**Ex.**

sum	12	5	-1	31	-61	59	26	-53	58	97	-93	-23	84	-15	6
187						+	+	+	+	+					

**Applications.** Computer vision, data mining, genomic sequence analysis, technical job interviews, etc.

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**Brute-force algorithm.**

- For each  $i$  and  $j$  : computer  $a[i] + a[i + 1] + \dots + a[j]$ .
- Takes  $\Theta(n^3)$  time.

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**Brute-force algorithm.**

- For each  $i$  and  $j$  : computer  $a[i] + a[i + 1] + \dots + a[j]$ .
- Takes  $\Theta(n^3)$  time.

**Apply “cumulative sum” trick.**

- Pre-compute cumulative sums:  $S[i] = a[0] + a[1] + \dots + a[i]$ .
- Now  $a[i] + a[i + 1] + \dots + a[j] = S[j] - S[i - 1]$ .
- Improves running time  $\Theta(n^2)$ .

# Kadane's algorithm

**Def.**  $OPT(i)$  = max sum of any sub-array of  $x$  whose rightmost index is  $i$ .

**Goal.**  $\max_i OPT(i)$

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**Bellman equation.**

$$OPT(i) = \begin{cases} x_1 & \text{if } i = 1 \\ \max\{x_i, x_i + OPT(i - 1)\} & \text{if } i > 1 \end{cases}$$

- take only element  $i$
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**Running time.**  $O(n)$ .

# Maximum Rectangle Problem

**Goal.** Given an  $n$ -by- $n$  matrix  $A$ , find a rectangle whose sum is maximum.

			+	+	+		
	-2	5	0	-5	-2	2	-3
+	4	-3	-1	3	2	1	-1
+	-5	6	3	-5	-1	-4	-2
+	-1	-1	3	-1	4	1	1
+	3	-3	2	0	3	-3	-2
+	-2	1	-2	1	1	3	-1
+	2	-4	0	1	0	-3	-1

**Applications.** Databases, image processing, maximum likelihood estimation, technical job interviews, etc.



# Bentley's algorithm

**Assumption.** Suppose you knew the left and right column indices  $j$  and  $j'$ .

<hr/>						
$j$			$j'$			
<hr/>						
-2	5	0	-5	-2	2	-3
<hr/>						
4	-3	-1	3	2	1	-1
<hr/>						
-5	6	3	-5	-1	-4	-2
<hr/>						
-1	-1	3	-1	4	1	1
<hr/>						
3	-3	2	0	3	-3	-2
<hr/>						
-2	1	-2	1	1	3	-1
<hr/>						
2	-4	0	1	0	-3	-1
<hr/>						

$x$
<hr/>
-7
<hr/>
4
<hr/>
-3
<hr/>
6
<hr/>
5
<hr/>
0
<hr/>
1
<hr/>

# Bentley's algorithm (cont.)

An  $O(n^3)$  algorithm.

1. Pre-compute cumulative row sums:  $\sum_{k=1}^j A_{ik}$ ;
2. For each  $j < j'$ :
  1. define array  $x$  using row-sum differences:  $x_i = S_{ij'} - S_{ij}$ ;
  2. run Kadane's algorithm in array  $x$ ;

**Open problem.**  $O(n^{3-\epsilon})$  for any constant  $\epsilon > 0$ .

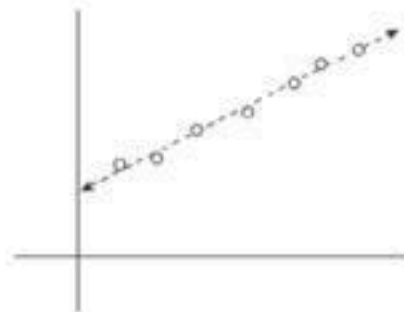
# Segmented least squares

# Least squares

**Least squares.** Foundational problem in statistics.

- Given  $n$  points in the plane:  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ .
- Find a line  $y = ax + b$  that minimizes the sum of the squared error:

$$SSE = \sum_{i=1}^n (y_i - ax_i - b)^2$$

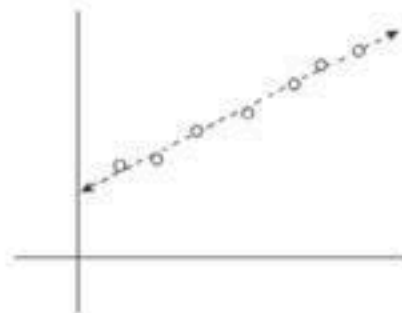


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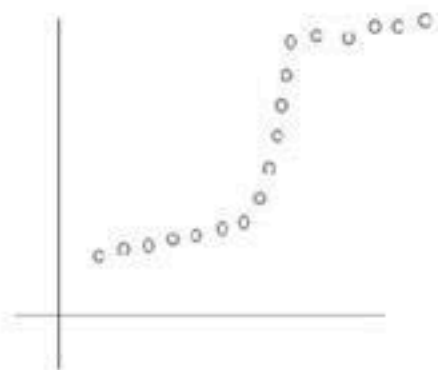
**Solution.** Calculus  $\Rightarrow$  min error is achieved when

$$a = \frac{n \sum_i x_i y_i - (\sum_i x_i)(\sum_i y_i)}{n \sum_i x_i^2 - (\sum_i x_i)^2}, b = \frac{\sum_i y_i - a \sum_i x_i}{n}$$

# Segmented Least Squares Problem

Segmented least squares.

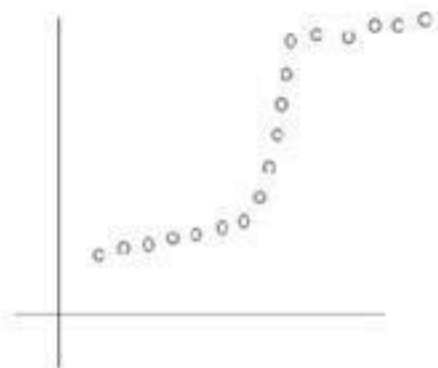
- Points lie roughly on a sequence of line segments.
- Given  $n$  points in the plane:  
 $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$  with  $x_1 < x_2 < \dots < x_n$ ,  
find a *sequence of lines* that minimizes  $f(x)$ .



# Segmented Least Squares Problem

## Segmented least squares.

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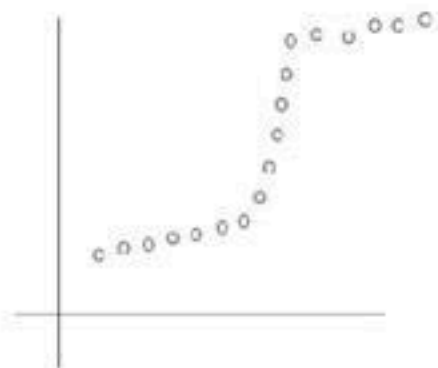
**Q.** What is a reasonable choice for  $f(x)$  to balance *accuracy* and *parsimony*?

- goodness of fit vs. number of lines

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find a *sequence of lines* that minimizes  $f(x)$ .



**Q.** What is a reasonable choice for  $f(x)$  to balance *accuracy* and *parsimony*?

- goodness of fit vs. number of lines

**Goal.** Minimize  $f(x) = E + cL$  for some constant  $c > 0$ , where

- $E$  = sum of SSEs in each segment.
- $L$  = number of lines.



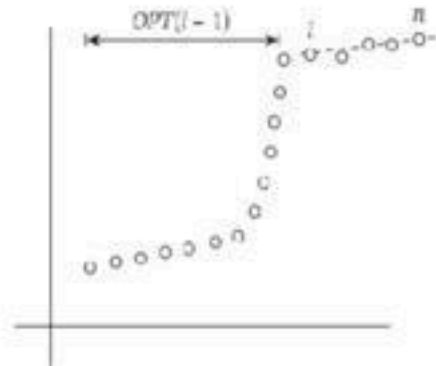
# Dynamic programming: multi-way choice

## Notation.

- $OPT(j)$  = minimum cost for points  $p_1, p_2, \dots, p_j$ .
- $e_{ij}$  = SSE for for points  $p_i, p_{i+1}, \dots, p_j$ .

## To compute $OPT(j)$ :

- Last segment uses points  $p_i, p_{i+1}, \dots, p_j$  for some  $i \leq j$ .
- Cost =  $e_{ij} + c + OPT(i-1)$ .



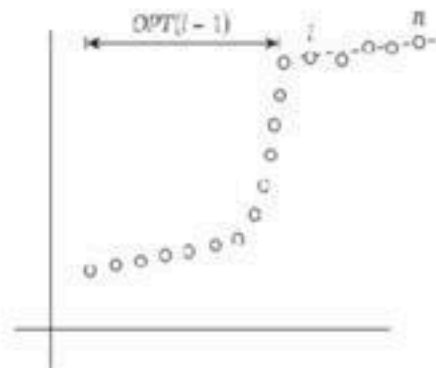
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## Bellman equation.

$$OPT(j) = \begin{cases} 0 & \text{if } j = 0 \\ \min_{1 \leq i \leq j} \{e_{ij} + c + OPT(i-1)\} & \text{if } j > 0 \end{cases}$$

# Segmented Least Squares: algorithm

SEGMENTED-LEAST-SQUARES( $n, p_1, \dots, p_n, c$ )

1. FOR  $j = 1..n$ :
  1. FOR  $i = 1..j$ :
    1. Compute the SSE  $e_{ij}$  for the points  $p_i, p_{i+1}, \dots, p_j$ ;
  2.  $M[0] = 0$ ;
  3. FOR  $j = 1..n$ :
    1.  $M[j] = \min_{1 \leq i \leq j} \{e_{ij} + c + M[i - 1]\}$ ;
4. RETURN  $M[n]$ ;

# Segmented Least Squares: analysis

**Theorem.** [Bellman 1961] DP algorithm solves the segmented least squares problem in  $O(n^3)$  time and  $O(n^2)$  space.

**Pf.**

- Bottleneck = computing SSE  $e_{ij}$  for each  $i$  and  $j$ .

$$a_{ij} = \frac{n \sum_k x_k y_k - (\sum_k x_k)(\sum_k y_k)}{n \sum_k x_k^2 - (\sum_k x_k)^2}, b_{ij} = \frac{\sum_k y_k - a_{ij} \sum_k x_k}{n}$$

- $O(n)$  to compute  $e_{ij}$ .

**Remark.** Can be improved to  $O(n^2)$  time.

- For each  $i$ : pre-compute cumulative sums:  $\sum_k x_k, \sum_k y_k, \sum_k x_k^2, \sum_k x_k y_k$
- Using cumulative sums, can compute  $e_{ij}$  in  $O(1)$  time.

# Knapsack problem

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**Goal.** Pack knapsack so as to maximize total value of items taken.

- There are  $n$  items: item  $i$  provides value  $v_i > 0$  and weighs  $w_i > 0$ .
- Value of a subset of items = sum of values of individual items.
- Knapsack has weight limit of  $W$ .

**Assumption.** All values and weights are integral.

**Ex.** The subset  $\{ 1, 2, 5 \}$  has value 35 (and weight 10).

**Ex.** The subset  $\{ 3, 4 \}$  has value 40 (and weight 11).

$i$	1	2	3	4	5
$v_i$	1	6	18	22	28
$w_i$	1	2	5	6	7

weight limit  $W = 11$

# Quiz: Knapsack via greedy

Which algorithm solves knapsack problem?

- A. Greedy-by-value: repeatedly add item with maximum  $v_i$ .
- B. Greedy-by-weight: repeatedly add item with minimum  $w_i$ .
- C. Greedy-by-ratio: repeatedly add item with maximum ratio  $v_i/w_i$ .
- D. None of the above.

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# Quiz: Knapsack via DP

Which sub-problems?

- A.  $OPT(w)$  = optimal value of knapsack problem with weight limit  $w$ .
- B.  $OPT(i)$  = optimal value of knapsack problem with items  $1, \dots, i$ .
- C.  $OPT(i, w)$  = optimal value of knapsack problem with items  $1, \dots, i$  subject to weight limit  $W$ .
- D. Any of the above.



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- C.**  $OPT(i, w)$  = optimal value of knapsack problem with items  $1, \dots, i$  subject to weight limit  $W$ .
- D.** Any of the above.

A/B: not eliminating any conflict, thus reduce to brute-force.

# Dynamic programming: two variables

**Def.**  $OPT(i, w)$  = optimal value of knapsack problem with items  $1, \dots, i$ , subject to weight limit  $w$ .

**Goal.**  $OPT(n, W)$ .

# Dynamic programming: two variables

**Def.**  $OPT(i, w)$  = optimal value of knapsack problem with items  $1, \dots, i$ , subject to weight limit  $w$ .

**Goal.**  $OPT(n, W)$ .

**Case 1.**  $OPT(i, w)$  does not select item  $i$ .

- $OPT(i, w)$  selects best of  $\{1, 2, \dots, i-1\}$  subject to weight limit  $w$ .

**Case 2.**  $OPT(i, w)$  selects item  $i$ .

- Collect value  $v_i$ .
- New weight limit =  $w - w_i$ .
- $OPT(i, w)$  selects best of  $\{1, 2, \dots, i-1\}$  subject to new weight limit.

# DP: two variables (cont.)

**Def.**  $OPT(i, w)$  = optimal value of knapsack problem with items  $1, \dots, i$ , subject to weight limit  $w$ .

**Goal.**  $OPT(n, W)$ .

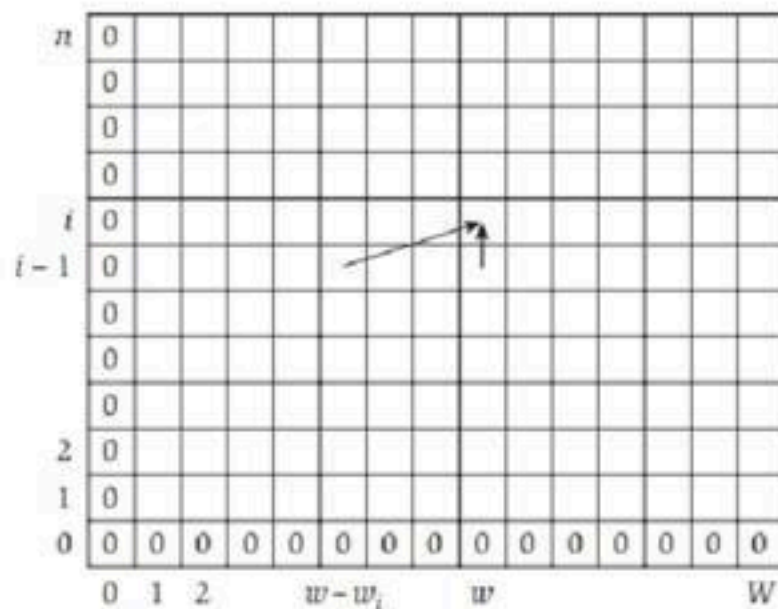
**Case 1.**  $OPT(i, w)$  does not select item  $i$ .

**Case 2.**  $OPT(i, w)$  selects item  $i$ .

**Bellman equation.**

$$OPT(i, w) = \begin{cases} 0 & \text{if } i = 0 \\ OPT(i - 1, w) & \text{if } w_i > w \\ \max\{OPT(i - 1, w), v_i + OPT(i - 1, w - w_i)\} & \text{otherwise} \end{cases}$$

# DP: two-dimensional table



$$OPT(i, w) = \begin{cases} 0 & \text{if } i = 0 \\ OPT(i-1, w) & \text{if } w_i > w \\ \max\{OPT(i-1, w), v_i + OPT(i-1, w - w_i)\} & \text{otherwise} \end{cases}$$

# Knapsack problem: bottom-up DP

$\text{KNAPSACK}(n, W, w_1, \dots, w_n, v_1, \dots, v_n)$

1. FOR  $w = 0..W$ :  $M[0, w] = 0$ ;
2. FOR  $i = 1..n$ :
  1. FOR  $w = 0..W$ :
    1. IF  $(w_i > w)$ :  $M[i, w] = M[i-1, w]$ ;
    2. ELSE:  $M[i, w] = \max\{M[i-1, w], v_i + M[i-1, w-w_i]\}$ ;
3. RETURN  $M[n, W]$ ;

$$\text{OPT}(i, w) = \begin{cases} 0 & \text{if } i = 0 \\ \text{OPT}(i-1, w) & \text{if } w_i > w \\ \max\{\text{OPT}(i-1, w), v_i + \text{OPT}(i-1, w-w_i)\} & \text{otherwise} \end{cases}$$

# Knapsack problem: bottom-up DP demo

Knapsack size  $W = 6$ , 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

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

Filling in values for  $i = 1$

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
	0	1	2	3	4	5	6

Filling in values for  $i = 2$

3							
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
	0	1	2	3	4	5	6

Filling in values for  $i = 3$

$$OPT(i, w) = \begin{cases} 0 & \text{if } i = 0 \\ OPT(i - 1, w) & \text{if } w_i > w \\ \max\{OPT(i - 1, w), v_i + OPT(i - 1, w - w_i)\} & \text{otherwise} \end{cases}$$

# Knapsack problem: analysis

**Theorem.** The DP algorithm solves the knapsack problem with  $n$  items and maximum weight  $W$  in  $\Theta(nW)$  time and  $\Theta(nW)$  space.

**Pf.**

- Takes  $O(1)$  time per table entry.
- There are  $\Theta(nW)$  table entries.
- After computing optimal values, can trace back to find solution:
  - $OPT(i, w)$  takes item  $i$  iff  $M[i, w] > M[i-1, w]$ .

**Remarks.**

- Algorithm depends critically on assumption that weights are *integral*.
  - weights are integers between 1 and  $W$



# Coin changing: revisit

**Problem.** Given  $n$  coin denominations  $\{d_1, d_2, \dots, d_n\}$  and a target value  $V$ , find the fewest coins needed to make change for  $V$  (or report impossible).

**Recall.** Greedy cashier's algorithm is optimal for U.S. coin denominations, but not for arbitrary coin denominations.

**Ex.**  $\{1, 10, 21, 34, 70, 100, 350, 1295, 1500\}$ .

**Optimal.**  $140\text{¢} = 70 + 70$ .

# Coin changing: DP solution

**Def.**  $OPT(v)$  = min number of coins to make change for  $v$ .

**Goal.**  $OPT(V)$ .

**Multiway choice.** To compute  $OPT(v)$ ,

- Select a coin of denomination  $c_i$  for some  $i$ .
- Select fewest coins to make change for  $v - c_i$ .

**Bellman equation.**

$$OPT(v) = \begin{cases} \infty & \text{if } v < 0 \\ 0 & \text{if } v = 0 \\ \min_{1 \leq i \leq n} \{1 + OPT(v - d_i)\} & \text{if } v > 0 \end{cases}$$

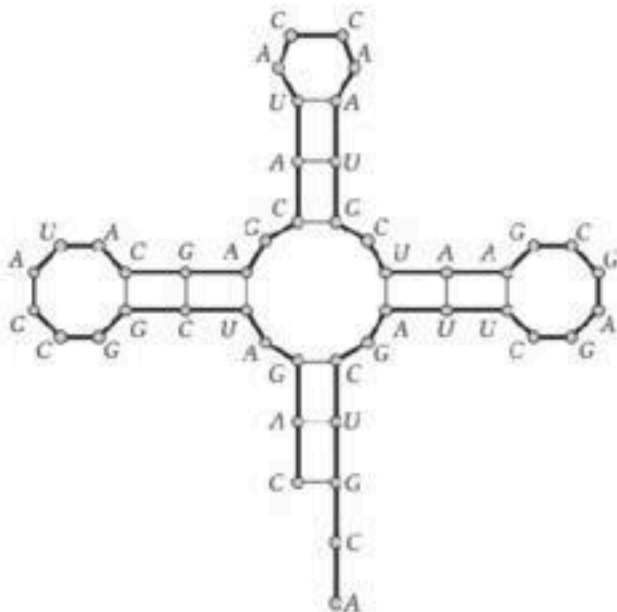
≡ **Running time.**  $O(nV)$ .

# RNA secondary structure

# RNA secondary structure

**RNA.** String  $B = b_1 b_2 \dots b_n$  over alphabet  $\{A, C, G, U\}$ .

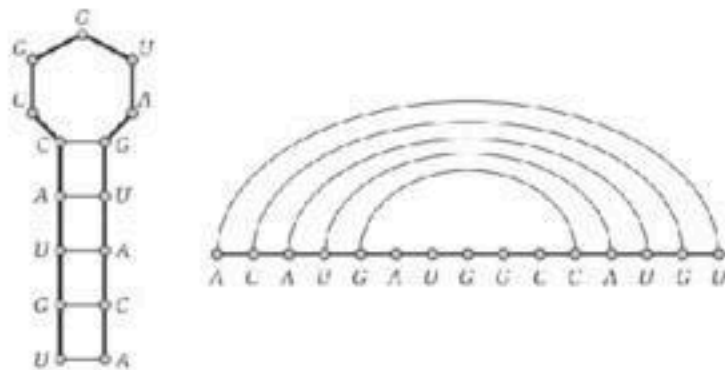
**Secondary structure.** RNA is single-stranded so it tends to loop back and form *base pairs* with itself. This structure is essential for understanding behavior of molecule.



# RNA: matching rule

**Secondary structure.** A set of pairs  $S = \{(b_i, b_j)\}$  that satisfy:

- [Watson–Crick]  $S$  is a matching and each pair in  $S$  is a Watson–Crick complement: A–U, U–A, C–G, or G–C.
- [No sharp turns] The ends of each pair are separated by at least 4 intervening bases. If  $(b_i, b_j) \in S$ , then  $i < j-4$ .
- [Non-crossing] If  $(b_i, b_j)$  and  $(b_k, b_l)$  are two pairs in  $S$ , then we cannot have  $i < k < j < l$ .



# RNA: hypothesis

**Secondary structure.** A set of pairs  $S = \{(b_i, b_j)\}$  that satisfy:

- [Watson–Crick]  $S$  is a matching and each pair in  $S$  is a Watson–Crick complement: A–U, U–A, C–G, or G–C.
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- [Non-crossing] If  $(b_i, b_j)$  and  $(b_k, b_l)$  are two pairs in  $S$ , then we cannot have  $i < k < j < l$ .

**Free-energy hypothesis.** RNA molecule will form secondary structure with *minimum total free energy*.

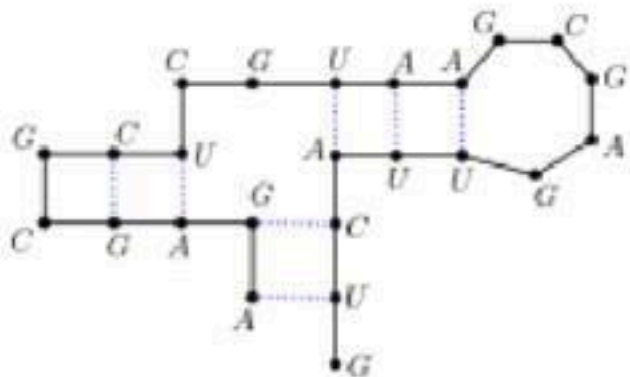
- approximate by # base pairs: more base pairs  $\Rightarrow$  lower free energy

**Goal.** Given an RNA molecule  $B = b_1 b_2 \dots b_n$ , find a secondary structure  $S$  that maximizes number of base pairs.

# Quiz: matching rule

Is the following a secondary structure?

- A. Yes.
- B. No, violates Watson–Crick condition.
- C. No, violates no-sharp-turns condition.
- D. No, violates no-crossing condition.



# Quiz: RNA secondary structure

Which sub-problems?

- A.  $OPT(j)$  = max number of base pairs in secondary structure of the substring  $b_1b_2 \dots b_j$ .
- B.  $OPT(j)$  = max number of base pairs in secondary structure of the substring  $b_jb_{j+1} \dots b_n$ .
- C. Either A or B.
- D. Neither A nor B.

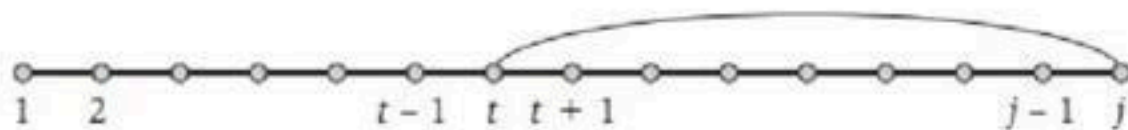


# RNA secondary structure: sub-problems

**First attempt.**  $OPT(j) = \max$  number of base pairs in secondary structure of the substring  $b_1b_2 \dots b_j$ .

**Goal.**  $OPT(n)$ .

**Choice.** Match bases  $b_t$  and  $b_j$ .

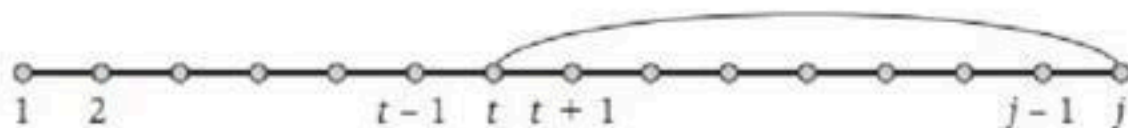


# RNA secondary structure: sub-problems

**First attempt.**  $OPT(j) = \max$  number of base pairs in secondary structure of the substring  $b_1b_2 \dots b_j$ .

**Goal.**  $OPT(n)$ .

**Choice.** Match bases  $b_t$  and  $b_j$ .



**Difficulty.** Results in two sub-problems (but one of wrong form).

- Find secondary structure in  $b_1b_2 \dots b_{t-1}$ :  $OPT(t-1)$ .
- Find secondary structure in  $b_{t+1}b_{t+2} \dots b_{j-1}$ .
  - break sub-structure: first base no longer  $b_1$

# DP: intervals

**Def.**  $OPT(i, j)$  = maximum number of base pairs in a secondary structure of the substring  $b_i b_{i+1} \dots b_j$ .

**Case 1.** If  $i \geq j-4$ .

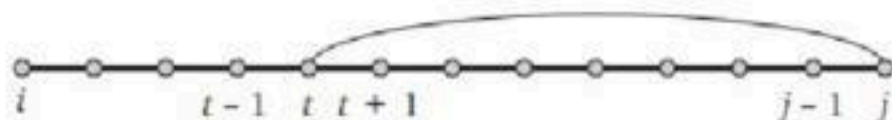
- $OPT(i, j) = 0$  by no-sharp-turns condition.

**Case 2.** Base  $b_j$  is not involved in a pair.

- $OPT(i, j) = OPT(i, j-1)$ .

**Case 3.** Base  $b_j$  pairs with  $b_t$  for some  $i \leq t < j-4$ .

- Non-crossing condition decouples resulting two sub-problems.
  - $OPT(i, j) = 1 + \max_t OPT(i, t-1) + OPT(t+1, j-1)$ .



# Quiz: DP for RNA

In which order to compute  $OPT(i, j)$ ?

- A. Increasing  $i$ , then  $j$ .
- B. Increasing  $j$ , then  $i$ .
- C. Either **A** or **B**.
- D. Neither **A** nor **B**.

# Quiz: DP for RNA

In which order to compute  $OPT(i, j)$ ?

- A. Increasing  $i$ , then  $j$ .
- B. Increasing  $j$ , then  $i$ .
- C. Either **A** or **B**.
- D. Neither **A** nor **B**.

B

# Bottom-up DP over intervals

Q. In which order to solve the sub-problems?

A. Do shortest intervals first—increasing order of  $|j - i|$ .

Ex. RNA sequence ACCGGUAGU.

4	0	0	0	
3	0	0		
2	0			
$i = 1$				

$j = 6 \ 7 \ 8 \ 9$   
Initial values

4	0	0	0	0
3	0	0	1	
2	0	0		
$i = 1$	1			

$j = 6 \ 7 \ 8 \ 9$   
Filling in the values  
for  $k = 5$

4	0	0	0	0
3	0	0	1	1
2	0	0	1	
$i = 1$	1	1		

$j = 6 \ 7 \ 8 \ 9$   
Filling in the values  
for  $k = 6$

4	0	0	0	0
3	0	0	1	1
2	0	0	1	1
$i = 1$	1	1	1	

$j = 6 \ 7 \ 8 \ 9$   
Filling in the values  
for  $k = 7$

4	0	0	0	0
3	0	0	1	1
2	0	0	1	1
$i = 1$	1	1	1	2

$j = 6 \ 7 \ 8 \ 9$   
Filling in the values  
for  $k = 8$

# DP for RNA: algorithm

RNA-SECONDARY-STRUCTURE( $n, b_1, \dots, b_n$ )

1. FOR  $k = 5..n-1$ :
  1. FOR  $i = 1..n-k$ :
    1.  $j = i + k$ ;
    2. Compute  $M[i, j]$  using formula;
2. RETURN  $M[1, n]$ ;

**Theorem.** The DP algorithm solves the RNA secondary structure problem in  $O(n^3)$  time and  $O(n^2)$  space.

# Dynamic programming summary

## Outline.

- Define a collection of (polynomial number of) sub-problems.
- Solution to original problem can be computed from sub-problems.
- Natural ordering of sub-problems from “smallest” to “largest” that enables determining a solution to a subproblem from solutions to smaller sub-problems.

## Techniques.

- Binary choice: weighted interval scheduling.
- Multi-way choice: segmented least squares.
- Adding a new variable: knapsack problem.
- Intervals: RNA secondary structure.

**Top-down vs. bottom-up DP.** recursive vs. iterative.