### Dynamic Programming\*

#### Xiaofeng Gao

Department of Computer Science and Engineering Shanghai Jiao Tong University, P.R.China

Algorithm Course: Shanghai Jiao Tong University

Algorithm Course @SJTU Xiaofeng Gao Dynamic Programming 1/2

<sup>\*</sup>Special thanks is given to *Prof. Kevin Wayne@Princeton* for sharing his slides, and also given to Mr. Chao Wang from CS2014@SJTU and Mr. Hongjian Cao from CS2015@SJTU for producing this lecture.

#### Outline

- Introduction
  - Background
  - Introductory Example: Weighted Interval Scheduling
- Popular Recipes
  - Segmented Least Squares
  - Knapsack Problem
  - RNA Secondary Structure
- 3 Hirschberg's Alignment Algorithm
  - String Similarity
  - Sequence Alignment in Linear Space

#### Outline

- Introduction
  - Background
  - Introductory Example: Weighted Interval Scheduling
- 2 Popular Recipes
  - Segmented Least Squares
  - Knapsack Problem
  - RNA Secondary Structure
- 3 Hirschberg's Alignment Algorithm
  - String Similarity
  - Sequence Alignment in Linear Space

## Algorithmic Paradigms

**Greedy:** Build up a solution incrementally, myopically optimizing some local criterion.

**Divide-and-conquer:** Break up a problem into sub-problems, solve each sub-problem independently, and combine solution to sub-problems to form solution to original problem.

**Dynamic programming:** Break up a problem into a series of overlapping sub-problems, and build up solutions to larger and larger sub-problems.

### History

**Richard E. Bellman (1920-1984)**: Pioneered the systematic study of dynamic programming in 1950s.

#### **Etymology:**

- Dynamic programming = planning over time
- Secretary of Defense had pathological fear of mathematical research.
- Bellman sought a "dynamic" adjective to avoid conflict.



### **Applications**

**Areas:** Bioinformatics, Control Theory, Information Theory, Operations Research, Computer Science (Theory, Graphics, AI, Compilers, Systems, ...)

#### **Some Famous Algorithms**

- Avidan-Shamir for seam carving.
- Unix diff for comparing two files.
- Viterbi for hidden Markov models.
- De Boor for evaluating spline curves.
- Knuth-Plass for word wrapping text in T<sub>E</sub>X.
- o Smith-Waterman for genetic sequence alignment.
- o Bellman-Ford-Moore for shortest path routing in networks.
- Cocke-Kasami-Younger for parsing context free grammars.
- Needleman-Wunsch/Smith-Waterman for sequence alignment.



6/59

### **Dynamic Programming Books**











































#### Outline

- Introduction
  - Background
  - Introductory Example: Weighted Interval Scheduling
- 2 Popular Recipes
  - Segmented Least Squares
  - Knapsack Problem
  - RNA Secondary Structure
- 3 Hirschberg's Alignment Algorithm
  - String Similarity
  - Sequence Alignment in Linear Space

### Weighted Interval Scheduling Problem

Job j starts at  $s_j$ , finishes at  $f_j$ , and has weight or value  $w_j > 0$ .

Two jobs are compatible if they don't overlap.

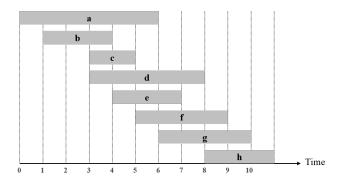
**Goal:** find maximum weight subset of mutually compatible jobs.

### Weighted Interval Scheduling Problem

Job j starts at  $s_j$ , finishes at  $f_j$ , and has weight or value  $w_j > 0$ .

Two jobs are compatible if they don't overlap.

Goal: find maximum weight subset of mutually compatible jobs.



### Unweighted Interval Scheduling Review

**Recall:** Greedy algorithm works if all weights are 1.

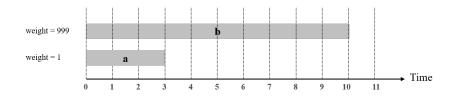
- o Consider jobs in ascending order of finish time.
- Add job to subset if it is compatible with previously chosen jobs.

## Unweighted Interval Scheduling Review

**Recall:** Greedy algorithm works if all weights are 1.

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

**Observation:** Greedy algorithm can fail spectacularly if arbitrary weights are allowed.



## Weighted Interval Scheduling

**Notation:** Label jobs by finishing time:  $f_1 \le f_2 \le \cdots \le f_n$ .

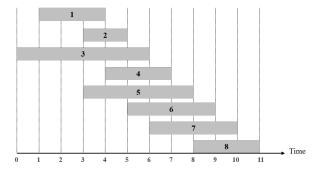
**Definition:** p(j) = largest index i < j such that job i is compatible with j.

# Weighted Interval Scheduling

**Notation:** Label jobs by finishing time:  $f_1 \le f_2 \le \cdots \le f_n$ .

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

**Example:** p(8) = 5, p(7) = 3, p(2) = 0.



### **Binary Choice**

**Recurrence template:** OPT(j) = value of optimal solution to the problem consisting of job requests  $1, 2, \dots, j$ .

### Binary Choice

**Recurrence template:** OPT(j) = value of optimal solution to the problem consisting of job requests  $1, 2, \dots, j$ .

#### **Optimal substructure:**

- Case 1: OPT selects job *j*.
  - collect weight  $w_i$ ,
  - o can't use incompatible jobs  $\{p(j) + 1, p(j) + 2, \dots, j 1\},\$
  - must include optimal solution to problem consisting of remaining compatible jobs  $1, 2, \dots, p(j)$ .
- Case 2: OPT does not select job *j*.
  - must include optimal solution to problem consisting of remaining compatible jobs  $1, 2, \dots, j-1$ .

### **Binary Choice**

**Recurrence template:** OPT(j) = value of optimal solution to the problem consisting of job requests  $1, 2, \dots, j$ .

#### **Optimal substructure:**

Case 1: OPT selects job *j*.

- collect weight  $w_i$ ,
- o can't use incompatible jobs  $\{p(j) + 1, p(j) + 2, \dots, j 1\},\$
- must include optimal solution to problem consisting of remaining compatible jobs  $1, 2, \dots, p(j)$ .

Case 2: OPT does not select job *j*.

• must include optimal solution to problem consisting of remaining compatible jobs  $1, 2, \dots, j-1$ .

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

Algorithm Course@SJTU Xiaofeng Gao Dynamic Programming 12/59

### Brute Force Algorithm

### **Algorithm 1:** Weighted Interval Scheduling – Brute Force

```
Input: n; s_1, \dots, s_n; f_1, \dots, f_n; w_1, \dots, w_n; Output: Optimal weight OPT(n).
```

- 1 Sort jobs by finish times so that  $f_1 \le f_2 \le \cdots \le f_n$ ;
- **2** Compute  $p(1), p(2), \dots, p(n)$ ;
- 3 return B-Sched(n);

#### **Algorithm 2:** B-Sched (j)

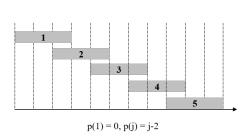
```
1 if j = 0 then
2 | return 0;
3 else
```

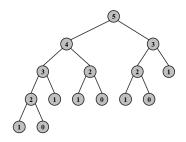
**return**  $\max\{w_j + B - Sched(p(j)), B - Sched(j-1)\};$ 

### Brute Force Algorithm

**Observation:** Recursive algorithm fails spectacularly because of redundant sub-problems  $\Rightarrow$  exponential algorithms.

**Example:** Number of recursive calls for family of "layered" instances grows like Fibonacci sequence.





### Memoization: Store sub-results in cache; lookup as needed

#### **Algorithm 3:** Weighted Interval Scheduling – Memoization

```
Input: n; s_1, \dots, s_n; f_1, \dots, f_n; w_1, \dots, w_n; Output: Optimal weight OPT(n).
```

- 1 Sort jobs by finish times so that  $f_1 \le f_2 \le \cdots \le f_n$ ;
- **2** Compute  $p(1), p(2), \dots, p(n)$ ;
- 3 M[0] = 0; // global array
- 4 return M-Sched (n);

#### **Algorithm 4:** M-Sched (j)

- 1 if M[j] is uninitialized then
- $\mathbf{2} \quad | \quad M[j] = \max\{w_j + \mathbf{M} \mathbf{Sched}(p(j)), \mathbf{M} \mathbf{Sched}(j-1)\};$
- 3 return M[j];



### **Running Time**

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

- Sort by finish time:  $O(n \log n)$ .
- Computing  $p(\cdot)$ :  $O(n \log n)$  via sorting by start time.
- M-Sched(j): each invocation takes O(1) time and either
  - (1) returns an existing value M[j]
  - (2) initializes M[j] and makes two recursive calls
- Progress measure  $\Phi =$  number nonempty entries of  $M[\cdot]$ .
  - $\triangleright$  initially  $\Phi = 0$ , throughout  $\Phi \le n$ .
  - $\triangleright$  (2) increases  $\Phi$  by  $1 \Rightarrow$  at most 2n recursive calls.
- Overall running time of M-Sched(n) is O(n).

### **Running Time**

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

- Sort by finish time:  $O(n \log n)$ .
- Computing  $p(\cdot)$ :  $O(n \log n)$  via sorting by start time.
- M-Sched(j): each invocation takes O(1) time and either
  - (1) returns an existing value M[j]
  - (2) initializes M[j] and makes two recursive calls
- Progress measure  $\Phi =$  number nonempty entries of  $M[\cdot]$ .
  - $\triangleright$  initially  $\Phi = 0$ , throughout  $\Phi \le n$ .
  - $\triangleright$  (2) increases  $\Phi$  by  $1 \Rightarrow$  at most 2n recursive calls.
- Overall running time of M-Sched(n) is O(n).

**Remark:** O(n) if jobs are pre-sorted by start and finish times.



## Finding a Solution from the OPT Value

```
Algorithm 5: Find-Solution (j)

if j=0 then

| return \emptyset; 

selse if w_j + M[p(j)] > M[j-1] then

| return \{j\} \cup Find-Solution (p(j)); 

selse

| return Find-Solution (j-1);
```

### Finding a Solution from the OPT Value

```
Algorithm 5: Find-Solution (j)

if j=0 then

| return \emptyset; 

selse if w_j + M[p(j)] > M[j-1] then

| return \{j\} \cup Find-Solution (p(j)); 

selse

| return Find-Solution (j-1);
```

- Run Find-Solution(*n*) to find optimal schedule;
- # of recursive calls  $1 \le n \Rightarrow O(n)$ ;

## Tabulation: Bottom-Up Dynamic Programming

#### Algorithm 6: Weighted Interval Scheduling – Tabulation

```
Input: n; s_1, \dots, s_n; f_1, \dots, f_n; w_1, \dots, w_n;
```

**Output:** Optimal weight OPT(n).

- 1 Sort jobs by finish times so that  $f_1 \le f_2 \le \cdots \le f_n$ ;
- 2 Compute  $p(1), p(2), \dots, p(n)$ ;
- M[0] = 0;
- 4 for  $j = 1 \rightarrow n$  do
- 5  $M[j] = \max\{w_j + M[p(j)], M[j-1]\};$

## Tabulation: Bottom-Up Dynamic Programming

#### Algorithm 6: Weighted Interval Scheduling – Tabulation

```
Input: n; s_1, \dots, s_n; f_1, \dots, f_n; w_1, \dots, w_n;
```

**Output:** Optimal weight OPT(n).

- 1 Sort jobs by finish times so that  $f_1 \le f_2 \le \cdots \le f_n$ ;
- 2 Compute  $p(1), p(2), \dots, p(n)$ ;
- M[0] = 0;
- 4 for  $j = 1 \rightarrow n$  do
- 5  $M[j] = \max\{w_j + M[p(j)], M[j-1]\};$

**Running Time**:  $O(n \log n)$ .



# Tabulation: Bottom-Up Dynamic Programming

#### Algorithm 6: Weighted Interval Scheduling – Tabulation

**Input:** 
$$n$$
;  $s_1, \dots, s_n$ ;  $f_1, \dots, f_n$ ;  $w_1, \dots, w_n$ ;

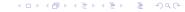
**Output:** Optimal weight OPT(n).

- 1 Sort jobs by finish times so that  $f_1 \le f_2 \le \cdots \le f_n$ ;
- 2 Compute  $p(1), p(2), \dots, p(n)$ ;
- M[0] = 0;
- 4 for  $j = 1 \rightarrow n$  do
- 5  $M[j] = \max\{w_j + M[p(j)], M[j-1]\};$

**Running Time**:  $O(n \log n)$ .

Those who cannot remember the past are condemned to repeat it.

— Kevin Wayne@Princeton

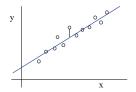


Algorithm Course@SJTU

#### Outline

- Introduction
  - Background
  - Introductory Example: Weighted Interval Scheduling
- Popular Recipes
  - Segmented Least Squares
  - Knapsack Problem
  - RNA Secondary Structure
- 3 Hirschberg's Alignment Algorithm
  - String Similarity
  - Sequence Alignment in Linear Space

- Foundational problem in statistic and numerical analysis.
- Given *n* points in the plane:  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ .
- $\circ$  Find a line y = ax + b to minimize the sum of the squared error:



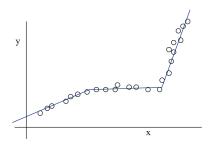
**Solution:** Calculus  $\Rightarrow$  min error is achieved when

$$a = \frac{n \sum_{i} x_{i} y_{i} - (\sum_{i} x_{i})(\sum_{i} y_{i})}{n \sum_{i} x_{i}^{2} - (\sum_{i} x_{i})^{2}}, b = \frac{\sum_{i} y_{i} - a \sum_{i} x_{i}}{n}$$

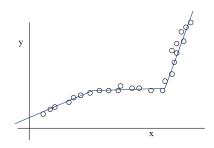


- Points lie roughly on a sequence of several line segments.
- Given *n* points in the plane:  $(x_1, y_1)$ ,  $(x_2, y_2)$ ,  $\cdots$ ,  $(x_n, y_n)$  with  $x_1 < x_2 < \cdots < x_n$ , find a sequence of lines that minimizes f(x).

Question: What's a reasonable choice for f(x) to balance accuracy (goodness of fit) and parsimony (number of lines)?



- Points lie roughly on a sequence of several line segments.
- Given *n* points in the plane:  $(x_1, y_1)$ ,  $(x_2, y_2)$ ,  $\cdots$ ,  $(x_n, y_n)$  with  $x_1 < x_2 < \cdots < x_n$ , find a sequence of lines that minimizes:
  - $\triangleright$  the sum of the sums of the squared errors E in each segment
  - $\triangleright$  the number of lines L
- Tradeoff function: E + cL, for some constant c > 0.



## Multiway Choice

#### **Notation:**

- $OPT(j) = \text{minimum cost for points } p_1, p_{i+1}, \cdots, p_j$ .
- $e(i,j) = \text{minimum sum of squares for points } p_i, p_{i+1}, \cdots, p_j$ .

#### Compute OPT(j):

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

$$OPT(j) = \begin{cases} 0, & j = 0, \\ \min_{1 \le i \le j} \{e(i,j) + c + OPT(i-1)\}, & otherwise \end{cases}$$

#### **Algorithm 7:** Segmented Square Error (SSE)

**Input:**  $n; p_1, \cdots, p_n; c;$ 

**Output:** Optimal square error for  $p_1, \dots, p_n$ .

- 1 for  $j = 1 \rightarrow n$  do
- 2 | for  $i = 1 \rightarrow j$  do
- 3 compute least square error  $e_{ij}$  for segment  $p_i, \dots, p_j$ ;
- 4 M[0] = 0;
- 5 for  $j = 1 \rightarrow n$  do
- 6  $M[j] = \min_{1 \le i \le j} \{e_{ij} + c + M[i-1]\};$
- 7 return M[n];

#### **Algorithm 7:** Segmented Square Error (SSE)

```
Input: n; p_1, \cdots, p_n; c;
```

**Output:** Optimal square error for  $p_1, \dots, p_n$ .

```
\begin{array}{c|c} \mathbf{1} & \mathbf{for} \ j = 1 \to n \ \mathbf{do} \\ \mathbf{2} & \mathbf{for} \ i = 1 \to j \ \mathbf{do} \\ \mathbf{3} & \mathbf{compute} \ \text{least square error} \ e_{ij} \ \text{for segment} \ p_i, \cdots, p_j; \end{array}
```

4 
$$M[0] = 0$$
;

5 for 
$$j = 1 \rightarrow n$$
 do

6 
$$M[j] = \min_{1 \le i \le j} \{e_{ij} + c + M[i-1]\};$$

7 return 
$$M[n]$$
;

**Time Complexity**:  $O(n^3)$  (can be improved to  $O(n^2)$ )

**Space Complexity**:  $O(n^2)$ .



## Algorithm Analysis

**Theorem** (Bellman, 1961) SSE solves the segmented least squares problem in  $O(n^3)$  time and  $O(n^2)$  space.

## Algorithm Analysis

**Theorem** (Bellman, 1961) SSE solves the segmented least squares problem in  $O(n^3)$  time and  $O(n^2)$  space.

**Proof**: Bottleneck = computing  $e_{ij}$  for  $O(n^2)$  pairs,

$$a = \frac{n \sum_{i} x_{i} y_{i} - (\sum_{i} x_{i})(\sum_{i} y_{i})}{n \sum_{i} x_{i}^{2} - (\sum_{i} x_{i})^{2}}, \ b = \frac{\sum_{i} y_{i} - a \sum_{i} x_{i}}{n},$$

O(n) per pair  $e_{ij}$  using previous formula.



## Algorithm Analysis

**Theorem** (Bellman, 1961) SSE solves the segmented least squares problem in  $O(n^3)$  time and  $O(n^2)$  space.

**Proof**: Bottleneck = computing  $e_{ij}$  for  $O(n^2)$  pairs,

$$a = \frac{n \sum_{i} x_{i} y_{i} - (\sum_{i} x_{i})(\sum_{i} y_{i})}{n \sum_{i} x_{i}^{2} - (\sum_{i} x_{i})^{2}}, \ b = \frac{\sum_{i} y_{i} - a \sum_{i} x_{i}}{n},$$

O(n) per pair  $e_{ij}$  using previous formula.

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

- o  $\forall i$ : precompute cumulative sums  $\sum_{k=1}^{i} x_k$ ,  $\sum_{k=1}^{i} y_k$ ,  $\sum_{k=1}^{i} x_k^2$ ,  $\sum_{k=1}^{i} x_k y_k$ ,
- Using cumulative sums, we can compute  $e_{ij}$  in O(1) time.



### Outline

- Introduction
  - Background
  - Introductory Example: Weighted Interval Scheduling
- Popular Recipes
  - Segmented Least Squares
  - Knapsack Problem
  - RNA Secondary Structure
- 3 Hirschberg's Alignment Algorithm
  - String Similarity
  - Sequence Alignment in Linear Space



## Knapsack Problem

Given *n* objects and a "knapsack".

Item *i* weighs  $w_i > 0$  kilograms and has value  $v_i > 0$ .

Knapsack has capacity of W kilograms.

**Goal:** fill knapsack so as to maximize total value.

## Knapsack Problem

Given *n* objects and a "knapsack".

Item *i* weighs  $w_i > 0$  kilograms and has value  $v_i > 0$ .

Knapsack has capacity of W kilograms.

Goal: fill knapsack so as to maximize total value.

**Example:**  $\{3,4\}$  has value 40.



	value	weight
1	1	1
2	6	2
3	18	5
4	22	6
5	28	7

## Knapsack Problem

Given *n* objects and a "knapsack".

Item *i* weighs  $w_i > 0$  kilograms and has value  $v_i > 0$ .

Knapsack has capacity of W kilograms.

Goal: fill knapsack so as to maximize total value.

**Example:**  $\{3,4\}$  has value 40.

W = 11

	value	weight
1	1	1
2	6	2
3	18	5
4	22	6
5	28	7

**Greedy:** repeatedly add item with maximum ratio  $v_i/w_i$ .

**Example:**  $\{5, 2, 1\}$  achieves only value =  $35 \Rightarrow$  greedy not optimal.

### First Attempt

**Definition:**  $OPT(i) = \max \text{ profit subset of items } 1, \dots, i.$ 

Case 1: OPT does not select item i.

• OPT selects best of  $\{1, 2, \dots, i-1\}$ .

Case 2: OPT selects item *i*.

- accepting item i does not immediately imply that we will have to reject other items,
- without knowing what other items were selected before i, we don't even know if we have enough room for i.

### First Attempt

**Definition:**  $OPT(i) = \max \text{ profit subset of items } 1, \dots, i.$ 

Case 1: OPT does not select item i.

• OPT selects best of  $\{1, 2, \dots, i-1\}$ .

Case 2: OPT selects item i.

- accepting item *i* does not immediately imply that we will have to reject other items,
- without knowing what other items were selected before i, we don't even know if we have enough room for i.

Conclusion: Need more sub-problems!

## Adding a New Variable

**Definiton:**  $OPT(i) = \max \text{ profit subset of items } 1, \dots, i \text{ with weight limit } w.$ 

Case 1: OPT does not select item i.

• OPT selects best of  $\{1, 2, \dots, i-1\}$  using weight limit w

Case 2: OPT selects item i.

- new weight  $limit = w w_i$
- OPT selects best of using  $\{1, 2, \dots, i-1\}$  this new weight limit

## Adding a New Variable

**Definiton:**  $OPT(i) = \max \text{ profit subset of items } 1, \dots, i \text{ with weight limit } w.$ 

Case 1: OPT does not select item i.

• OPT selects best of  $\{1, 2, \dots, i-1\}$  using weight limit w

Case 2: OPT selects item *i*.

- new weight  $limit = w w_i$
- OPT selects best of using  $\{1, 2, \dots, i-1\}$  this new weight limit

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



## Bottom-Up Algorithm (Fill up an *n*-by-*W* array)

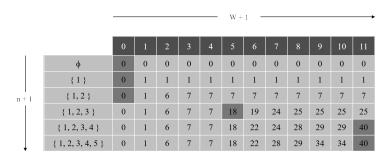
#### **Algorithm 8:** Knapsack Algorithm using *n*-by-*W* Array

```
Input: n, W, w_1, \dots, w_n, v_1, \dots, v_n;
  Output: Optimal value of knapsack with W.
1 for w = 0 \rightarrow W do
  M[0, w] = 0;
3 for i=1 \rightarrow n do
      for w = 1 \rightarrow W do
          if w_i > w then
5
         M[i, w] = M[i - 1, w];
6
          else
            M[i, w] = \max\{M[i-1, w], v_i + M[i-1, w-w_i]\}; 
8
```

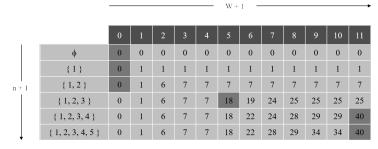
9 return M[n, W];



## Knapsack Algorithm



## Knapsack Algorithm



OPT: 
$$\{4, 3\}$$
  
value =  $22 + 18 = 40$ 

Item	Value	Weight
1	1	1
2	6	2
3	18	5
4	22	6
5	28	7

### Running Time

**Running time:**  $\Theta(nW)$ .

- Not polynomial in input size!
- "Pseudo-polynomial".
- Decision version of Knapsack is NP-complete.

**Knapsack approximation algorithm:** There exists a poly-time algorithm that produces a feasible solution that has value within 0.01% of optimum.

#### Outline

- Introduction
  - Background
  - Introductory Example: Weighted Interval Scheduling
- 2 Popular Recipes
  - Segmented Least Squares
  - Knapsack Problem
  - RNA Secondary Structure
- 3 Hirschberg's Alignment Algorithm
  - String Similarity
  - Sequence Alignment in Linear Space

### RNA Secondary Structure

**RNA:**String  $B = b_1 b_2 \cdots b_n$  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 Secondary Structure

**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.

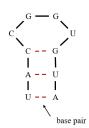
[No sharp turns] The ends of each pair are separated by at least 4 intervening bases. If  $(b_i, b_j) \in S$ , then i < j - 4.

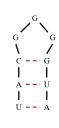
[Non-crossing] If  $(b_i, b_j)$  and  $(b_k, b_l)$  are two pairs in S, then we cannot have i < k < j < l.

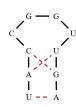
**Free energy:** Usual hypothesis is that an RNA molecule will form the secondary structure with the optimum total free energy.

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

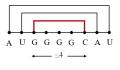
### Examples













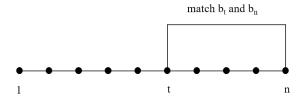
ok

sharp turn

crossing

### Subproblems

**First attempt:**  $OPT(j) = \text{maximum number of base pairs in a secondary structure of the substring <math>b_1b_2 \cdots b_j$ .



**Difficulty:** Results in two sub-problems.

- Finding secondary structure in:  $b_1b_2 \cdots b_{t-1}$ .
- Finding secondary structure in:  $b_{t+1}b_{t+2}\cdots b_{n-1}$ .



## **Dynamic Programming Over Intervals**

**Notation:**  $OPT(j) = \text{maximum number of base pairs in a secondary structure of the substring <math>b_i b_{i+1} \cdots b_j$ .

- Case 1: If  $i \ge j 4$ .
  - OPT(i,j) = 0 by no-sharp turns condition.
- Case 2: Base  $b_i$  is not involved in a pair.
  - $\circ$  OPT(i,j) = OPT(i,j-1)
- Case 3: Base  $b_j$  pairs with  $b_t$  for some  $i \le t < j 4$ .
  - o non-crossing constraint decouples resulting sub-problems
  - $\circ OPT(i,j) = 1 + \max_{t} \{ OPT(i,t-1) + OPT(t+1,j-1) \}$

**Remark:** Same core idea in CKY algorithm to parse context-free grammars.

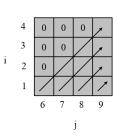


## **Bottom Up Dynamic Programming Over Intervals**

Question: What order to solve the sub-problems?

Answer: Do shortest intervals first.

```
RNA(b_{1},...,b_{n}) \{
for k = 5, 6, ..., n-1
for i = 1, 2, ..., n-k
j = i + k
Compute M[i, j]
return M[1, n]
using recurrence
\}
```



Running time:  $O(n^3)$ .

# **Dynamic Programming Summary**

#### Recipe

- Characterize structure of problem.
- o Recursively define value of optimal solution.
- o Compute value of optimal solution.
- Construct optimal solution from computed information.

#### **Dynamic programming techniques**

- o Binary choice: weighted interval scheduling.
- o Multi-way choice: segmented least squares.
- o Adding a new variable: knapsack.
- Dynamic programming over interval

**Top-down vs. bottom-up:** different people have different intuitions.



#### Outline

- Introduction
  - Background
  - Introductory Example: Weighted Interval Scheduling
- 2 Popular Recipes
  - Segmented Least Squares
  - Knapsack Problem
  - RNA Secondary Structure
- 3 Hirschberg's Alignment Algorithm
  - String Similarity
  - Sequence Alignment in Linear Space

## String Similarity: How similar are two strings?

0	c	u	r	r	a	n	c	e	-
0	с	c	u	r	r	e	n	c	e

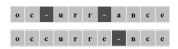
6 mismatches, 1 gap

#### How similar are two strings?

- ocurrance
- occurrence



1 mismatch, 1 gap



0 mismatches, 3 gaps

#### Edit Distance

#### Applications.

- Basis for Unix diff.
- Speech recognition.
- Computational biology.

#### Edit distance. [Levenshtein 1966, Needleman-Wunsch 1970]

- Gap penalty  $\delta$ ; mismatch penalty  $\alpha_{pq}$ .
- Cost = sum of gap and mismatch penalties.



### Sequence Alignment

**Goal:** Given two strings  $X = x_1 x_2 \cdots x_m$  and  $Y = y_1 y_2 \cdots y_n$  find alignment of minimum cost.

**Definiton:** An alignment M is a set of ordered pairs  $x_i - y_j$  such that each item occurs in at most one pair and no crossings.

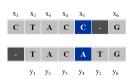
**Definiton:** The pair  $x_i - y_j$  and  $x_{i'} - y_{j'}$  cross if i < i', but j > j'.

$$M = \sum_{\substack{(x_i, y_j) \in M \\ \uparrow \\ \text{mismatch}}} \alpha_{x_i y_j} + \sum_{i: x_i \text{ unmatched}} \delta + \sum_{j: y_j \text{unmatched}} \delta$$

**Example:** CTACCG vs. TACATG.

**Solution:** 
$$M = x_2 - y_1, x_3 - y_2, x_4 - y_3, x_5 -$$

$$y_4, x_6 - y_6$$
.



#### **Problem Structure**

```
Definition: OPT(i,j) = \min \text{ cost of aligning strings } x_1x_2 \cdots x_i \text{ and } y_1y_2 \cdots y_j.
```

Case 1: OPT matches  $x_i - y_j$ .

pay mismatch for  $x_i - y_j$  + min cost of aligning two strings

$$x_1x_2\cdots x_{i-1}$$
 and  $y_1y_2\cdots y_{j-1}$ 

Case 2a: OPT leaves  $x_i$  unmatched.

pay gap for  $x_i$  and min cost of aligning  $x_1x_2 \cdots x_{i-1}$  and  $y_1y_2 \cdots y_j$ 

Case 2b: OPT leaves  $y_j$  unmatched.

pay gap for  $y_j$  and min cost of aligning  $x_1x_2 \cdots x_i$  and  $y_1y_2 \cdots y_{j-1}$ 

## Sequence Alignment

#### **Algorithm 9:** Sequence Alignment

```
Input: m, n, x_1x_2 \cdots x_m, y_1y_2 \cdots y_n, \alpha, \delta;

1 for i = 0 \to m do M[i, 0] = i\delta;

2 for j = 0 \to n do M[0, j] = j\delta;

3 for i = 1 \to m do

4 for j = 1 \to n do

5 M[i, j] = \min(\alpha[x_i, y_j] + M[i - 1, j - 1], \delta + M[i - 1, j], \delta + M[i, j - 1]);

6 return M[m, n];
```

## Sequence Alignment

#### **Algorithm 9:** Sequence Alignment

```
Input: m, n, x_1x_2 \cdots x_m, y_1y_2 \cdots y_n, \alpha, \delta;

1 for i = 0 \to m do M[i, 0] = i\delta;

2 for j = 0 \to n do M[0, j] = j\delta;

3 for i = 1 \to m do

4  for j = 1 \to n do

5  M[i, j] = \min(\alpha[x_i, y_j] + M[i - 1, j - 1], \delta + M[i - 1, j], \delta + M[i, j - 1]);

6 return M[m, n];
```

**Analysis:**  $\Theta(mn)$  time and space.

English words or sentences:  $m, n \le 10$ .

**Computational biology:** m = n = 100,000. 10 billions ops OK, but 10GB array?

#### Outline

- Introduction
  - Background
  - Introductory Example: Weighted Interval Scheduling
- 2 Popular Recipes
  - Segmented Least Squares
  - Knapsack Problem
  - RNA Secondary Structure
- 3 Hirschberg's Alignment Algorithm
  - String Similarity
  - Sequence Alignment in Linear Space

### Linear Space

Question: Can we avoid using quadratic space?

Easy. Optimal value in O(m + n) space\* and O(mn) time.

- Compute  $OPT(i, \cdot)$  from  $OPT(i-1, \cdot)$ .
- No longer a simple way to recover alignment itself.

### Linear Space

Question: Can we avoid using quadratic space?

Easy. Optimal value in O(m + n) space\* and O(mn) time.

- Compute  $OPT(i, \cdot)$  from  $OPT(i-1, \cdot)$ .
- No longer a simple way to recover alignment itself.

**Theorem.** [Hirschberg 1975] Optimal alignment in O(m+n) space and O(mn) time.

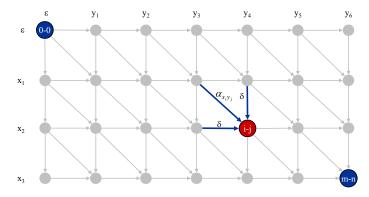
- Clever combination of divide-and-conquer and dynamic programming.
- Inspired by idea of Savitch from complexity theory.

Programming G. Manacher Endergon A Linear Space Algorithm for Computing Maximal Common Subsequences D.s. Hirschberg Princeton University

The profiles of fielding a longer common subsequence and appear appear and appear appear and appear appear and appear and appear appear and appear appear appear appear appear and appear appear

<sup>\*</sup>including space storing original strings

- Let f(i,j) be shortest path from (0,0) to (i,j).
- Observation: f(i,j) = OPT(i,j).



- Let f(i,j) be shortest path from (0,0) to (i,j).
- Observation: f(i,j) = OPT(i,j).



**Proof:** (by strong induction on i + j)

Base case: 
$$f(0,0) = OPT(0,0) = 0$$

Inductive hypothesis: assume true for all (i',j') with i'+j' < i+j.

Induction: Last edge on shortest path to (i,j) is from (i-1,j-1), (i-1,j), or (i,j-1).

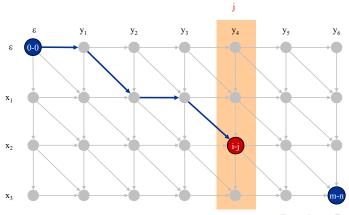
$$f(i,j) = \min\{a_{x_i y_i} + f(i-1,j-1), \delta + f(i-1,j), \delta + f(i,j-1)\}$$

$$= \min\{a_{x_i y_i} + OPT(i-1,j-1), \delta + OPT(i-1,j), \delta + OPT(i,j-1)\}$$

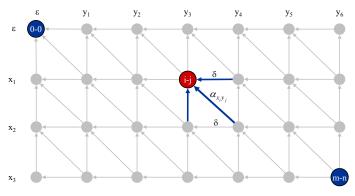
$$= OPT(i,j)$$



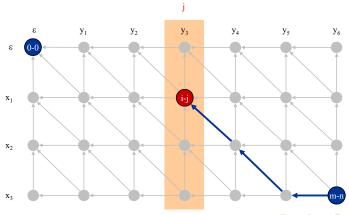
- Let f(i,j) be shortest path from (0,0) to (i,j).
- Can compute  $f(\cdot,j)$  for any j in O(mn) time and O(m+n) space.



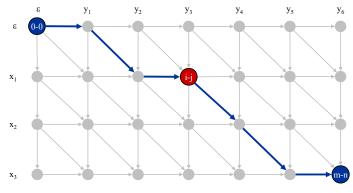
- Let g(i,j) be shortest path from (i,j) to (m,n).
- Can compute by reversing the edge orientations and inverting the roles of (0,0) and (m,n)



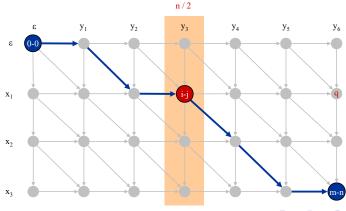
- Let g(i,j) be shortest path from (i,j) to (m,n).
- Can compute  $g(\cdot,j)$  for any j in O(mn) time and O(m+n) space.



**Observation 1:** The cost of the shortest path that uses (i,j) is f(i,j) + g(i,j).

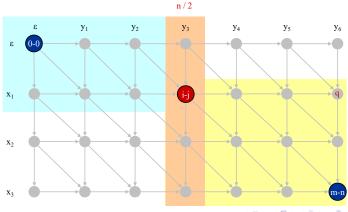


**Observation 2:** Let q be an index that minimizes f(q, n/2) + g(q, n/2). Then, the shortest path from (0, 0) to (m, n) uses (q, n/2).



**Divide:** find index q that minimizes f(q, n/2) + g(q, n/2) using DP. Align  $x_q$  and  $y_{n/2}$ .

**Conquer:** recursively compute optimal alignment in each piece.



## Running Time Analysis Warmup

**Theorem:** Let  $T(m, n) = \max$  running time of algorithm on strings of length at most m and n.  $T(m, n) = O(mn \log n)$ .

$$T(m,n) \le 2T(m,n/2) + O(mn) \Rightarrow T(m,n) = O(mn \log n)$$

**Remark:** Analysis is not tight because two sub-problems are of size (q, n/2) and (m - q, n/2). In next slide, we save  $\log n$  factor.

## Running Time Analysis

**Theorem.** Let  $T(m, n) = \max$  running time of algorithm on strings of length m and n. T(m, n) = O(mn)

**Proof:** (by induction on *n*)

- o O(mn) time to compute  $f(\cdot, n/2)$  and  $g(\cdot, n/2)$  and find index q.
- o T(q, n/2) + T(m q, n/2) time for two recursive calls
- Choose constant c so that:

$$T(m,2) \le cm$$

$$T(2,n) \le cn$$

$$T(m,n) \le cmn + T(q,n/2) + T(m-q,n/2)$$



### Running Time Analysis (Continued)

**Theorem.** Let  $T(m, n) = \max$  running time of algorithm on strings of length m and n. T(m, n) = O(mn)

#### **Proof:**

- Base cases: m = 2 or n = 2.
- Inductive hypothesis:  $T(m, n) \leq 2cmn$ .

$$T(m,n) \le T(q,n/2) + T(m-q,n/2) + cmn$$

$$\le 2cqn/2 + 2c(m-q)n/2 + cmn$$

$$= cqn + cmn - cqn + cmn$$

$$= 2cmn$$