Weighted Interval Scheduling

### **Dynamic Programming**

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  - Con: usually reduces time for a problem known to be solvable in polynomial time.

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#### 4. Dynamic programming

- More powerful than greedy and divide-and-conquer strategies.
- Implicitly explore space of all possible solutions.
- Solve multiple sub-problems and build up correct solutions to larger and larger sub-problems.
- Careful analysis needed to ensure number of sub-problems solved is polynomial in the size of the input.

## **History of Dynamic Programming**

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- ▶ The Secretary of Defense at that time was hostile to mathematical research.
- Bellman sought an impressive name to avoid confrontation.
  - "it's impossible to use dynamic in a pejorative sense"
  - "something not even a Congressman could object to" (Bellman, R. E., Eye of the Hurricane, An Autobiography).

### **Applications of Dynamic Programming**

- Computational biology: Smith-Waterman algorithm for sequence alignment.
- Operations research: Bellman-Ford algorithm for shortest path routing in networks.
- Control theory: Viterbi algorithm for hidden Markov models.
- Computer science (theory, graphics, Al, ...): Unix diff command for comparing two files.

### **Review: Interval Scheduling**

#### Interval Scheduling

**INSTANCE:** Nonempty set  $\{(s_i, f_i), 1 \le i \le n\}$  of start and finish times of n jobs.

**SOLUTION:** The largest subset of mutually compatible jobs.

▶ Two jobs are *compatible* if they do not overlap.

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**SOLUTION:** The largest subset of mutually compatible jobs.

- Two jobs are compatible if they do not overlap.
- Greedy algorithm: sort jobs in increasing order of finish times. Add next job to current subset only if it is compatible with previously-selected jobs.

### Weighted Interval Scheduling

#### WEIGHTED INTERVAL SCHEDULING

**INSTANCE:** Nonempty set  $\{(s_i, f_i), 1 \le i \le n\}$  of start and finish times of n jobs and a weight  $v_i \ge 0$  associated with each job.

**SOLUTION:** A set S of mutually compatible jobs such that  $\sum_{i \in S} v_i$  is maximised.

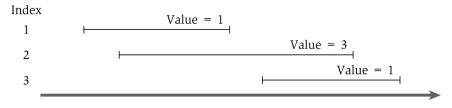


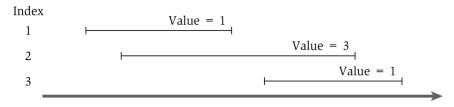
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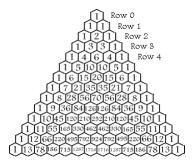
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**Figure 6.1** A simple instance of weighted interval scheduling.

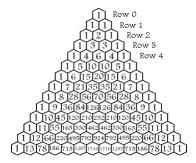
Greedy algorithm can produce arbitrarily bad results for this problem.

## **Detour: a Binomial Identity**



Shortest Paths in Graphs

#### **Detour: a Binomial Identity**

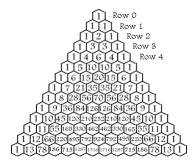


► Pascal's triangle:

Weighted Interval Scheduling

- Each element is a binomial co-efficient.
- ▶ Each element is the sum of the two elements above it.

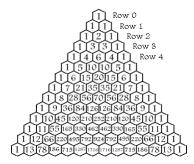
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$$\binom{n}{r} = \binom{n-1}{r-1} + \binom{n-1}{r}$$

Proof: either we select the nth element or not ...

Shortest Paths in Graphs

### **Approach**

- ▶ Sort jobs in increasing order of finish time and relabel:  $f_1 \le f_2 \le ... \le f_n$ .
- ▶ Job *i* comes before job *j* if i < j.

Weighted Interval Scheduling

- ▶ p(j) is the largest index i < j such that job i is compatible with job j. p(j) = 0 if there is no such job i.
- All jobs that come before job p(j) are also compatible with job j.

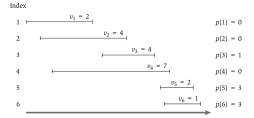


Figure 6.2 An instance of weighted interval scheduling with the functions p(j) defined for each interval i.

▶ We will develop optimal algorithm from obvious statements about the problem.

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- O cannot use incompatible jobs  $\{p(n)+1,p(n)+2,\ldots,n-1\}.$
- $\triangleright$  Remaining jobs in  $\mathcal{O}$  must be the optimal solution for jobs  $\{1, 2, \ldots, p(n)\}.$

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- O must be the best of these two choices!
- Suggests finding optimal solution for sub-problems consisting of jobs  $\{1, 2, \dots, i-1, i\}$ , for all values of i.

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$$\mathsf{OPT}(j) = \mathsf{max}(v_j + \mathsf{OPT}(p(j)), \mathsf{OPT}(j-1))$$

▶ When does request j belong to  $\mathcal{O}_j$ ? If and only if  $v_j + \mathsf{OPT}(p(j)) \ge \mathsf{OPT}(j-1)$ .

## **Recursive Algorithm**

```
Compute-Opt(j)
  If j=0 then
    Return 0
  Else
    Return \max(v_i + \text{Compute-Opt}(p(j)), \text{Compute-Opt}(j-1))
  Endif
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### **Recursive Algorithm**

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Correctness of algorithm follows by induction (see textbook for proof).

#### **Example of Recursive Algorithm**

#### 

**Figure 6.2** An instance of weighted interval scheduling with the functions p(j) defined for each interval j.

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OPT(6) = OPT(5) = OPT(4) = OPT(3) = OPT(2) = OPT(1) = OPT(0) = 0
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Segmented Least Squares

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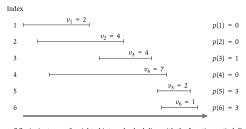
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OPT(2) = OPT(1) = OPT(0) = 0
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**Figure 6.2** An instance of weighted interval scheduling with the functions p(j) defined for each interval j.

```
\begin{array}{l} \mathsf{OPT}(6) = \; \mathsf{max}(v_6 + \mathsf{OPT}(p(6)), \mathsf{OPT}(5)) = \mathsf{max}(1 + \mathsf{OPT}(3), \mathsf{OPT}(5)) \\ \mathsf{OPT}(5) = \; \mathsf{max}(v_5 + \mathsf{OPT}(p(j)), \mathsf{OPT}(4)) = \mathsf{max}(2 + \mathsf{OPT}(3), \mathsf{OPT}(4)) \\ \mathsf{OPT}(4) = \; \mathsf{max}(v_4 + \mathsf{OPT}(p(4)), \mathsf{OPT}(3)) = \mathsf{max}(7 + \mathsf{OPT}(0), \mathsf{OPT}(3)) \\ \mathsf{OPT}(3) = \; \mathsf{max}(v_3 + \mathsf{OPT}(p(3)), \mathsf{OPT}(2)) = \mathsf{max}(4 + \mathsf{OPT}(1), \mathsf{OPT}(2)) \\ \mathsf{OPT}(2) = \; \mathsf{max}(v_2 + \mathsf{OPT}(p(2)), \mathsf{OPT}(1)) = \mathsf{max}(4 + \mathsf{OPT}(0), \mathsf{OPT}(1)) \\ \mathsf{OPT}(1) = \\ \mathsf{OPT}(0) = 0 \end{array}
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Segmented Least Squares

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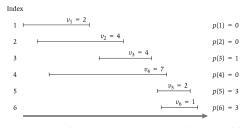
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OPT(3) = max(v_3 + OPT(p(3)), OPT(2)) = max(4 + OPT(1), OPT(2)) = 6
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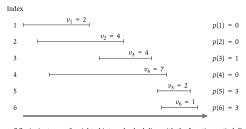
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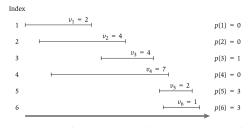
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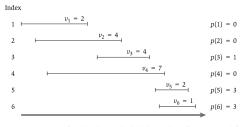


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Optimal solution is

### **Example of Recursive Algorithm**



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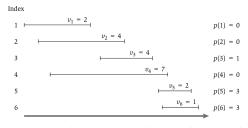
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```

Optimal solution is job 5, job 3, and job 1.

## Running Time of Recursive Algorithm

```
Compute-Opt(j)
  If j=0 then
     Return 0
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What is the running time of the algorithm?

```
\label{eq:compute-Opt(j)} \begin{split} &\text{If } j = 0 \text{ then} \\ &\text{Return 0} \\ &\text{Else} \\ &\text{Return max}(v_j + \text{Compute-Opt}(\texttt{p(j)}), \text{ Compute-Opt}(j-1)) \\ &\text{Endif} \end{split}
```

▶ What is the running time of the algorithm? Can be exponential in *n*.

## Running Time of Recursive Algorithm

$$\label{eq:compute-Opt} \begin{split} & \text{Compute-Opt}(j) \\ & \text{If } j = 0 \text{ then} \\ & \text{Return } 0 \\ & \text{Else} \\ & \text{Return } \max(\nu_j + \text{Compute-Opt}(\texttt{p}(\texttt{j})) \text{, } \text{Compute-Opt}(j-1)) \\ & \text{Endif} \end{split}$$

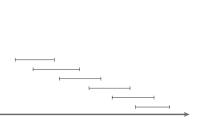


Figure 6.4 An instance of weighted interval scheduling on which the simple Compute— Opt recursion will take exponential time. The values of all intervals in this instance are 1.

- ▶ What is the running time of the algorithm? Can be exponential in *n*.
- ▶ When p(j) = j 2, for all  $j \ge 2$ : recursive calls are for j 1 and j 2.

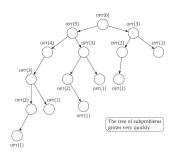


Figure 6.3 The tree of subproblems called by Compute-Opt on the problem instance of Figure 6.2.

#### **Memoisation**

Shortest Paths in Graphs

ightharpoonup Store OPT(j) values in a cache and reuse them rather than recompute them.

#### **Memoisation**

▶ Store OPT(j) values in a cache and reuse them rather than recompute them.

```
M-Compute-Opt(j)

If j=0 then

Return 0

Else if M[j] is not empty then

Return M[j]

Else

Define M[j] = \max(v_j + \text{M-Compute-Opt}(p(j)), \text{M-Compute-Opt}(j-1))

Return M[j]

Endif
```

```
\label{eq:m-compute-opt} \begin{aligned} & \text{M-Compute-Opt}(j) \\ & \text{If } j = 0 \text{ then} \\ & \text{Return } 0 \\ & \text{Else if } M[j] \text{ is not empty then} \\ & \text{Return } M[j] \\ & \text{Else} \\ & \text{Define } M[j] = \max(v_j + \text{M-Compute-Opt}(p(j)), \text{ M-Compute-Opt}(j-1)) \\ & \text{Return } M[j] \\ & \text{Endif} \end{aligned}
```

Claim: running time of this algorithm is O(n) (after sorting).

## **Running Time of Memoisation**

```
M-Compute-Opt(i)
  If i = 0 then
    Return 0
  Else if M[i] is not empty then
    Return M[i]
  Else
   Define M[j] = \max(v_i + M - Compute - Opt(p(j)), M - Compute - Opt(j-1))
    Return M[i]
  Endif
```

- Claim: running time of this algorithm is O(n) (after sorting).
- Time spent in a single call to M-Compute-Opt is O(1) apart from time spent in recursive calls.
- Total time spent is the order of the number of recursive calls to M-Compute-Opt.
- How many such recursive calls are there in total?

Shortest Paths in Graphs

```
M-Compute-Opt(j)  \begin{tabular}{ll} If $j=0$ then \\ Return 0 \\ Else if $M[j]$ is not empty then \\ Return $M[j]$ \\ Else \\ Define $M[j]=\max(v_j+M-Compute-Opt(p(j))$, M-Compute-Opt(j-1)) \\ Return $M[j]$ \\ Endif \\ \end{tabular}
```

- ▶ Claim: running time of this algorithm is O(n) (after sorting).
- ▶ Time spent in a single call to M-Compute-Opt is O(1) apart from time spent in recursive calls.
- Total time spent is the order of the number of recursive calls to M-Compute-Opt.
- ▶ How many such recursive calls are there in total?

Weighted Interval Scheduling

- $\blacktriangleright$  Use number of filled entries in M as a measure of progress.
- $\blacktriangleright$  Each time M-Compute-Opt issues two recursive calls, it fills in a new entry in M.
- Therefore, total number of recursive calls is O(n).

▶ Explicitly store  $\mathcal{O}_j$  in addition to  $\mathsf{OPT}(j)$ .

**Explicitly store**  $\mathcal{O}_i$  in addition to OPT(j). Running time becomes  $O(n^2)$ .

- **Explicitly store**  $\mathcal{O}_i$  in addition to OPT(i). Running time becomes  $O(n^2)$ .
- Recall: request j belong to  $\mathcal{O}_i$  if and only if  $v_i + \mathsf{OPT}(p(j)) \geq \mathsf{OPT}(j-1)$ .
- Can recover  $\mathcal{O}_i$  from values of the optimal solutions in  $\mathcal{O}(i)$  time.

- ▶ Explicitly store  $\mathcal{O}_j$  in addition to OPT(j). Running time becomes  $O(n^2)$ .
- ▶ Recall: request j belong to  $\mathcal{O}_j$  if and only if  $v_j + \mathsf{OPT}(p(j)) \ge \mathsf{OPT}(j-1)$ .
- ▶ Can recover  $\mathcal{O}_i$  from values of the optimal solutions in O(j) time.

```
Find-Solution(j)

If j=0 then

Output nothing

Else

If v_j+M[p(j)]\geq M[j-1] then

Output j together with the result of Find-Solution(p(j))

Else

Output the result of Find-Solution(j-1)

Endif

Endif
```

#### From Recursion to Iteration

- Unwind the recursion and convert it into iteration.
- Can compute values in M iteratively in O(n) time.
- Find-Solution works as before.

```
Iterative-Compute-Opt
  M[0] = 0
  For i = 1, 2, ..., n
    M[j] = \max(v_i + M[p(j)], M[j-1])
  Endfor
```

## **Basic Outline of Dynamic Programming**

- ➤ To solve a problem, we need a collection of sub-problems that satisfy a few properties:
  - 1. There are a polynomial number of sub-problems.
  - The solution to the problem can be computed easily from the solutions to the sub-problems.
  - 3. There is a natural ordering of the sub-problems from "smallest" to "largest".
  - 4. There is an easy-to-compute recurrence that allows us to compute the solution to a sub-problem from the solutions to some smaller sub-problems.

## **Basic Outline of Dynamic Programming**

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  - 3. There is a natural ordering of the sub-problems from "smallest" to "largest".
  - 4. There is an easy-to-compute recurrence that allows us to compute the solution to a sub-problem from the solutions to some smaller sub-problems.
- ▶ Difficulties in designing dynamic programming algorithms:
  - 1. Which sub-problems to define?
  - 2. How can we tie together sub-problems using a recurrence?
  - 3. How do we order the sub-problems (to allow iterative computation of optimal solutions to sub-problems)?

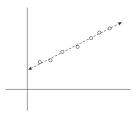


Figure 6.6 A "line of best fit."

- Given scientific or statistical data plotted on two axes.
- ▶ Find the "best" line that "passes" through these points.

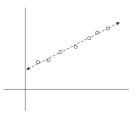


Figure 6.6 A "line of best fit."

- Given scientific or statistical data plotted on two axes.
- ► Find the "best" line that "passes" through these points.
- ► How do we formalise the problem?

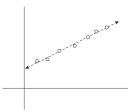


Figure 6.6 A "line of best fit."

- Given scientific or statistical data plotted on two axes.
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- How do we formalise the problem?

Least Squares

**INSTANCE:** Set  $P = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$  of *n* points.

**SOLUTION:** Line L: y = ax + b that minimises

$$Error(L, P) = \sum_{i=1}^{\infty} (y_i - ax_i - b)^2.$$

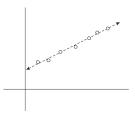


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**SOLUTION:** Line L: y = ax + b that minimises

$$Error(L, P) = \sum_{i=1}^{m} (y_i - ax_i - b)^2.$$

▶ Minimisation is over all possible choices of

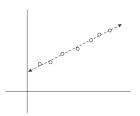


Figure 6.6 A "line of best fit."

Given scientific or statistical data plotted on two axes.

- ► Find the "best" line that "passes" through these points.
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#### Least Squares

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**SOLUTION:** Line L: y = ax + b that minimises

$$Error(L, P) = \sum_{i=1} (y_i - ax_i - b)^2.$$

- Minimisation is over all possible choices of a and b.
- ► Solution is achieved by

$$a = \frac{n \sum_{i} x_{i} y_{i} - \left(\sum_{i} x_{i}\right) \left(\sum_{i} y_{i}\right)}{n \sum_{i} x_{i}^{2} - \left(\sum_{i} x_{i}\right)^{2}} \text{ and } b = \frac{\sum_{i} y_{i} - a \sum_{i} x_{i}}{n}$$

## **Segmented Least Squares**

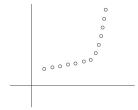


Figure 6.7 A set of points that lie approximately on two lines.

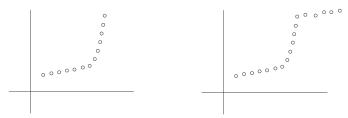


Figure 6.7 A set of points that lie approximately on two lines. Figure 6.8 A set of points that lie approximately on three lines.

## **Segmented Least Squares**

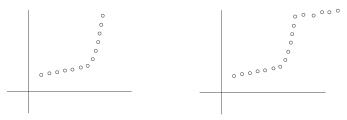
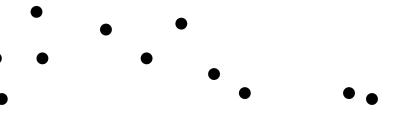
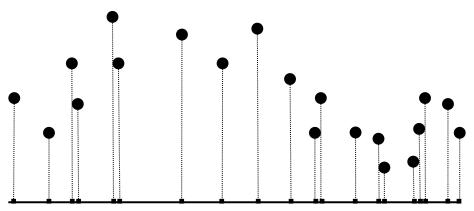


Figure 6.7 A set of points that lie approximately on two lines. Figure 6.8 A set of points that lie approximately on three lines.

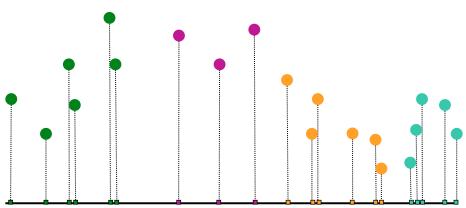
- Want to fit multiple lines through P.
- Each line must fit contiguous set of x-coordinates.
- Lines must minimise total error.



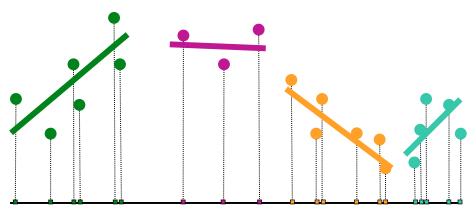
Input contains a set of two-dimensional points.



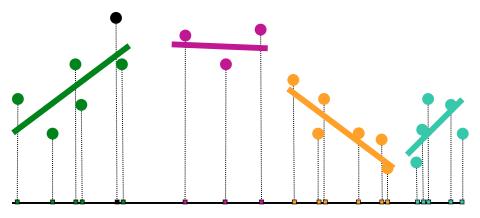
Consider the x-coordinates of the points in the input.



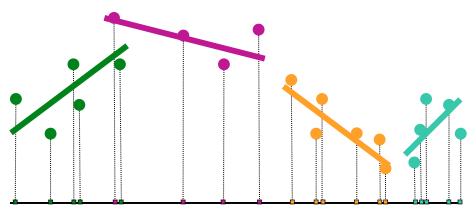
Divide the points into segments; each segment contains consecutive points in the sorted order by *x*-coordinate.



Fit the best line for each segment.



Illegal solution: black point is not in any segment.



Illegal solution: leftmost purple point has *x*-coordinate between last two points in green segment.

#### **Segmented Least Squares**



Figure 6.7 A set of points that lie approximately on two lines. Figure 6.8 A set of points that lie approximately on three lines.

#### Segmented Least Squares



Figure 6.7 A set of points that lie approximately on two lines. Figure 6.8 A set of points that lie approximately on three lines.

#### SEGMENTED LEAST SQUARES

**INSTANCE:** Set 
$$P = \{p_i = (x_i, y_i), 1 \le i \le n\}$$
 of *n* points,  $x_1 < x_2 < \dots < x_n$ .

**SOLUTION:** A integer k, a partition of P into k segments  $\{P_1, P_2, \dots, P_k\}$ , k lines  $L_i: y = a_i x + b_i, 1 \le i \le k$  that minimise

$$\sum_{j=1}^{\kappa} \mathsf{Error}(L_j, P_j)$$

▶ A subset P' of P is a segment if  $1 \le i < j \le n$  exist such that  $P' = \{(x_i, y_i), (x_{i+1}, y_{i+1}), \dots, (x_{i-1}, y_{i-1}), (x_i, y_i)\}.$ 

RNA Secondary Structure



Figure 6.7 A set of points that lie approximately on two lines. Figure 6.8 A set of points that lie approximately on three lines.

#### SEGMENTED LEAST SQUARES

Weighted Interval Scheduling

**INSTANCE:** Set  $P = \{p_i = (x_i, y_i), 1 \le i \le n\}$  of *n* points,  $x_1 < x_2 < \cdots < x_n$  and a parameter C > 0.

**SOLUTION:** A integer k, a partition of P into k segments  $\{P_1, P_2, \dots, P_k\}$ , k lines  $L_i: y = a_i x + b_i, 1 \le i \le k$  that minimise

$$\sum_{j=1}^{k} \operatorname{Error}(L_j, P_j) + Ck$$

▶ A subset P' of P is a segment if  $1 \le i < j \le n$  exist such that  $P' = \{(x_i, y_i), (x_{i+1}, y_{i+1}), \dots, (x_{i-1}, y_{i-1}), (x_i, y_i)\}.$ 

#### Formulating the Recursion I

- $\triangleright$  Observation:  $p_n$  is part of some segment in the optimal solution. This segment starts at some point  $p_i$ .
- Let OPT(i) be the optimal value for the points  $\{p_1, p_2, \dots, p_i\}$ .
- Let  $e_{i,i}$  denote the minimum error of a (single) line that fits  $\{p_i, p_2, \dots, p_i\}$ .
- $\blacktriangleright$  We want to compute  $\mathsf{OPT}(n)$ .

Figure 6.9 A possible solution: a single line segment fits points  $p_i, p_{i+1}, \dots, p_n$ , and then an optimal solution is found for the remaining points  $p_1, p_2, \dots, p_{i-1}$ 

▶ If the last segment in the optimal partition is  $\{p_i, p_{i+1}, \dots, p_n\}$ , then

$$OPT(n) = e_{i,n} + C + OPT(i-1)$$

### Formulating the Recursion II

- Consider the sub-problem on the points  $\{p_1, p_2, \dots p_i\}$
- $\triangleright$  To obtain OPT(i), if the last segment in the optimal partition is  $\{p_i, p_{i+1}, \dots, p_i\}$ , then

$$\mathsf{OPT}(j) = e_{i,j} + C + \mathsf{OPT}(i-1)$$

### Formulating the Recursion II

- ▶ Consider the sub-problem on the points  $\{p_1, p_2, \dots p_j\}$
- ▶ To obtain OPT(j), if the last segment in the optimal partition is  $\{p_i, p_{i+1}, \dots, p_j\}$ , then

$$\mathsf{OPT}(j) = e_{i,j} + C + \mathsf{OPT}(i-1)$$

Since i can take only j distinct values,

$$\mathsf{OPT}(j) = \min_{1 \le i \le j} \left( e_{i,j} + C + \mathsf{OPT}(i-1) \right)$$

▶ Segment  $\{p_i, p_{i+1}, \dots p_j\}$  is part of the optimal solution for this sub-problem if and only if the minimum value of  $\mathsf{OPT}(j)$  is obtained using index i.

## **Dynamic Programming Algorithm**

$$\mathsf{OPT}(j) = \min_{1 \leq i \leq j} \left( e_{i,j} + C + \mathsf{OPT}(i-1) \right)$$

```
Segmented-Least-Squares(n)
  Array M[0...n]
  Set M[0] = 0
  For all pairs i \leq j
    Compute the least squares error e_{i,j} for the segment p_i, \ldots, p_j
  Endfor
  For i = 1, 2, ..., n
    Use the recurrence (6.7) to compute M[j]
  Endfor
  Return M[n]
```

### **Dynamic Programming Algorithm**

$$\mathsf{OPT}(j) = \min_{1 \leq i \leq j} \left( e_{i,j} + C + \mathsf{OPT}(i-1) \right)$$

```
Segmented-Least-Squares(n)  \begin{array}{l} \text{Array } M[0 \ldots n] \\ \text{Set } M[0] = 0 \\ \text{For all pairs } i \leq j \\ \text{Compute the least squares error } e_{i,j} \text{ for the segment } p_i, \ldots, p_j \\ \text{Endfor} \\ \text{For } j = 1, 2, \ldots, n \\ \text{Use the recurrence (6.7) to compute } M[j] \\ \text{Endfor} \\ \text{Return } M[n] \\ \end{array}
```

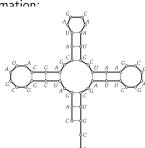
- ▶ Running time is  $O(n^3)$ , can be improved to  $O(n^2)$ .
- ▶ We can find the segments in the optimal solution by backtracking.

#### **RNA** Molecules

- RNA is a basic biological molecule. It is single stranded.
- RNA molecules fold into complex "secondary structures."
- Secondary structure often governs the behaviour of an RNA molecule.
- Various rules govern secondary structure formation:

#### **RNA Molecules**

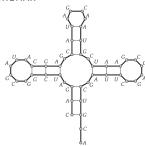
- ▶ RNA is a basic biological molecule. It is single stranded.
- RNA molecules fold into complex "secondary structures."
- ▶ Secondary structure often governs the behaviour of an RNA molecule.
- ► Various rules govern secondary structure formation:
- 1. Pairs of bases match up; each base matches with  $\leq 1$  other base.
- 2. Adenine always matches with Uracil.
- 3. Cytosine always matches with Guanine.
- 4. There are no kinks in the folded molecule.
- 5. Structures are "knot-free".



**Figure 6.13** An RNA secondary structure. Thick lines connect adjacent elements of the sequence; thin lines indicate pairs of elements that are matched.

#### RIVA Molecule

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- ► Various rules govern secondary structure formation:
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- 3. Cytosine always matches with Guanine.
- 4. There are no kinks in the folded molecule.
- 5. Structures are "knot-free".

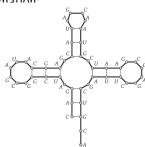


 $\label{eq:Figure 6.13} \textbf{An RNA secondary structure. Thick lines connect adjacent elements of the sequence; thin lines indicate pairs of elements that are matched.}$ 

Problem: given an RNA molecule, predict its secondary structure.

#### **RNA Molecules**

- ▶ RNA is a basic biological molecule. It is single stranded.
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 ${\bf Figure~6.13~An~RNA~secondary~structure.~Thick~lines~connect~adjacent~elements~of~the~sequence;~thin~lines~indicate~pairs~of~elements~that~are~matched.}$ 

- Problem: given an RNA molecule, predict its secondary structure.
- Hypothesis: In the cell, RNA molecules form the secondary structure with the lowest total free energy.

#### Formulating the Problem



Figure 6.14 Two views of an RNA secondary structure. In the second view, (b), the string has been "stretched" lengthwise, and edges connecting matched pairs appear as noncrossing "bubbles" over the string.

- ▶ An RNA molecule is a string  $B = b_1 b_2 \dots b_n$ ; each  $b_i \in \{A, C, G, U\}$ .
- ▶ A secondary structure on B is a set of pairs  $S = \{(i,j)\}$ , where  $1 \le i,j \le n$  and

#### Formulating the Problem

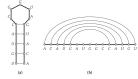
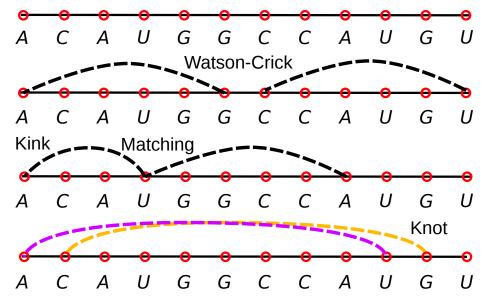
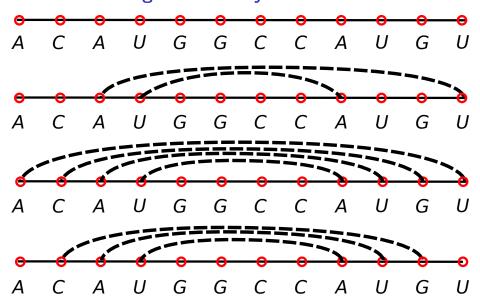


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- ▶ An RNA molecule is a string  $B = b_1 b_2 \dots b_n$ ; each  $b_i \in \{A, C, G, U\}$ .
- ▶ A secondary structure on B is a set of pairs  $S = \{(i,j)\}$ , where  $1 \le i,j \le n$  and
  - 1. (No kinks.) If  $(i,j) \in S$ , then i < j 4.
  - 2. (Watson-Crick) The elements in each pair in S consist of either  $\{A, U\}$  or  $\{C, G\}$  (in either order).
  - 3. *S* is a *matching*: no index appears in more than one pair.
  - 4. (No knots) If (i,j) and (k,l) are two pairs in S, then we cannot have i < k < j < l.
- ▶ The *energy* of a secondary structure  $\propto$  the number of base pairs in it.
- Problem: Compute the largest secondary structure, i.e., with the largest number of base pairs.

# **Illegal Secondary Structures**





▶ OPT(j) is the maximum number of base pairs in a secondary structure for  $b_1b_2...b_j$ .

 $\triangleright$  OPT(j) is the maximum number of base pairs in a secondary structure for  $b_1 b_2 \dots b_i$ . OPT(j) = 0, if  $j \le 5$ .

- ▶ OPT(i) is the maximum number of base pairs in a secondary structure for  $b_1 b_2 \dots b_i$ . OPT(j) = 0, if  $j \leq 5$ .
  - In the optimal secondary structure on  $b_1 b_2 \dots b_i$

- $\triangleright$  OPT(j) is the maximum number of base pairs in a secondary structure for  $b_1 b_2 \dots b_j$ . OPT(j) = 0, if  $j \le 5$ .
- ▶ In the optimal secondary structure on  $b_1b_2...b_i$ 
  - 1. if j is not a member of any pair, use OPT(j-1).

- $\triangleright$  OPT(j) is the maximum number of base pairs in a secondary structure for  $b_1 b_2 \dots b_i$ . OPT(i) = 0, if  $i \le 5$ .
- ▶ In the optimal secondary structure on  $b_1b_2...b_i$ 
  - 1. if j is not a member of any pair, use OPT(j-1).
  - 2. if j pairs with some t < j 4,

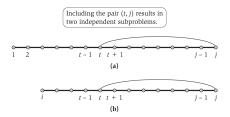


Figure 6.15 Schematic views of the dynamic programming recurrence using (a) one variable, and (b) two variables,

- ▶ OPT(j) is the maximum number of base pairs in a secondary structure for  $b_1b_2...b_j$ . OPT(j) = 0, if  $j \le 5$ .
- ▶ In the optimal secondary structure on  $b_1b_2...b_j$ 
  - 1. if j is not a member of any pair, use OPT(j-1).
  - 2. if j pairs with some t < j-4, knot condition yields two independent sub-problems!

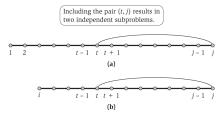


Figure 6.15 Schematic views of the dynamic programming recurrence using (a) one variable, and (b) two variables.

- ▶ OPT(j) is the maximum number of base pairs in a secondary structure for  $b_1b_2...b_j$ . OPT(j) = 0, if  $j \le 5$ .
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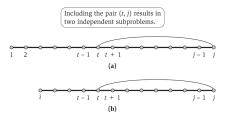


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- Insight: need sub-problems indexed both by start and by end.

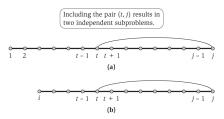


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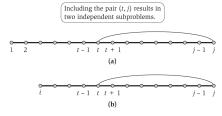


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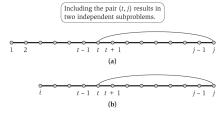
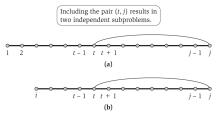


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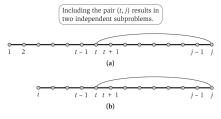
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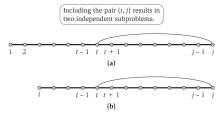
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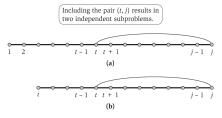
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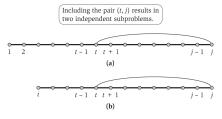


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#### Correct Dynamic Programming Approach

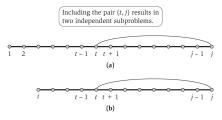


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### **Correct Dynamic Programming Approach**

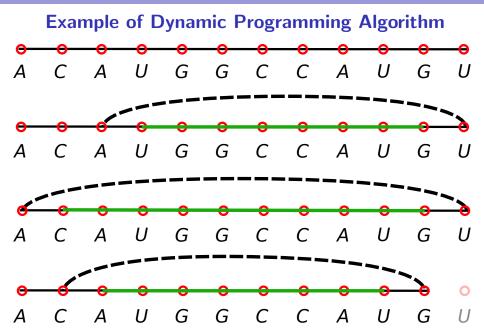


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▶ In the "inner" maximisation, t runs over all indices between i and j-5 that are allowed to pair with j.



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- ▶ There are  $O(n^2)$  sub-problems.
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### **Dynamic Programming Algorithm**

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```
Initialize \mathsf{OPT}(i,j) = 0 whenever i \ge j-4

For k = 5, 6, \ldots, n-1

For i = 1, 2, \ldots n-k

Set j = i+k

Compute \mathsf{OPT}(i,j) using the recurrence in (6.13)

Endfor

Endfor

Return \mathsf{OPT}(1,n)
```

### **Dynamic Programming Algorithm**

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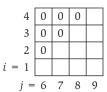
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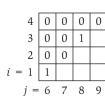
Running time of the algorithm is  $O(n^3)$ .

### **Example of Algorithm**

RNA sequence ACCGGUAGU



**Initial values** 



Filling in the values for k = 5

Filling in the values for k = 6

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

March 24, 26, 31, 2014

T. M. Murali

#### **Motivation**

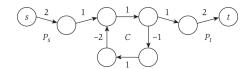
- Computational finance:
  - Each node is a financial agent.
  - The cost  $c_{uv}$  of an edge (u, v) is the cost of a transaction in which we buy from agent u and sell to agent v.
  - Negative cost corresponds to a profit.
- Internet routing protocols
  - Dijkstra's algorithm needs knowledge of the entire network.
  - Routers only know which other routers they are connected to.
  - Algorithm for shortest paths with negative edges is decentralised.
  - ▶ We will not study this algorithm in the class. See Chapter 6.9.

#### Problem Statement

- ▶ Input: a directed graph G = (V, E) with a cost function  $c : E \to \mathbb{R}$ , i.e.,  $c_{uv}$ is the cost of the edge  $(u, v) \in E$ .
- ▶ A negative cycle is a directed cycle whose edges have a total cost that is negative.
- ► Two related problems:
  - 1. If G has no negative cycles, find the shortest s-t path: a path of from source s to destination t with minimum total cost.
  - 2. Does G have a negative cycle?

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**Figure 6.20** In this graph, one can find s-t paths of arbitrarily negative cost (by going around the cycle C many times).

# **Approaches for Shortest Path Algorithm**

1. Dijsktra's algorithm.

2. Add some large constant to each edge.

#### Approaches for Shortest Path Algorithm

- 1. Dijsktra's algorithm. Computes incorrect answers because it is greedy.
- 2. Add some large constant to each edge. Computes incorrect answers because the minimum cost path changes.





Figure 6.21 (a) With negative edge costs, Dijkstra's Algorithm can give the wrong answer for the Shortest-Path Problem. (b) Adding 3 to the cost of each edge will make all edges nonnegative, but it will change the identity of the shortest s-t path.

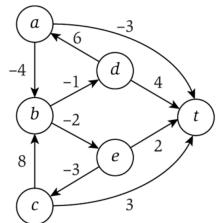
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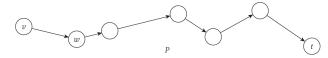
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- ► How do we define sub-problems?
  - ▶ Shortest s-t path has < n-1edges: how we can reach t using i edges, for different values of *i*?
  - We do not know which nodes will be in shortest s-t path: how we can reach t from each node in V?

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- ▶ Claim: There is a shortest path from s to t that is simple (does not repeat a node) and hence has at most n-1 edges.
- ▶ How do we define sub-problems?
  - Shortest s-t path has ≤ n − 1 edges: how we can reach t using i edges, for different values of i?
  - We do not know which nodes will be in shortest s-t path: how we can reach t from each node in V?
- Sub-problems defined by varying the number of edges in the shortest path and by varying the starting node in the shortest path.



- ightharpoonup OPT(i, v): minimum cost of a v-t path that uses at most i edges.
- t is not explicitly mentioned in the sub-problems.
- Goal is to compute OPT(n-1, s).

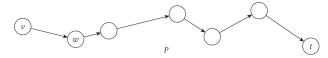
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**Figure 6.22** The minimum-cost path P from v to t using at most i edges.

Let P be the optimal path whose cost is OPT(i, v).

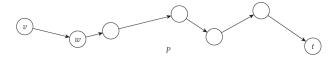
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- Let P be the optimal path whose cost is OPT(i, v).
  - 1. If P actually uses i-1 edges, then OPT(i, v) = OPT(i-1, v).
  - 2. If first node on P is w, then  $OPT(i, v) = c_{vw} + OPT(i-1, w)$ .

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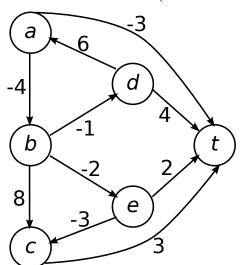


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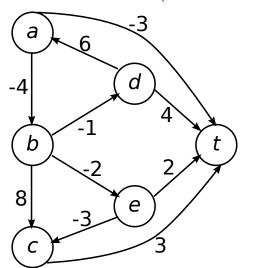
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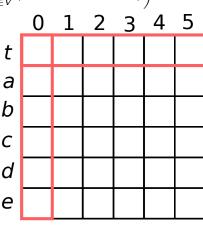
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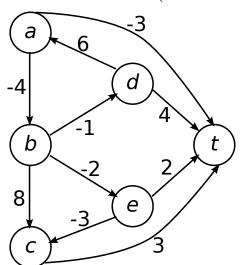
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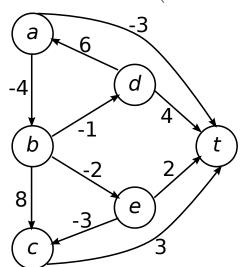


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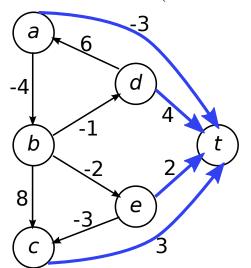
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e	$\infty$					

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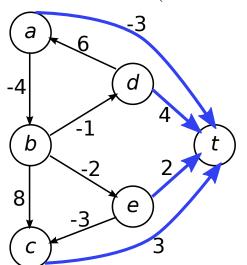
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e	8					

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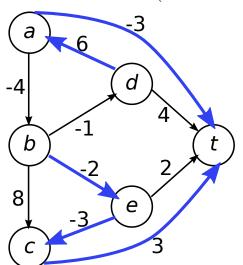
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t	0	0	0	0	0	0
a	8	-3				
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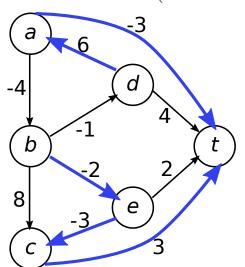
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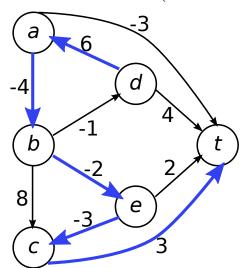
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c	8	3	3			
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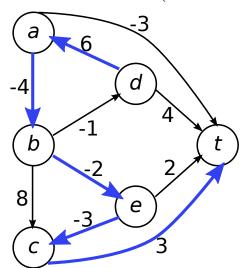
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	0	1	2	3	4	5
t	0	0	0	0	0	0
a	8	-3	-3			
b	8	8	0			
C	8	3	3			
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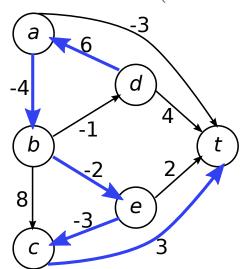
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t	0	0	0	0	0	0
a	8	-3	-3	-4		
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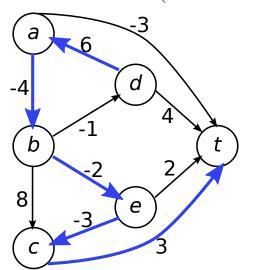
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C	8	3	3	3		
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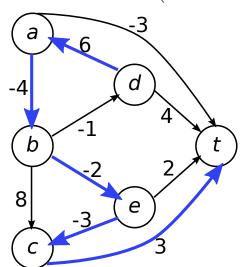
v					/	
	0	1	2	3	4	5
t			0			0
			-3			
b	8	8	0	-2	-2	
c	8	3	3	3	3	
d	8	4	3	3	2	
e	8	2	0	0	0	

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



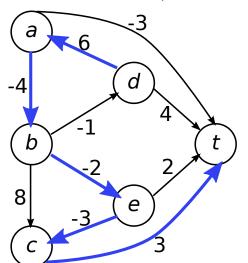
V `			-	. ,	/	
	0	1	2	3	4	5
t	0			0		0
a	8		-უ			
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ĘV`	` '')						
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	0		0	0	0	0	
	8		-უ				
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d	8	4	3	3	2	0	
e	8	2	0	0	0	0	

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	0	1	2	3	4	5	
t	0	0	0	0	0	0	
a	8	-3	-3	-4	-6	-6	
b	8	8	0	-2	-2	-2	
	8					3	
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Compare the two desired solutions:

$$\min_{i=1}^{n-1} \mathsf{OPT}_=(\mathsf{i},\,\mathsf{s}) = \min_{i=1}^{n-1} \left( \, \min_{\mathsf{w} \in V} \left( c_{\mathsf{sw}} + \mathsf{OPT}_=(\mathsf{i} \, \text{-} \, \mathsf{1},\, \mathsf{w}) \right) \, \right)$$

$$\mathsf{OPT}(n-1,s) = \min\left(\mathsf{OPT}(n-2,s), \min_{w \in V}\left(c_{sw} + \mathsf{OPT}(n-2,w)\right)\right)$$

#### **Bellman-Ford Algorithm**

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

```
Shortest-Path(G, s, t)
n = \text{number of nodes in } G
Array M[0 \dots n-1, V]
Define M[0, t] = 0 and M[0, v] = \infty for all other v \in V
For i = 1, \dots, n-1
For v \in V in any order
Compute M[i, v] using the recurrence (6.23)
Endfor
Endfor
Return M[n-1, s]
```

#### Bellman-Ford Algorithm

Segmented Least Squares

```
\mathsf{OPT}(i, v) = \mathsf{min}\left(\mathsf{OPT}(i-1, v), \min_{w \in V}\left(c_{vw} + \mathsf{OPT}(i-1, w)\right)\right)
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    For v \in V in any order
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  Endfor
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```

- ▶ Space used is  $O(n^2)$ . Running time is  $O(n^3)$ .
- If shortest path uses k edges, we can recover it in O(kn) time by tracing back through smaller sub-problems.

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▶ Suppose G has n nodes and  $m \ll \binom{n}{2}$  edges. Can we demonstrate a better upper bound on the running time?

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$$\sum_{v\in V}n_v=m.$$

▶ The total running time is O(mn).

# **Improving the Memory Requirements**

$$M[i,v] = \min\left(M[i-1,v], \min_{w \in N_v}\left(c_{vw} + M[i-1,w]\right)\right)$$

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Shortest Paths in Graphs

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Weighted Interval Scheduling

- 1. Maintain two arrays M and M' indexed over V.
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- ▶ Claim: at the beginning of iteration i, M stores values of  $\mathsf{OPT}(i-1,v)$  for all nodes  $v \in V$ .
- ▶ Space used is O(n).

# Computing the Shortest Path: Algorithm

$$M[v] = \min \left( M'[v], \min_{w \in N_v} \left( c_{vw} + M'[w] \right) \right)$$

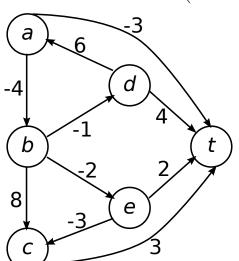
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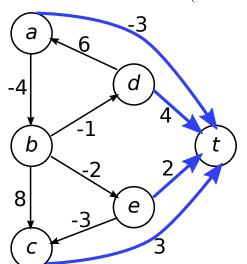
- ▶ How can we recover the shortest path that has cost M[v]?
- For each node v, maintain f(v), the first node after v in the current shortest path from v to t.
- ▶ To update f(v), if we ever set M[v] to  $\min_{w \in N_v} (c_{vw} + M'[w])$ , set f(v) to be the node w that attains this minimum.
- ▶ At the end, follow f(v) pointers from s to t.

$$M[v] = \min \left( M'[v], \min_{w \in N_v} \left( c_{vw} + M'[w] \right) \right)$$



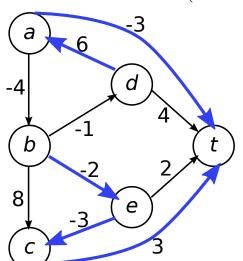
		,	/			
	0	1	2	3	4	5
t	0	0	0	0	0	0
а	∞					
b	∞					
С	$\infty$					
d	∞					
e	∞					

$$M[v] = \min \left( M'[v], \min_{w \in N_v} \left( c_{vw} + M'[w] \right) \right)$$



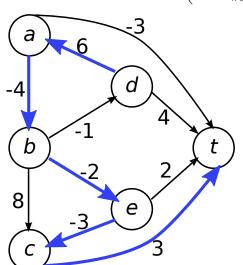
	0	1	<u></u>	3	4	5
t	0	0	0	0	0	0
a	8	-3				
b	8	∞				
C	8	3				
d	8	4				
e	8	2				

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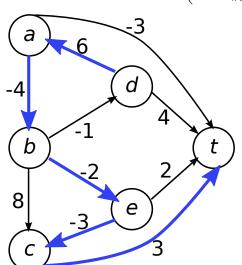
			/			
	0	1	2	3	4	5
t	0	0	0	0	0	0
a	8	-3	-3			
b	8	8	0			
C	8	3	3			
d	8	4	3			
9	8	2	0			

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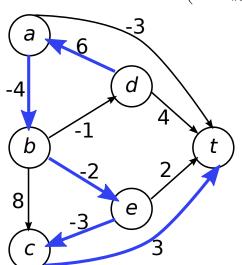
			/			
	0	1	2	3	4	5
t	0	0	0	0	0	0
a	8	-3	-3	-4		
b	8	8	0	-2		
c	8	3	3	3		
d	8	4	3	3		
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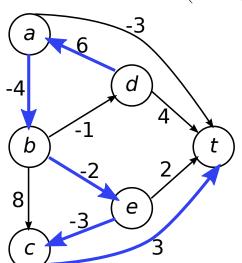
			/			
	0	1	2	3	4	5
t	0	0	0	0	0	0
a	8	-3	-3	-4	-6	
b	8	8	0	-2	-2	
C	8	3	3	3	3	
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e	8	2	0	0	0	

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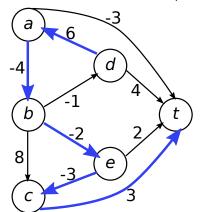
/			/			
	0	1	2	3	4	5
t	0	0	0	0	0	0
	8					
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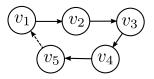


	0	1	2	3	4	5
t	0	0	0	0	0	0
a	8	-3	-3	-4	-6	-6
b	8	8	0	-2	-2	-2
C	8	3	3	3	3	3
d	8	4	3	3	2	0
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- ▶ Pointer graph P(V, F): each edge in F is (v, f(v)).
  - Can P have cycles?
  - ▶ Is there a path from s to t in P?
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  - Which of these is the shortest path?

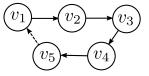


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t	0	0	0	0	0	0
а	8	-3	-3	-4	-6	-6
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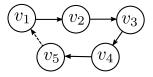
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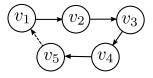
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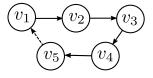
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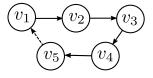
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  - ▶  $M[v_i] M[v_{i+1}] \ge c_{v_i v_{i+1}}$ , for all  $1 \le i < k-1$ .
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- ▶ Corollary: if G has no negative cycles that P does not either.

### **Computing the Shortest Path: Paths in** *P*

- ▶ Let *P* be the pointer graph upon termination of the algorithm.
- ▶ Consider the path  $P_v$  in P obtained by following the pointers from v to  $f(v) = v_1$ , to  $f(v_1) = v_2$ , and so on.

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- Claim:  $P_v$  is the shortest path in G from v to t.

# **Bellman-Ford Algorithm: One Array**

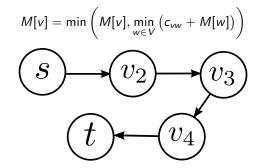
$$M[v] = \min\left(M[v], \min_{w \in N_v} \left(c_{vw} + M[w]\right)\right)$$

▶ We can prove algorithm's correctness in this case as well.

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- ▶ In general, after i iterations, the path whose length is M[v] may have many more than i edges.
- ► Early termination: If *M* does not change after processing all the nodes, we have computed all the shortest paths to *t*.