T. M. Murali

February 28, March 5, 17, 19, 21, 2013

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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

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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.

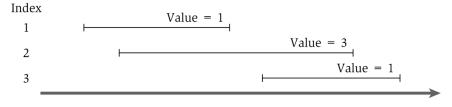


Figure 6.1 A simple instance of weighted interval scheduling.

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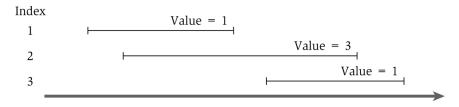


Figure 6.1 A simple instance of weighted interval scheduling.

Greedy algorithm can produce arbitrarily bad results for this problem.

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.
- ▶ 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.

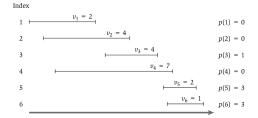
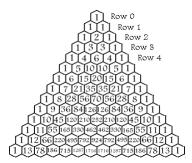


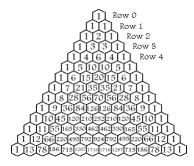
Figure 6.2 An instance of weighted interval scheduling with the functions p(j) defined for each interval j.

We will develop optimal algorithm from obvious statements about the problem. Weighted Interval Scheduling

Detour: a Binomial Identity

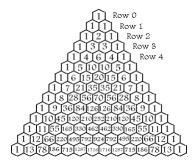


Detour: a Binomial Identity



- Pascal's triangle:
 - ▶ Each element is a binomial co-efficient.
 - Each element is the sum of the two elements above it.

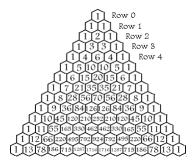
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Segmented Least Squares

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

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Case 1 job n is not in \mathcal{O} .

Case 2 job n is in \mathcal{O} .

RNA Secondary Structure

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 - O cannot use incompatible jobs $\{p(n)+1,p(n)+2,\ldots,n-1\}.$
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 - O cannot use incompatible jobs $\{p(n)+1, p(n)+2, \ldots, n-1\}.$
 - ightharpoonup Remaining jobs in $\mathcal O$ must be the optimal solution for jobs $\{1, 2, \ldots, p(n)\}.$
- O must be the best of these two choices!
- Suggests finding optimal solution for sub-problems consisting of jobs $\{1, 2, ..., j - 1, j\}$, for all values of j.

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$$OPT(j) = max(v_j + OPT(p(j)), OPT(j-1))$$

▶ When does request j belong to \mathcal{O}_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}_i ? If and only if $v_i + \mathsf{OPT}(p(i)) > \mathsf{OPT}(i-1)$.

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
```

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(v_j + \text{Compute-Opt}(\texttt{p(j)}), \text{ Compute-Opt}(j-1)) \\ & \text{Endif} \end{split}
```

Correctness of algorithm follows by induction.



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.

Example of Recursive Algorithm

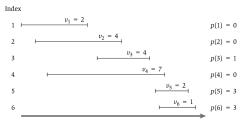


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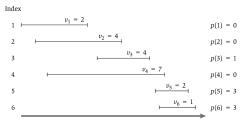


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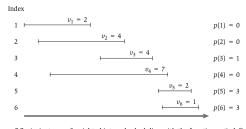
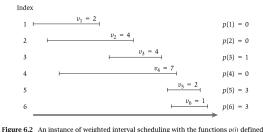


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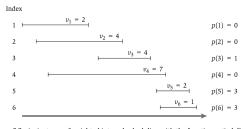


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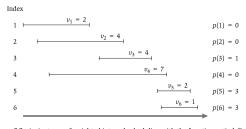


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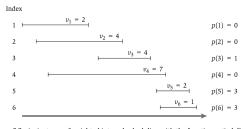


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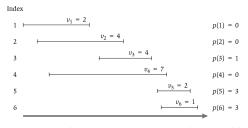


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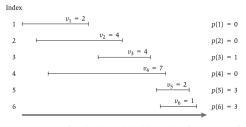


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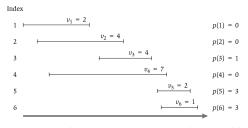


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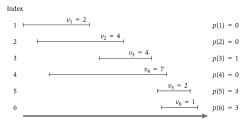


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OPT(2) = \max(v_2 + \text{OPT}(p(2)), \text{OPT}(1)) = \max(4 + \text{OPT}(0), \text{OPT}(1)) = 4

OPT(1) = v_1 = 2

OPT(0) = 0
```

Optimal solution is

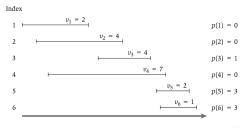


Figure 6.2 An instance of weighted interval scheduling with the functions p(j) defined for each interval j.

```
OPT(6) = \max(v_6 + \text{OPT}(p(6)), \text{OPT}(5)) = \max(1 + \text{OPT}(3), \text{OPT}(5)) = 8

OPT(5) = \max(v_5 + \text{OPT}(p(j)), \text{OPT}(4)) = \max(2 + \text{OPT}(3), \text{OPT}(4)) = 8

OPT(4) = \max(v_4 + \text{OPT}(p(4)), \text{OPT}(3)) = \max(7 + \text{OPT}(0), \text{OPT}(3)) = 7

OPT(3) = \max(v_3 + \text{OPT}(p(3)), \text{OPT}(2)) = \max(4 + \text{OPT}(1), \text{OPT}(2)) = 6

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OPT(1) = v_1 = 2

OPT(0) = 0
```

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

```
\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(j)}), \text{ Compute-Opt}(j-1)) \\ & \text{Endif} \end{split}
```

```
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
```

▶ What is the running time of the algorithm?

```
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```

 \triangleright What is the running time of the algorithm? Can be exponential in n.

```
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```

- \blacktriangleright 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 6.4 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.

Memoisation

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

Sequence Alignment

Memoisation

► Store OPT(i) 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[i]
  Else
   Define M[j] = \max(v_i + M - Compute - Opt(p(j)), M - Compute - Opt(j-1))
    Return M[i]
  Endif
```

Running Time of Memoisation

```
M-Compute-Opt(j)
  If i = 0 then
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  Else if M[i] is not empty then
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  Else
   Define M[j] = \max(v_i + M - Compute - Opt(p(j)), M - Compute - Opt(j-1))
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Claim: running time of this algorithm is O(n) (after sorting).

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  Endif
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- 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?

Running Time of Memoisation

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  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?
- Use number of filled entries in M as a measure of progress.
- 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}_i in addition to OPT(j).

Weighted Interval Scheduling

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.

```
\begin{aligned} &\text{Find-Solution}(j) \\ &\text{If } j = 0 \text{ then} \\ &\text{Output nothing} \\ &\text{Else} \\ &\text{If } v_j + M[p(j)] \geq M[j-1] \text{ then} \\ &\text{Output } j \text{ together with the result of Find-Solution}(p(j)) \\ &\text{Else} \\ &\text{Output the result of Find-Solution}(j-1) \\ &\text{Endif} \end{aligned}
```

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.

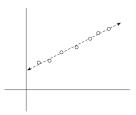
```
Iterative-Compute-Opt
  M[0] = 0
  For i = 1, 2, ..., n
    M[j] = \max(v_i + M[p(j)], M[j-1])
  Endfor
```

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.
 - 2. 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

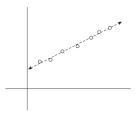
- ➤ To solve a problem, we need a collection of sub-problems that satisfy a few properties:
 - 1. There are a polynomial number of sub-problems.
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 - 3. There is a natural ordering of the sub-problems from "smallest" to "largest".
 - 4. There is an easy-to-compute 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)?



Weighted Interval Scheduling

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.



Weighted Interval Scheduling

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- ▶ How do we formalise the problem?

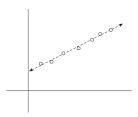


Figure 6.6 A "line of best fit."

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

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

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

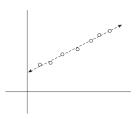


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SOLUTION: Line L: y = ax + b that minimises

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

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

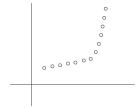


Figure 6.7 A set of points that lie approximately on two lines.

Sequence Alignment

Segmented Least Squares

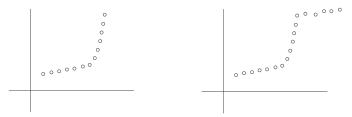


Figure 6.7 A set of points that lie approximately on two lines. Figure 6.8 A set of points that lie approximately on three lines.

Weighted Interval Scheduling

Segmented Least Squares

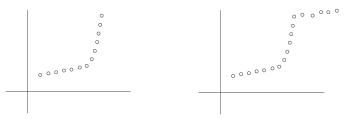


Figure 6.7 A set of points that lie approximately on two lines. Figure 6.8 A set of points that lie approximately on three lines.

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

Weighted Interval Scheduling

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.

Shortest Paths in Graphs

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 $P' = \{(x_i, y_i), (x_{i+1}, y_{i+1}), \dots, (x_{i-1}, y_{i-1}), (x_i, y_i)\}.$

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

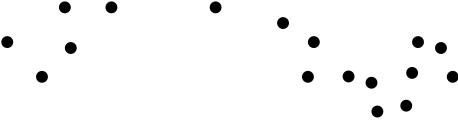
INSTANCE: Set $P = \{p_i = (x_i, y_i), 1 \le i \le n\}$ of *n* points, $x_1 < x_2 < \cdots < x_n$ and a parameter C > 0.

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

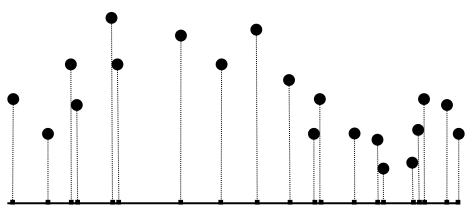
$$\sum_{i=1}^{k} \operatorname{Error}(L_j, P_j) + Ck$$

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

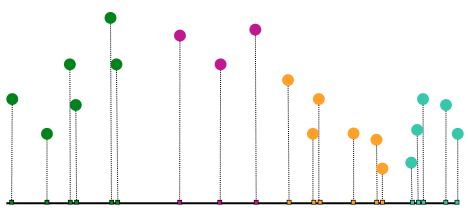




Input contains a set of two-dimensional points.



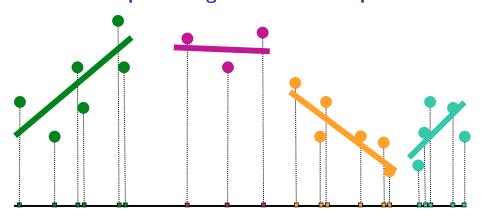
Consider the *x*-coordinates of the points in the input.



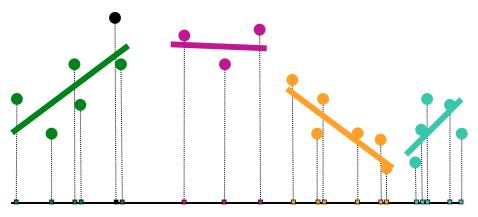
Divide the points into segments; each segment contains consecutive points in the sorted order by *x*-coordinate.

Sequence Alignment

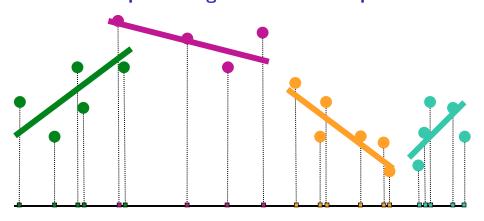
Example of Segmented Least Squares



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.

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 $e_{i,j}$ denote the minimum error of any line that fits $\{p_i, p_2, \dots, p_i\}$.
- \blacktriangleright We want to compute $\mathsf{OPT}(n)$.

Weighted Interval Scheduling

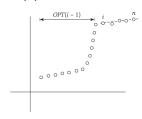


Figure 6.9 A possible solution: a single line segment fits points p_i, p_{i+1}, \dots, p_n , and then an optimal solution is found for the remaining points p_1, p_2, \dots, p_{i-1}

▶ 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

RNA Secondary Structure

- 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

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- \triangleright To obtain OPT(i), if the last segment in the optimal partition is $\{p_i, p_{i+1}, \dots, p_i\}$, then

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

Since i can take only i distinct values,

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

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

Dynamic Programming Algorithm

RNA Secondary Structure

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

```
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

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

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  Endfor
  For i = 1, 2, ..., n
    Use the recurrence (6.7) to compute M[i]
  Endfor
  Return M[n]
```

- 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 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:

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- ▶ Various rules govern secondary structure formation:
- 1. Pairs of bases match up; each base matches with ≤ 1 other base.
- 2. Adenine always matches with Uracil.
- 3. Cytosine always matches with Guanine.
- There are no kinks in the folded molecule.
- 5. Structures are "knot-free".

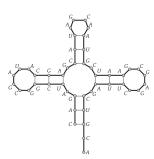


Figure 6.13 An RNA secondary structure. Thick lines connect adjacent elements of the sequence; thin lines indicate pairs of elements that are matched.

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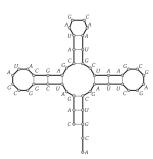


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Problem: given an RNA molecule, predict its secondary structure.

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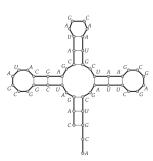


Figure 6.13 An RNA secondary structure. Thick lines connect adjacent elements of the sequence; thin lines indicate pairs of elements that are matched.

- ▶ 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

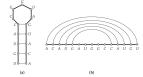


Figure 6.14 Two views of an RNA secondary structure. In the second view, (b), the string has been "stretched" lengthwise, and edges connecting matched pairs appear as noncrossing "bubbles" over the string.

- ▶ 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

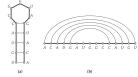
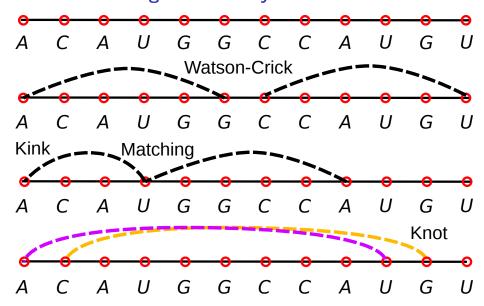
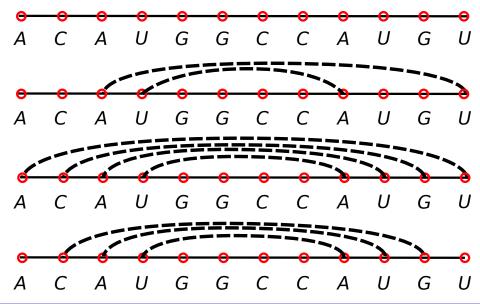


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- ▶ An RNA molecule is a string $B = b_1 b_2 \dots b_n$; each $b_i \in \{A, C, G, U\}$.
- A secondary structure on B is a set of pairs $S = \{(i, j)\}$, where $1 \le i, j \le n$ and
 - 1. (No kinks.) If $(i, j) \in S$, then i < j 4.
 - 2. (Watson-Crick) 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 < 1.
- ▶ 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.



Legal Secondary Structures



 \triangleright OPT(j) is the maximum number of base pairs in a secondary structure for $b_1b_2\ldots b_i$.

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- ▶ 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 $b_1b_2\dots b_j$

Sequence Alignment

- \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,

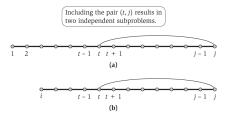


Figure 6.15 Schematic views of the dynamic programming recurrence using (a) one variable, and (b) two variables,

- ▶ OPT(i) 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 $b_1b_2 \dots b_i$
 - 1. if j is not a member of any pair, use OPT(j-1).
 - 2. if j pairs with some t < j 4, knot condition yields two independent sub-problems!

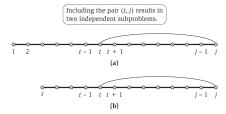


Figure 6.15 Schematic views of the dynamic programming recurrence using (a) one variable, and (b) two variables,

- ▶ OPT(j) is the maximum number of base pairs in a secondary structure for $b_1b_2...b_j$. OPT(j) = 0, if $j \le 5$.
- ▶ 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! OPT(t 1) and ???

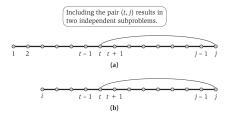


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 - 1. if j is not a member of any pair, use OPT(j-1).
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- Insight: need sub-problems indexed both by start and by end.

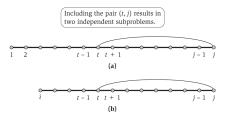


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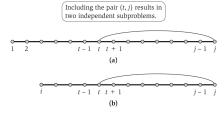


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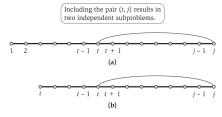


Figure 6.15 Schematic views of the dynamic programming recurrence using (a) one variable, and (b) two variables.

 \triangleright OPT(i, j) is the maximum number of base pairs in a secondary structure for $b_i b_2 \dots b_i$. OPT(i, j) = 0, if $i \ge j - 4$.

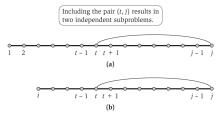


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$$\mathsf{OPT}(i,j) = \mathsf{max}\left(\begin{array}{c} \\ \end{array} \right)$$

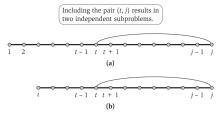


Figure 6.15 Schematic views of the dynamic programming recurrence using (a) one variable, and (b) two variables.

- ▶ OPT(i,j) is the maximum number of base pairs in a secondary structure for $b_ib_2...b_j$. OPT(i,j) = 0, if $i \ge j 4$.
- ▶ In the optimal secondary structure on $b_i b_2 \dots b_j$
 - 1. if j is not a member of any pair, compute OPT(i, j-1).

$$\mathsf{OPT}(i,j) = \mathsf{max}\left(\mathsf{OPT}(i,j-1),
ight.$$

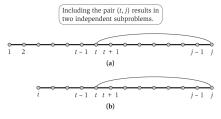


Figure 6.15 Schematic views of the dynamic programming recurrence using (a) one variable, and (b) two variables.

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- ▶ In the optimal secondary structure on $b_i b_2 ... b_i$
 - 1. if j is not a member of any pair, compute OPT(i, j-1).
 - 2. if j pairs with some t < j 4, compute $\mathsf{OPT}(i, t 1)$ and $\mathsf{OPT}(t + 1, j 1)$.

$$\mathsf{OPT}(i,j) = \mathsf{max}\left(\mathsf{OPT}(i,j-1),
ight)$$

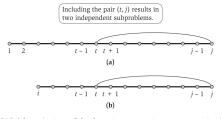


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 - 1. if i is not a member of any pair, compute OPT(i, j-1).
 - 2. if j pairs with some t < j 4, compute OPT(i, t 1) and OPT(t + 1, j 1).
- ▶ Since t can range from i to i 5,

$$\mathsf{OPT}(i,j) = \mathsf{max}\left(\mathsf{OPT}(i,j-1),
ight)$$

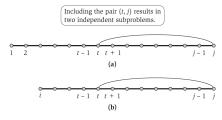
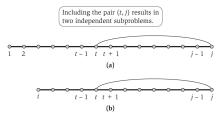


Figure 6.15 Schematic views of the dynamic programming recurrence using (a) one variable, and (b) two variables.

- ▶ OPT(i, j) is the maximum number of base pairs in a secondary structure for $b_i b_2 ... b_i$. OPT(i, j) = 0, if $i \ge j 4$.
- ▶ In the optimal secondary structure on $b_i b_2 \dots b_j$
 - 1. if j is not a member of any pair, compute OPT(i, j-1).
 - 2. if j pairs with some t < j 4, compute $\mathsf{OPT}(i, t 1)$ and $\mathsf{OPT}(t + 1, j 1)$.
- ▶ Since t can range from i to i 5,

$$\mathsf{OPT}(i,j) = \mathsf{max}\left(\mathsf{OPT}(i,j-1),\, \mathsf{max}_t \left(1 + \mathsf{OPT}(i,t-1) + \mathsf{OPT}(t+1,j-1)\right)\right)$$



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

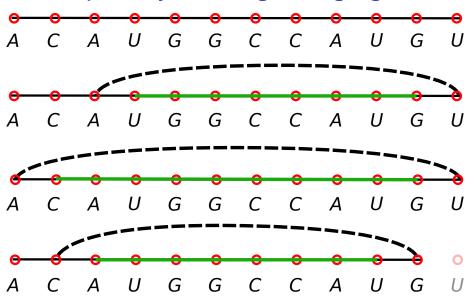
- ▶ OPT(i,j) is the maximum number of base pairs in a secondary structure for $b_ib_2...b_j$. OPT(i,j) = 0, if $i \ge j 4$.
- ▶ In the optimal secondary structure on $b_i b_2 \dots b_j$
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▶ In the "inner" maximisation, t runs over all indices between i and j-5 that are allowed to pair with j.

Weighted Interval Scheduling





Weighted Interval Scheduling

$$\mathsf{OPT}(i,j) = \mathsf{max}\left(\mathsf{OPT}(i,j-1), \mathsf{max}_t \left(1 + \mathsf{OPT}(i,t-1) + \mathsf{OPT}(t+1,j-1)\right)\right)$$

▶ There are $O(n^2)$ sub-problems.

Weighted Interval Scheduling

How do we order them from "smallest" to "largest"?

$$\mathsf{OPT}(i,j) = \mathsf{max}\left(\mathsf{OPT}(i,j-1), \mathsf{max}_t \left(1 + \mathsf{OPT}(i,t-1) + \mathsf{OPT}(t+1,j-1)\right)\right)$$

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Weighted Interval Scheduling

- How do we order them from "smallest" to "largest"?
- Note that computing OPT(i, j) involves sub-problems OPT(I, m) where m-1 < i-i.

$$\mathsf{OPT}(i,j) = \mathsf{max}\left(\mathsf{OPT}(i,j-1), \mathsf{max}_t \left(1 + \mathsf{OPT}(i,t-1) + \mathsf{OPT}(t+1,j-1)\right)\right)$$

- ▶ There are $O(n^2)$ sub-problems.
- How do we order them from "smallest" to "largest"?
- Note that computing $\mathsf{OPT}(i,j)$ involves sub-problems $\mathsf{OPT}(I,m)$ where m-l < j-i.

```
Initialize \mathsf{OPT}(i,j) = 0 whenever i \geq 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)
```

$$\mathsf{OPT}(i,j) = \mathsf{max}\left(\mathsf{OPT}(i,j-1), \mathsf{max}_t \left(1 + \mathsf{OPT}(i,t-1) + \mathsf{OPT}(t+1,j-1)\right)\right)$$

- ▶ There are $O(n^2)$ sub-problems.
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Set j = i+k

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Endfor

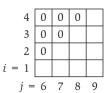
Endfor

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

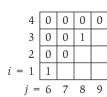
Running time of the algorithm is $O(n^3)$.

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

Filling in the values for k = 8

Weighted Interval Scheduling



▶ How do they know "Dynamic" and "Dymanic" are similar?

Sequence Similarity

- Given two strings, measure how similar they are.
- Given a database of strings and a query string, compute the string most similar to query in the database.
- Applications:
 - Online searches (Web, dictionary).
 - Spell-checkers.
 - Computational biology
 - Speech recognition.
 - Basis for Unix diff.

Defining Sequence Similarity

•	"ocurrance"	(wrong)	VS	"occurrence"	(right).
---	-------------	---------	----	--------------	----------

o-currance

occurrence

o-curr-ance occurre-nce

Defining Sequence Similarity

• "ocurrance" (wrong) vs "occurrence" (right).				
o-currance				
occurrence				
o-curr-ance				
occurre-nce				
ahhhaahhhhaah				
ababaaabbbbba-b				
abbbaabbbbaab				

Defining Sequence Similarity

"ocurrance" (wrong) vs "occurrence" (right).
-currance
ccurrence
-curr-ance
ccurre-nce
bbbaabbbbaab
pabaaabbbbba-b

- ► Edit distance model: how many changes must you to make to one string to transform it into another?
- Changes allowed are deleting a letter, adding a letter, changing a letter.

Edit Distance

- ▶ Proposed by Needleman and Wunsch in the early 1970s.
- Input: two strings $x = x_1 x_2 x_3 \dots x_m$ and $y = y_1 y_2 \dots y_n$.
- ▶ Sequences $\{1, 2, ..., m\}$ and $\{1, 2, ..., n\}$ represent positions in x and y.

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- Input: two strings $x = x_1 x_2 x_3 \dots x_m$ and $y = y_1 y_2 \dots y_n$.
- ▶ Sequences $\{1, 2, ..., m\}$ and $\{1, 2, ..., n\}$ represent positions in x and y.
- ▶ A matching of these sets is a set M of ordered pairs such that
 - 1. in each pair (i,j), $1 \le i \le m$ and $1 \le j \le n$ and
 - 2. no index from x (respectively, from y) appears as the first (respectively, second) element in more than one ordered pair.
- An index is *not matched* if it does not appear in the matching.

Weighted Interval Scheduling

- currance o-currance o-currance

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- A matching M is an alignment if there are no "crossing pairs" in M: if $(i,j) \in M$ and $(i',j') \in M$ and i < i' then j < j'.

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- Cost of an alignment is the sum of gap and mismatch penalties: Gap penalty Penalty $\delta > 0$ for every unmatched index. Mismatch penalty Penalty $\alpha_{x_iy_j} > 0$ if $(i,j) \in M$ and $x_i \neq y_j$.

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- Output: compute an alignment of minimal cost.

▶ Consider index $m \in x$ and index $n \in y$. Is $(m, n) \in M$?

- Consider index $m \in x$ and index $n \in y$. Is $(m, n) \in M$?
- Claim: $(m, n) \notin M$

- Consider index $m \in x$ and index $n \in y$. Is $(m, n) \in M$?
- Claim: $(m, n) \notin M \Rightarrow m \in x$ not matched or $n \in y$ not matched.

```
O - C u r r a n c e

Not matched with each other
```

- ▶ Consider index $m \in x$ and index $n \in y$. Is $(m, n) \in M$?
- ▶ Claim: $(m, n) \notin M \Rightarrow m \in x$ not matched or $n \in y$ not matched.
- How should we define sub-problems?

```
O C C U r r e n C e

Not matched
with each othe
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- How should we define sub-problems?
- ▶ OPT(i, j): cost of optimal alignment between $x = x_1x_2x_3...x_i$ and $y = y_1y_2...y_j$.
 - $(i,j) \in M$:

- ► Consider index $m \in x$ and index $n \in y$. Is $(m, n) \in M$?
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 - $(i,j) \in M: \mathsf{OPT}(i,j) = \alpha_{x_iy_j} + \mathsf{OPT}(i-1,j-1).$
 - *i* not matched: $OPT(i, j) = \delta + OPT(i 1, j)$.

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 - i not matched: $OPT(i,j) = \delta + OPT(i-1,j)$.
 - ▶ j not matched: $\mathsf{OPT}(i,j) = \delta + \mathsf{OPT}(i,j-1)$.

$$\mathsf{OPT}(i,j) = \min\left(\alpha_{x_iy_j} + \mathsf{OPT}(i-1,j-1), \delta + \mathsf{OPT}(i-1,j), \delta + \mathsf{OPT}(i,j-1)\right)$$

- $(i,j) \in M$ if and only if minimum is achieved by the first term.
- What are the base cases?

Weighted Interval Scheduling

RNA Secondary Structure

- Consider index $m \in x$ and index $n \in y$. Is $(m, n) \in M$?
- Claim: $(m, n) \notin M \Rightarrow m \in x$ not matched or $n \in y$ not matched.
- How should we define sub-problems?
- ▶ OPT(i, j): cost of optimal alignment between $x = x_1x_2x_3...x_i$ and $y = y_1 y_2 \dots y_i$.
 - ▶ $(i,j) \in M$: $\mathsf{OPT}(i,j) = \alpha_{x_i v_i} + \mathsf{OPT}(i-1,j-1)$.
 - i not matched: $OPT(i, j) = \delta + OPT(i 1, j)$.
 - ▶ j not matched: $\mathsf{OPT}(i,j) = \delta + \mathsf{OPT}(i,j-1)$.

$$\mathsf{OPT}(i,j) = \min \left(\alpha_{\mathsf{x}_i \mathsf{y}_j} + \mathsf{OPT}(i-1,j-1), \delta + \mathsf{OPT}(i-1,j), \delta + \mathsf{OPT}(i,j-1) \right)$$

- $(i,j) \in M$ if and only if minimum is achieved by the first term.
- ▶ What are the base cases? $OPT(i, 0) = OPT(0, i) = i\delta$.

Weighted Interval Scheduling

Dynamic Programming Algorithm

$$\mathsf{OPT}(i,j) = \mathsf{min}\left(\alpha_{\mathsf{x}_i\mathsf{y}_j} + \mathsf{OPT}(i-1,j-1), \delta + \mathsf{OPT}(i-1,j), \delta + \mathsf{OPT}(i,j-1)\right)$$

```
Alignment(X,Y)
  Array A[0...m,0...n]
  Initialize A[i,0] = i\delta for each i
  Initialize A[0, j] = i\delta for each j
  For i = 1, \ldots, n
     For i = 1, ..., m
          Use the recurrence (6.16) to compute A[i, i]
     Endfor
  Endfor
  Return A[m, n]
```

Dynamic Programming Algorithm

$$\mathsf{OPT}(i,j) = \mathsf{min}\left(\alpha_{\mathsf{x}_i\mathsf{y}_j} + \mathsf{OPT}(i-1,j-1), \delta + \mathsf{OPT}(i-1,j), \delta + \mathsf{OPT}(i,j-1)\right)$$

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Running time is O(mn). Space used in O(mn).

```
\mathsf{OPT}(i,j) = \mathsf{min}\left(\alpha_{\mathsf{x}_i\mathsf{y}_j} + \mathsf{OPT}(i-1,j-1), \delta + \mathsf{OPT}(i-1,j), \delta + \mathsf{OPT}(i,j-1)\right)
```

```
\begin{aligned} & \text{Alignment}(X,Y) \\ & \text{Array } A[0\dots m,0\dots n] \\ & \text{Initialize } A[i,0] = i\delta \text{ for each } i \\ & \text{Initialize } A[0,j] = j\delta \text{ for each } j \\ & \text{For } j = 1,\dots,n \\ & \text{For } i = 1,\dots,m \\ & \text{Use the recurrence (6.16) to compute } A[i,j] \\ & \text{Endfor} \\ & \text{Endfor} \\ & \text{Return } A[m,n] \end{aligned}
```

- ▶ Running time is O(mn). Space used in O(mn).
- ▶ Can compute OPT(m, n) in O(mn) time and O(m + n) space (Hirschberg 1975, Chapter 6.7).

```
\mathsf{OPT}(i,j) = \mathsf{min}\left(\alpha_{\mathsf{x}_i\mathsf{y}_j} + \mathsf{OPT}(i-1,j-1), \delta + \mathsf{OPT}(i-1,j), \delta + \mathsf{OPT}(i,j-1)\right)
```

```
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Array A[0 \dots m, 0 \dots n]

Initialize A[i,0] = i\delta for each i

Initialize A[0,j] = j\delta for each j

For j=1,\dots,n

Use the recurrence (6.16) to compute A[i,j]

Endfor

Endfor

Return A[m,n]
```

- ▶ Running time is O(mn). Space used in O(mn).
- ► Can compute OPT(m, n) in O(mn) time and O(m + n) space (Hirschberg 1975, Chapter 6.7).
- ► Can compute *alignment* in the same bounds by combining dynamic programming with divide and conquer.

Graph-theoretic View of Sequence Alignment

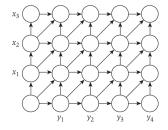


Figure 6.17 A graph-based picture of sequence alignment.

- Grid graph G_{xv} :
 - Rows labelled by symbols in x and columns labelled by symbols in y.
 - Edges from node (i, j) to (i, j + 1), to (i + 1, j), and to (i + 1, j + 1).
 - Edges directed upward and to the right have cost δ .
 - Edge directed from (i,j) to (i+1,j+1) has cost $\alpha_{x_{i+1}y_{i+1}}$.

Graph-theoretic View of Sequence Alignment

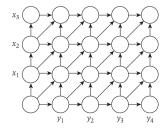


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- Grid graph G_{xy} :
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 - ▶ Edges from node (i,j) to (i,j+1), to (i+1,j), and to (i+1,j+1).
 - Edges directed upward and to the right have cost δ .
 - ▶ Edge directed from (i,j) to (i+1,j+1) has cost $\alpha_{x_{i+1}y_{i+1}}$.
- f(i, j): minimum cost of a path in G_{XY} from (0, 0) to (i, j).
- ▶ Claim: $f(i,j) = \mathsf{OPT}(i,j)$ and diagonal edges in the shortest path are the matched pairs in the alignment.

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:
 - 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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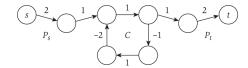


Figure 6.20 In this graph, one can find *s-t* paths of arbitrarily negative cost (by going around the cycle *C* many times).

Approaches for Shortest Path Algorithm

1. Dijsktra's algorithm.

2. Add some large constant to each edge.

1. Dijsktra's algorithm. Computes incorrect answers because it is greedy.

Weighted Interval Scheduling

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.

Assume G has no negative cycles.

Weighted Interval Scheduling

Claim: There is a shortest path from s to t that is simple (does not repeat a node)

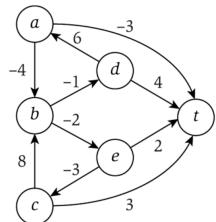
- Assume G has no negative cycles.
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- ► How do we define sub-problems?
 - ▶ Shortest s-t path has < n-1edges: how we can reach t using i edges, for different values of *i*?
 - We do not know which nodes will be in shortest s-t path: how we can reach t from each node in V?

▶ Assume *G* has no negative cycles.

- ▶ 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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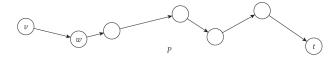


Figure 6.22 The minimum-cost path P from v to t using at most i edges.

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

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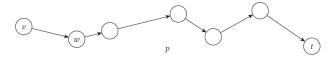


Figure 6.22 The minimum-cost path P from v to t using at most i edges.

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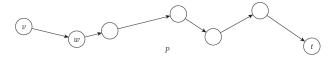
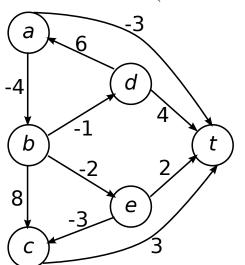


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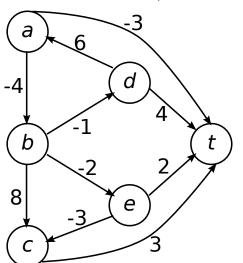
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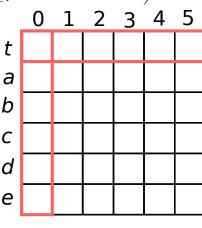
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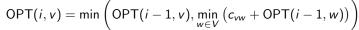
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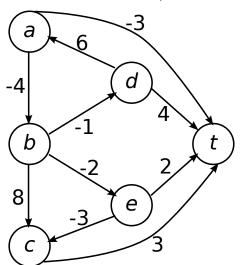




T. M. Murali

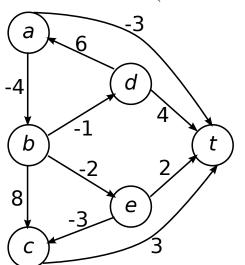
Weighted Interval Scheduling





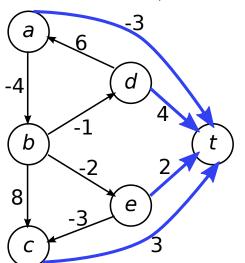
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$$\mathsf{OPT}(i, v) = \min\left(\mathsf{OPT}(i-1, v), \min_{w \in V}\left(c_{vw} + \mathsf{OPT}(i-1, w)\right)\right)$$



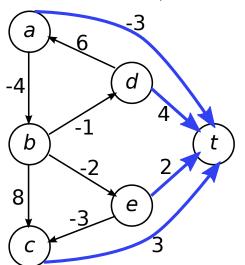
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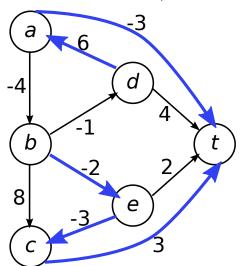
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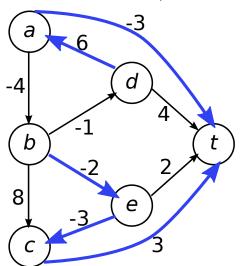
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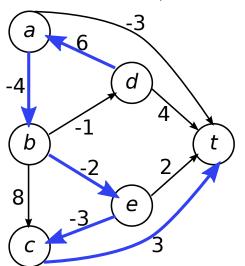
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d	8	4	3			
e	8	2	0			

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



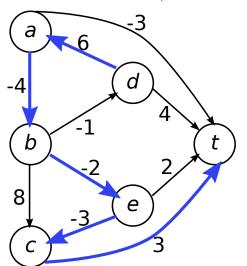
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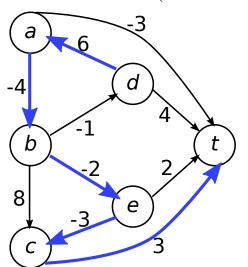
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d	8	4	3	3		
e	8	2	0	0		
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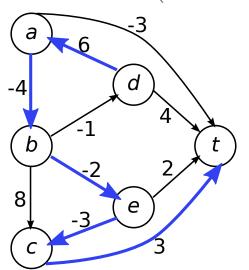
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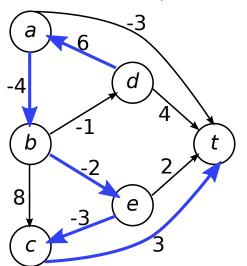
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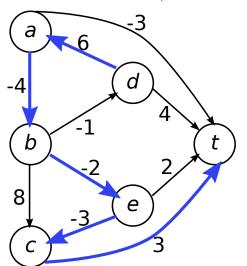
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d	8	4	3	3	2	
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b	8	8	0	-2	-2	-2
c	8	3	3	3	3	3
d	8	4	3	3	2	0
e	8	2	0	0	0	0

▶ OPT(i, v): minimum cost of a v-t path that uses exactly i edges. Goal is to compute

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RNA Secondary Structure

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Compare the two desired solutions:

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

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

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 = number of nodes in G
  Array M[0...n-1, V]
  Define M[0,t]=0 and M[0,v]=\infty for all other v \in V
  For i = 1, ..., 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]
```

Sequence Alignment

Bellman-Ford Algorithm

```
\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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    Endfor
  Endfor
  Return M[n-1,s]
```

- ▶ 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.

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

An Improved Bound on the Running Time

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- If n_v is the number of neighbours of v, then in each round, we spend time equal to

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- w only needs to range over neighbours of v.
- If n_v is the number of neighbours of v, then in each round, we spend time equal to

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

▶ The total running time is O(mn).

Improving the Memory Requirements

RNA Secondary Structure

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

▶ The algorithm uses $O(n^2)$ space to store the array M.

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- Modified algorithm:

- 1. Maintain two arrays M and M' indexed over V.
- 2. At the beginning of each iteration, copy M into M'.
- 3. To update M, use

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

- ▶ Claim: at the beginning of iteration i, M stores values of OPT(i-1, v) for all nodes $v \in V$.
- \triangleright Space used is O(n).

Computing the Shortest Path: Algorithm

RNA Secondary Structure

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

How can we recover the shortest path that has cost M[v]?

Computing the Shortest Path: Algorithm

RNA Secondary Structure

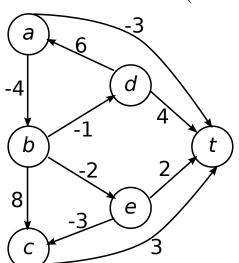
$$M[v] = \min \left(M'[v], \min_{w \in V} \left(c_{vw} + M'[w] \right) \right)$$

- 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 $\min_{w \in V} (c_{vw} + M'[w])$, set f(v) to be the node w that attains this minimum.
- At the end, follow f(v) pointers from s to t.

Weighted Interval Scheduling

Example of Maintaining Pointers

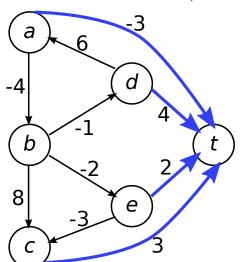
$$M[v] = \min \left(M'[v], \min_{w \in N_v} \left(c_{vw} + M'[w] \right) \right)$$



	0	1	2	3	4	5
t	0		0			
a	∞					
b	∞					
С	∞					
d	∞					
e	∞					

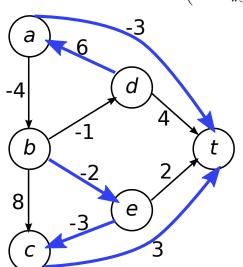
T. M. Murali

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



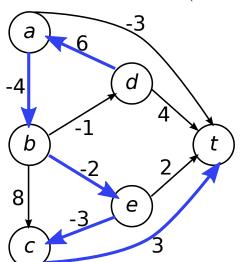
	0	1	<u></u>	3	4	5
t	0	0	0	0	0	0
a	8	-3				
b	8	∞				
C	8	3				
d	8	4				
e	8	2				

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



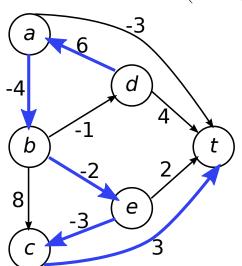
			/			
	0	1	2	3	4	5
t	0	0	0	0	0	0
a	8	-3	-3			
b	8	8	0			
C	8	3	3			
d	8	4	3			
e	8	2	0			

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



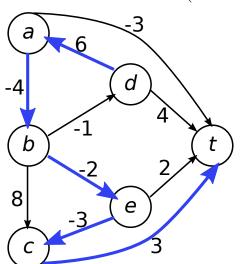
	0	1	[^] 2	3	4	5
t	0	0	0	0	0	0
a	8		-3	-4		
b	8	8	0	-2		
C	8	3	3	3		
d	8	4	3	3		
e	8	2	0	0		

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



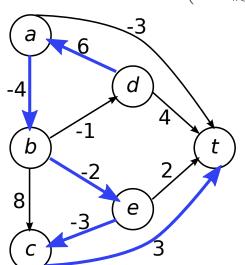
			/			
	0	1	2	3	4	5
t	0	0	0		0	0
٠.	8	-3	-3	-4	-6	
b	8	8	0	-2	-2	
C	8	3	3	3	3	
d	8	4	3	3	2	
e	8	2	0	0	0	

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



V			/			
	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
С	8	3	3	3	3	3
d	8	4	3	3	2	0
e	8	2	0	0	0	0

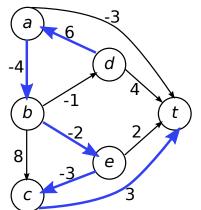
$$M[v] = \min \left(M'[v], \min_{w \in N_v} \left(c_{vw} + M'[w] \right) \right)$$



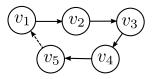
	0	1	2	3	4	5
t	0	0	0	0	0	0
						-6
b	8	8	0	-2	-2	-2
C	8	3	3	3	3	3
d	8	4	3	3	2	0
e	8	2	0	0	0	0

Computing the Shortest Path: Correctness

- ▶ 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?
 - Can there be multiple paths s to t in P?
 - Which of these is the shortest path?



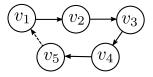
	0	1	2	3	4	5
t	0		0		0	0
a	8	-3	-3	-4	-6	-6
b	8	8	0	-2	-2	-2
C	8	3	3	3	3	3
d	8	4	3	3	2	0
e	8	2	0	0	0	0



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

▶ Claim: If P has a cycle C, then C has negative cost.

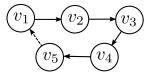
RNA Secondary Structure



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

- ▶ Claim: If P has a cycle C, then C has negative cost.
 - ▶ Suppose we set f(v) = w. Between this assignment and the assignment of f(v) to some other node, $M[v] \ge c_{vw} + M[w]$ (because M[w] may itself decrease).

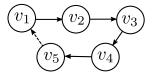
RNA Secondary Structure



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 - Let $v_1, v_2, \dots v_k$ be the nodes in C and assume that (v_k, v_1) is the last edge to have been added.
 - What is the situation just before this addition?

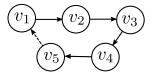
RNA Secondary Structure



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 - ▶ $M[v_i] M[v_{i+1}] \ge c_{v_i v_{i+1}}$, for all $1 \le i < k-1$.
 - $M[v_k] M[v_1] > c_{v_k,v_1}$

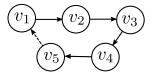
RNA Secondary Structure



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 - Adding all these inequalities, $0 > \sum_{i=1}^{k-1} c_{v_i v_{i+1}} + c_{v_k v_1} = \text{cost of } C$.

RNA Secondary Structure



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 - Adding all these inequalities, $0 > \sum_{i=1}^{k-1} c_{v_i v_{i+1}} + c_{v_k v_1} = \text{cost of } C$.
- 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.

Sequence Alignment

Computing the Shortest Path: Paths in *P*

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- ► Claim: P_v terminates at t.
- Claim: P_v is the shortest path in G from v to t.

Bellman-Ford Algorithm: One Array

RNA Secondary Structure

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

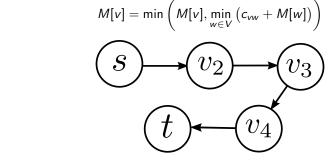
We can prove algorithm's correctness in this case as well.

Bellman-Ford Algorithm: Early Termination

▶ In general, after i iterations, the path whose length is M[v] may have many more than i edges.

Bellman-Ford Algorithm: Early Termination

RNA Secondary Structure



- 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.