Dynamic Programming

T. M. Murali

October 14, 19, 21, 26, 28, 2009

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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

Bellman pioneered the systematic study of dynamic programming in the 1950s.

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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 (CS 6604, MCB 110, 3:30-4:45pm on Oct 15).
- 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 $v_i > 0$ associated with each job.

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

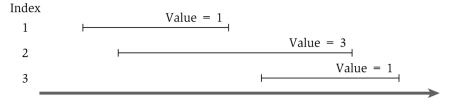


Figure 6.1 A simple instance of weighted interval scheduling.

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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.

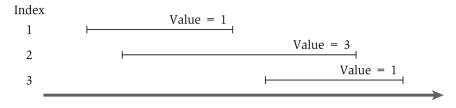


Figure 6.1 A simple instance of weighted interval scheduling.

Greedy algorithm can produce arbitrarily bad results for this problem.

Approach

- ▶ Sort jobs in increasing order of finish time and relabel: $f_1 \le f_2 \le ... \le f_n$.
- Request *i* comes before request *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.
 - ▶ Jobs at indices $\{p(j) + 1, p(j) + 2, ..., j 1\}$ are incompatible with job j.

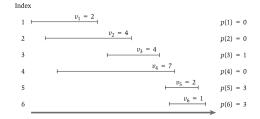
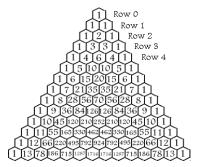


Figure 6.2 An instance of weighted interval scheduling with the functions p(j) defined for each interval j.

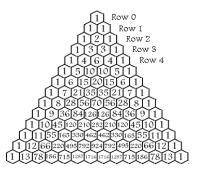
We will develop optimal algorithm from obvious statements about the problem.

Detour: a Binomial Identity

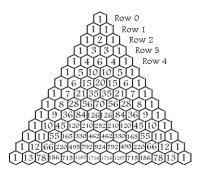


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Detour: a Binomial Identity



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



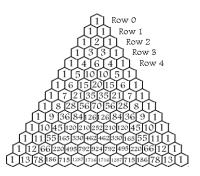
Segmented Least Squares

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Segmented Least Squares

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

- Proof: Consider any subset *S* of *r* elements.
 - Case 1 S contains the nth element: $\binom{n-1}{r-1}$ such subsets.
 - Case 2 S does not contain the nth element: $\binom{n-1}{r}$ such subsets.

▶ Let \mathcal{O} be the optimal solution. Let us reason about \mathcal{O} . Case 1 job n is not in \mathcal{O} .

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RNA Secondary Structure

- Let \mathcal{O} be the optimal solution. Let us reason about \mathcal{O} .
 - Case 1 job n is not in \mathcal{O} . \mathcal{O} must be the optimal solution for jobs $\{1, 2, \ldots, n-1\}.$
 - Case 2 job n is in \mathcal{O} .
 - 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 $\{1, 2, ..., j 1, j\}$, for all values of j.

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Final recurrence:

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

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▶ To compute \mathcal{O}_i : 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
```

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Correctness of algorithm follows by induction.

Example of Recursive Algorithm

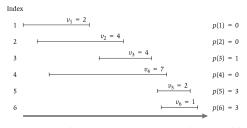


Figure 6.2 An instance of weighted interval scheduling with the functions p(j) defined for each interval j.

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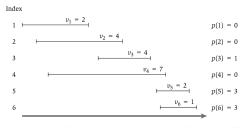


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OPT(4) = \max(v_4 + OPT(p(4)), OPT(3)) = \max(7 + OPT(0), OPT(3))

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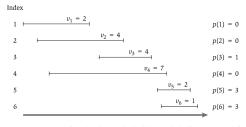


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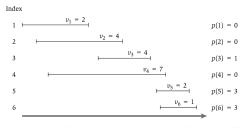


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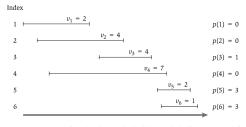


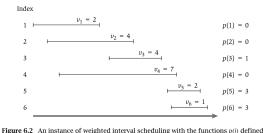
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for each interval i.

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OPT(3) = max(v_3 + OPT(p(3)), OPT(2)) = max(4 + OPT(1), OPT(2)) = 6
OPT(2) = max(v_2 + OPT(p(2)), OPT(1)) = max(4 + OPT(0), OPT(1)) = 4
OPT(1) = v_1 = 2
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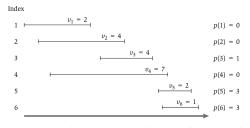


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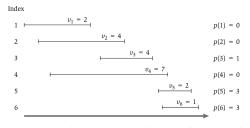


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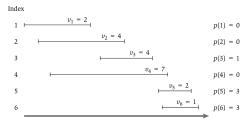


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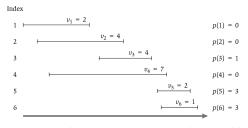


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Optimal solution is

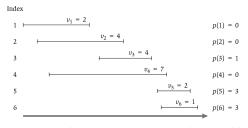


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```

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

```
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
```

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

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  Endif
```

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

Sequence Alignment

Memoisation

▶ 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

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

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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?

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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?
- 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).

Computing \mathcal{O} in Addition to OPT(n)

Computing \mathcal{O} in Addition to OPT(n)

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

Weighted Interval Scheduling

Computing \mathcal{O} in Addition to OPT(n)

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

Computing \mathcal{O} in Addition to OPT(n)

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

Computing \mathcal{O} in Addition to OPT(n)

- **Explicitly store** \mathcal{O}_j in addition to OPT(j). Running time becomes $O(n^2)$.
- ▶ Recall: request j belongs to \mathcal{O}_j if and only if $v_j + \mathsf{OPT}(p(j)) \ge \mathsf{OPT}(j-1)$.
- ▶ Can recover 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.

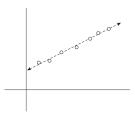
```
Iterative-Compute-Opt
  M[0] = 0
  For i = 1, 2, ..., n
    M[j] = \max(v_i + M[p(j)], M[j-1])
  Endfor
```

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".
 - 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

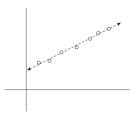
- ▶ To solve a problem, we need a collection of sub-problems that satisfy a few properties:
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 - 3. There is a natural ordering of the sub-problems from "smallest" to "largest".
 - 4. There is an easy-to-compute recurrence that allows us to compute the 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.



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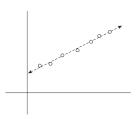


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Least Squares

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

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

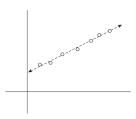


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Solution is achieved by

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

Segmented Least Squares

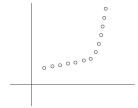


Figure 6.7 A set of points that lie approximately on two lines.

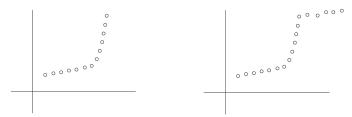


Figure 6.7 A set of points that lie approximately on two lines. Figure 6.8 A set of points that lie approximately on three lines.

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.

Segmented Least Squares

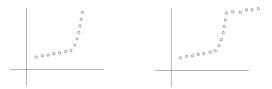


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Weighted Interval Scheduling

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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 $\{P_1, P_2, \ldots, P_k\}$, k lines $L_j: y = a_j x + b_j, 1 \le j \le k$ 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



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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

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

▶ 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 $e_{i,j}$ 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

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

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.

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

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

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

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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.

T. M. Murali

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:

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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.
- Cytosine always matches with Guanine.
- 4 There are no kinks in the folded molecule.
- 5. Structures are "knot-free".

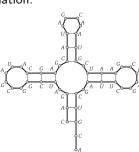


Figure 6.13 An RNA secondary structure. Thick lines connect adjacent elements of the sequence; thin lines indicate pairs of elements that are matched.

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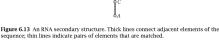
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sequence; thin lines indicate pairs of elements that are matched.

- 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

- ▶ 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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- 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 < i < 1.

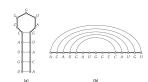


Figure 6.14 Two views of an RNA secondary structure. In the second view, (b), the string has been "stretched" lengthwise, and edges connecting matched pairs appear as noncrossing "bubbles" over the string

 \triangleright The energy of a secondary structure \propto the number of base pairs in it.

 \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 $b_1b_2 \dots b_j$
 - 1. if j is not a member of any pair, use OPT(j-1).

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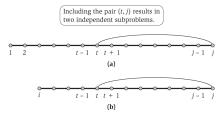


Figure 6.15 Schematic views of the dynamic programming recurrence using (a) one variable, and (b) two variables.

- ▶ 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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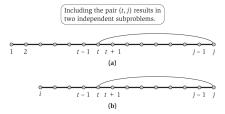


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 - 1. if j is not a member of any pair, use OPT(j-1).
 - 2. if j pairs with some t < j 4, knot condition yields two independent sub-problems! OPT(t-1) and ???
- Insight: need sub-problems indexed both by start and by end.

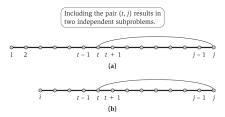


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 \triangleright OPT(i, j) is the maximum number of base pairs in a secondary structure for $b_i b_2 \dots b_i$.

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Sequence Alignment

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 - 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 OPT(i, t 1) and OPT(t + 1, j 1).

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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.

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

- ▶ There are $O(n^2)$ sub-problems.
- How do we order them from "smallest" to "largest"?

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

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

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

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

Set j = i+k

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

Endfor

Endfor

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

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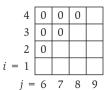
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Running time of the algorithm is $O(n^3)$.

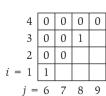
Example of Algorithm

RNA sequence ACCGGUAGU



Weighted Interval Scheduling

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

Google Search for "Dymanic Programming"



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

Sequence Alignment

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

o-currance occurrence

o-curr-ance occurre-nce

abbbaa--bbbbaab ababaaabbbbba-b

Defining Sequence Similarity

o-currance
occurrence
o-currance
occurrence
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- ► 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.

o-currance occurrence

o-curr-ance occurre-nce

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

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- ▶ Sets $\{1, 2, ..., m\}$ 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.

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o-currance occurrence

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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 $\alpha_{x_iy_i} > 0$ if $(i,j) \in M$ and $x_i \neq y_j$.

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Weighted Interval Scheduling

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- Output: compute an alignment of minimal cost.

Dynamic Programming Approach

▶ 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 $(m, n) \in M$?
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- Dynamic Frogramming Approach
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 - ▶ 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?

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

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 \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

For i=1,\dots,m

Use the recurrence (6.16) to compute A[i,j]
Endfor
Endfor
Return A[m,n]
```

Dynamic Programming Algorithm

```
\mathsf{OPT}(i,j) = \min \left( \alpha_{\mathsf{x};\mathsf{v}_i} + \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]
```

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

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

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).
- ► 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

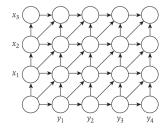


Figure 6.17 A graph-based picture of sequence alignment.

- 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

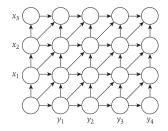


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- Grid graph G_{xy} :
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 - ▶ Edges from node (i,j) to (i,j+1), to (i+1,j), and to (i+1,j+1).
 - Edges directed upward and to the right have cost δ .
 - ▶ Edge directed from (i,j) to (i+1,j+1) has cost $\alpha_{x_{i+1}y_{j+1}}$.
- 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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- ► 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?

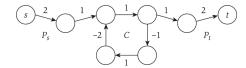


Figure 6.20 In this graph, one can find s-t paths of arbitrarily negative cost (by going around the cycle C many times).

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

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 5-t path.

- Assume G has no negative cycles.
- 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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Assume G has no negative cycles.

Weighted Interval Scheduling

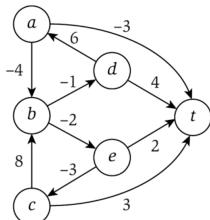
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- ▶ How do we define sub-problems?

- 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-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.

Weighted Interval Scheduling

- ▶ 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.



Dynamic Programming Recursion

- ▶ 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).

Dynamic Programming Recursion

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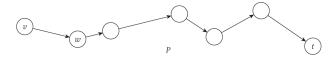


Figure 6.22 The minimum-cost path P from v to t using at most i edges.

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

RNA Secondary Structure

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Weighted Interval Scheduling

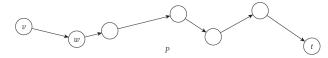


Figure 6.22 The minimum-cost path P from v to t using at most i edges.

- 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).
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Weighted Interval Scheduling

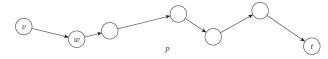
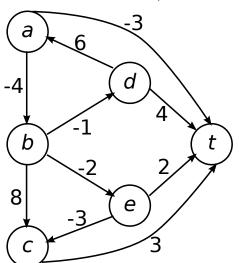


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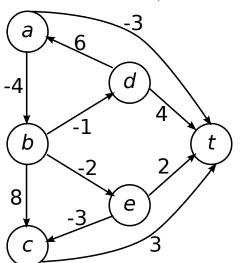


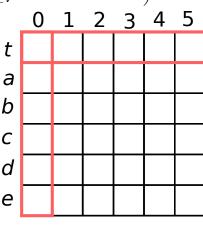
= V					/	
	0	1	2	3	4	5
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Weighted Interval Scheduling

Example of Dynamic Programming Recursion

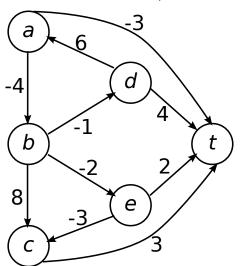
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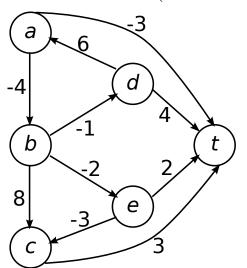
T. M. Murali

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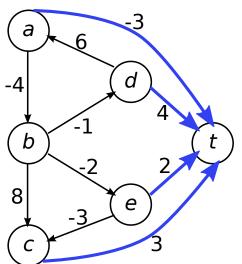
∈ <i>V</i> `			•	• • •	/	
	0	1	2	3	4	5
t	0	0	0	0	0	0
а	∞					
b	∞					
С	∞					
d	∞					
e	∞			·		

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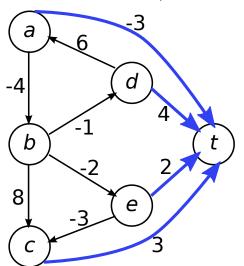
= V					/	
	0	1	2	3	4	5
t	0	0	0	0	0	0
a b	8					
b	8					
С	8					
d	8					
e	8					

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



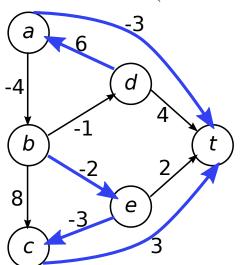
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\in V$ `				. ,	/	
		0	1	2	3	4	5
a ∞ -3	t	0	0	0	0	0	0
	a	8	-3				
$b \infty \infty$	b	8	∞				
c ∞ 3	С	8	3				
d ∞ 4	d	8	4				
e ∞ 2	e	8	2				

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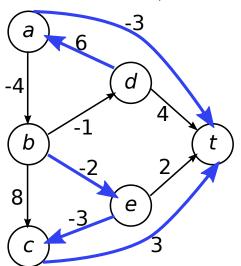
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	∈ <i>V</i> `			`	. ,,	/	
a ∞ -3 b ∞ ∞ c ∞ 3 d ∞ 4		0	1	2	3	4	5
b ∞ ∞ c ∞ 3 d ∞ 4	t	0	0	0	0	0	0
c ∞ 3 d ∞ 4	а	8	-3				
d ∞ 4	b	8	8				
	C	8	3				
e ∞ 2	d	8	4				
	e	8	2				

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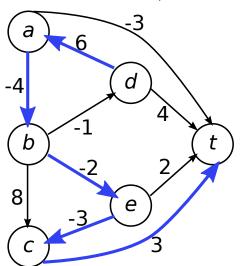
- v					/	
	0	1	2	3	4	5
t	0	0	0	0	0	0
a	8	-3	-3			
b	8	8	0			
С	8	3	3			
d	8	4	3			
e	8	2	0			

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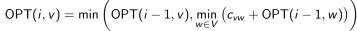


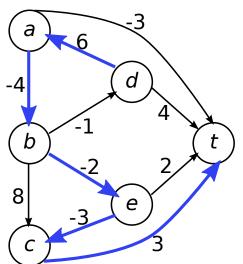
= v					/	
	0	1	2	3	4	5
t	0	0	0	0	0	0
a	8	ო	-3			
b	8	8	0			
С	8	3	3			
d	8	4	3			
e	8	2	0			

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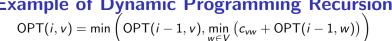


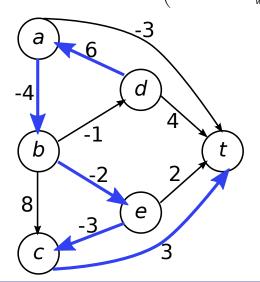
= V					/	
	0	1	2	3	4	5
t	0	0	0	0	0	0
a	8	-3	-3	-4		
b	8	8	0	-2		
C	8	3	3	3		
d	8	4	3	3		
e	8	2	0	0		
	•			,		•





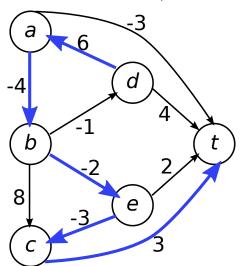
: V					/	
	0	1	2	3	4	5
t	0		0	0	0	0
a	8	-3	-3	-4		
b	8	8	0	-2		
C	8	3	3	3		
d	8	4	3	3		
e	8	2	0	0		





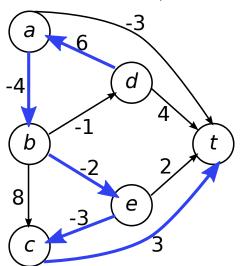
įV`	•••		`	' ')	/	
	0	1	2	3	4	5
t	0		0	0	0	0
a	8	-3	-3	-4	-6	
b	8	8	0	-2	-2	
C	8	3	3	3	3	
d	8	4	3	3	2	
e	8	2	0	0	0	

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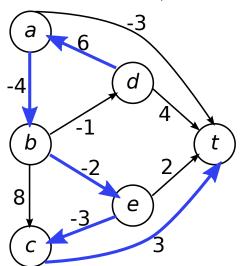
⊂ v					/	
	0	1	2	3	4	5
t	0	0	0	0	0	0
a	8	-3	-3	-4	-6	
b	8	8	0	-2	-2	
C	8	3	3	3	3	
d	8	4	3	3	2	
e	8	2	0	0	0	

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				/	
0	1	2	3	4	5
8	4	3	3	2	0
8	2	0	0	0	0
	8 8 8 8	0 0 ∞ -3 ∞ ∞ ∞ 3 ∞ 4	0 0 0 2 -3 -3 2 2 0 3 3 3 4 3	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	$\begin{array}{c ccccc} 0 & 1 & 2 & 3 & 4 \\ \hline 0 & 0 & 0 & 0 & 0 \\ \hline \infty & -3 & -3 & -4 & -6 \\ \hline \infty & \infty & 0 & -2 & -2 \\ \hline \infty & 3 & 3 & 3 & 3 \\ \hline \infty & 4 & 3 & 3 & 2 \\ \hline \infty & 2 & 0 & 0 & 0 \end{array}$

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= V					/	
	0	1	2	3	4	5
	0					0
						-6
b	8	8	0	-2	-2	-2
	8					3
d	8	4	3	3	2	0
e	8	2	0	0	0	0

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Compare the recurrence above to the previous recurrence:

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

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)
```

```
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]
```

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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.

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

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

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- w only needs to range over neighbours of $v(N_v)$.
- 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

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

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

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- ▶ Observe that M[i, v] depends only on M[i-1, *] and no other indices.

RNA Secondary Structure

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

Computing the Shortest Path: Algorithm

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

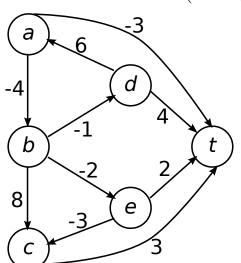
▶ How can we recover the shortest path that has cost M[v]?

Computing the Shortest Path: Algorithm

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

- ▶ 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 maintain 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.

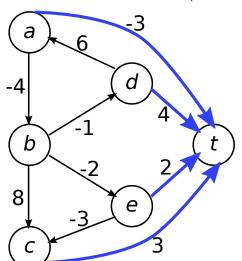
$$M[v] = \min \left(M'[v], \min_{w \in N_v} \left(c_{vw} + M'[w] \right) \right)$$



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

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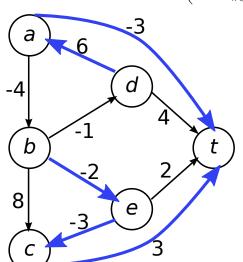
$$M[v] = \min \left(M'[v], \min_{w \in N_v} \left(c_{vw} + M'[w] \right) \right)$$



			/			
	0	1	<u>2</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				

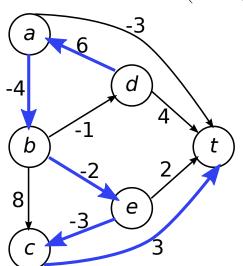
T. M. Murali

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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			
С	8	3	3			
d	8	4	3			
e	8	2	0			

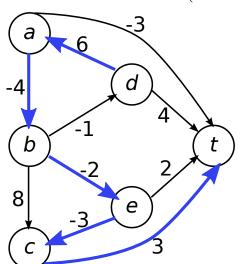
$$M[v] = \min \left(M'[v], \min_{w \in N_v} \left(c_{vw} + M'[w] \right) \right)$$



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

Example of Maintaining Pointers

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

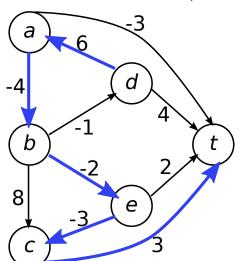


		/			
0	1	2	3	4	5
0	0	0	0	0	0
8	-3	-3	-4	-6	
8	8	0	-2	-2	
8	3	3	3	3	
8	4	3	3	2	
8	2	0	0	0	
	8 8 8 8	8 -38 88 34	0 0 0 ∞ -3 -3 ∞ ∞ 0 ∞ 3 3 ∞ 4 3	0 0 0 0 ∞ -3 -3 -4 ∞ ∞ 0 -2 ∞ 3 3 3 ∞ 4 3 3	0 0 0 0 ∞ -3 -3 -4 -6 ∞ ∞ 0 -2 -2 ∞ 3 3 3 3 ∞ 4 3 3 2

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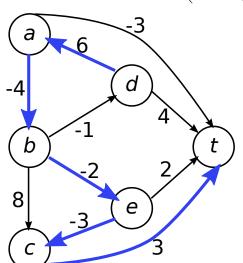
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V			/			
	0	1	2	3	4	5
t	0	0	0	0	0	0
a	8	-3	-3	-4	-6	-6
b	8	8	0	-2	-2	-2
С	8	3	3	3	3	3
d	8	4	3	3	2	0
e	8	2	0	0	0	0

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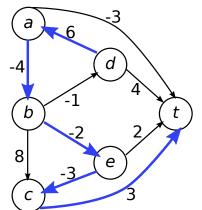


/			/			
	0	1	2	3	4	5
t	0	0	0	0	0	0
a	8	-3	-3	-4	-6	-6
					-2	
C	8	3	3	3	3	3
d	8	4	3	3	2	0
e	8	2	0	0	0	0

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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
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RNA Secondary Structure

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

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

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 - ▶ 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).

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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?

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

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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

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

- ▶ Claim: If P has a cycle C, then C has negative cost.
 - f(v) to some other node, $M[v] \ge c_{vw} + M[w]$ (because M[w] may itself decrease).

▶ Suppose we set f(v) = w. Between this assignment and the assignment of

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

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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: Early Termination

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

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

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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 equals N after processing all the nodes, we have computed all the shortest paths to t.