Dynamic Programming

T. M. Murali

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Oynamic 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, AI, ...): Unix diff command for comparing two files.

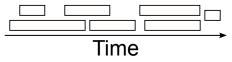






- Input: Start and end time of each ride.
- Constraint: Cannot be in two places at one time.
- Goal: Compute the largest number of rides you can be on in one day.

Review: Interval Scheduling



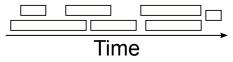
INTERVAL SCHEDULING

INSTANCE: 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.
- For any input set of jobs, algorithm must provably compute the largest set of compatible jobs.

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SOLUTION: The largest subset of mutually compatible jobs.

- Two jobs are *compatible* if they do not overlap.
- For any input set of jobs, algorithm must provably compute the largest set of compatible jobs.
- Greedy algorithm: sort jobs in increasing order of finish times. Add next job to current subset only if it is compatible with previously-selected jobs.

Weighted Interval Scheduling

WEIGHTED INTERVAL SCHEDULING

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

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

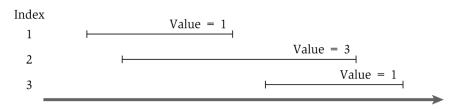


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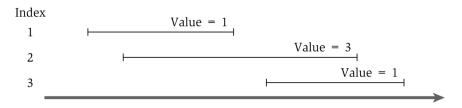
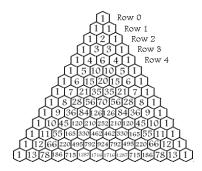
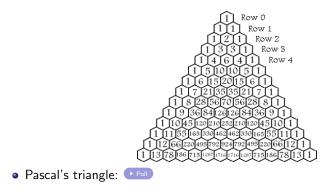
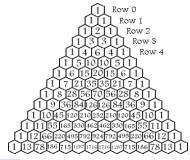


Figure 6.1 A simple instance of weighted interval scheduling.

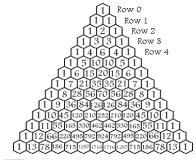
Greedy algorithm can produce arbitrarily bad results for this problem.





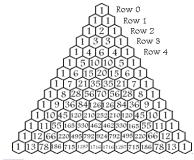


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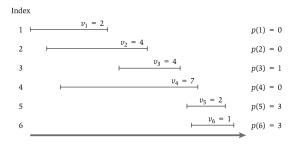
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• Proof: either we include the *n*th element in a subset or not

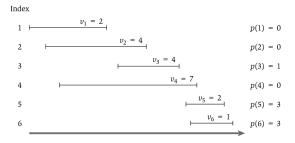
Approach

- Sort jobs in increasing order of finish time and relabel: $f_1 \leq f_2 \leq \ldots \leq f_n$.
- 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. Poil

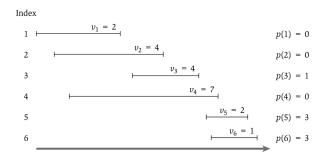


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- All jobs that come before job p(j) are also compatible with job j.

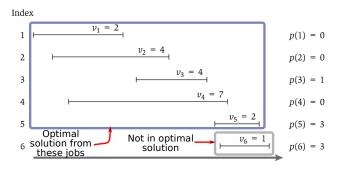


• We will develop optimal algorithm from obvious statements about the problem.

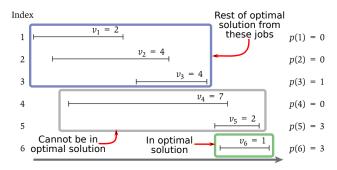


Let O be the optimal solution: it contains a subset of the input jobs. Two cases to consider. One of these cases must be true.
 Case 1: job n is not in O.

Case 2: job n is in O.



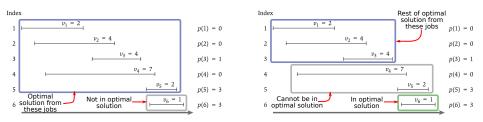
Let O be the optimal solution: it contains a subset of the input jobs. Two cases to consider. One of these cases must be true.
 Case 1: job n is not in O. O must be the optimal solution for jobs {1,2,...,n-1}.
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• Let \mathcal{O} be the optimal solution: it contains a subset of the input jobs. Two cases to consider. One of these cases must be true.

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} .

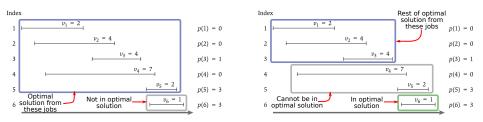
- * \mathcal{O} cannot use incompatible jobs $\{p(n) + 1, p(n) + 2, \dots, n-1\}$.
- * Remaining jobs in \mathcal{O} must be the optimal solution for jobs $\{1, 2, \dots, p(n)\}$.



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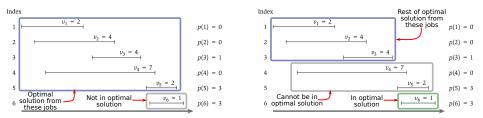
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- $\bullet \ \mathcal{O}$ must be the best of these two choices!



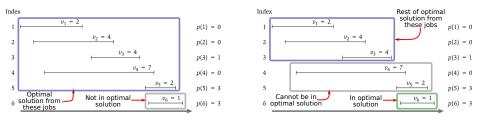
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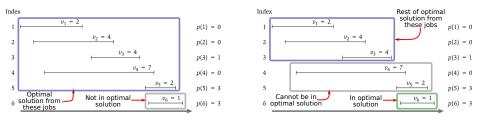
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- $\bullet \ \mathcal{O}$ must be the best of these two choices!
- Suggests finding optimal solution for sub-problems consisting of jobs $\{1, 2, \ldots, j 1, j\}$, for all values of j.



Let O_j be the optimal solution for jobs {1, 2, ..., j} and OPT(j) be the value of this solution (OPT(0) = 0).

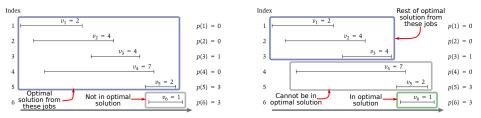


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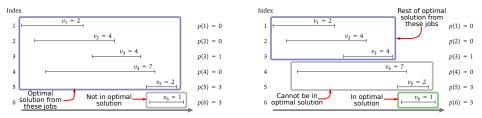
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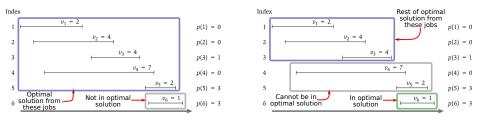
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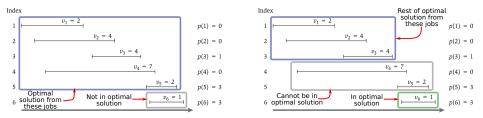
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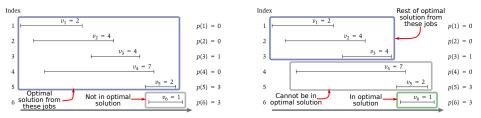
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$$OPT(j) = \max(v_j + OPT(p(j)), OPT(j-1))$$

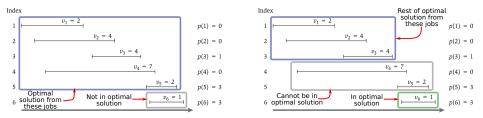


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• When does job *j* belong to \mathcal{O}_i ? • Poll



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

Recursive Algorithm

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

```
Compute-Opt(j)
If j = 0 then
Return 0
Else
Return max(v<sub>j</sub>+Compute-Opt(p(j)), Compute-Opt(j - 1))
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• Correctness of algorithm follows by induction (see textbook for proof).

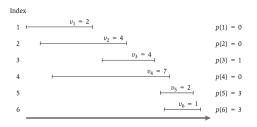


Figure 6.2 An instance of weighted interval scheduling with the functions p(j) defined for each interval *j*.

OPT(6) = PollOPT(5) =OPT(4) =OPT(3) =OPT(2) =OPT(1) =OPT(0) = 0

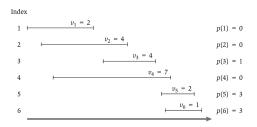


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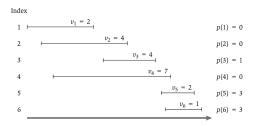


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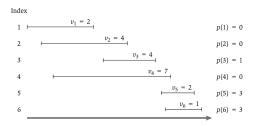


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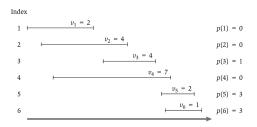


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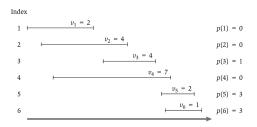


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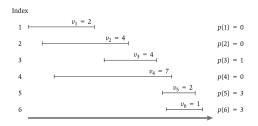


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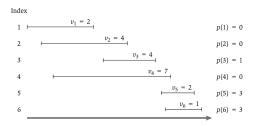


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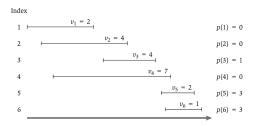


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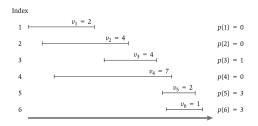


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$$\begin{array}{l} \mathsf{OPT}(6) = \max(v_6 + \mathsf{OPT}(p(6)), \mathsf{OPT}(5)) = \max(1 + \mathsf{OPT}(3), \mathsf{OPT}(5)) \\ \mathsf{OPT}(5) = \max(v_5 + \mathsf{OPT}(p(5)), \mathsf{OPT}(4)) = \max(2 + \mathsf{OPT}(3), \mathsf{OPT}(4)) \\ \mathsf{OPT}(4) = \max(v_4 + \mathsf{OPT}(p(4)), \mathsf{OPT}(3)) = \max(7 + \mathsf{OPT}(0), \mathsf{OPT}(3)) = 7 \\ \mathsf{OPT}(3) = \max(v_3 + \mathsf{OPT}(p(3)), \mathsf{OPT}(2)) = \max(4 + \mathsf{OPT}(1), \mathsf{OPT}(2)) = 6 \\ \mathsf{OPT}(2) = \max(v_2 + \mathsf{OPT}(p(2)), \mathsf{OPT}(1)) = \max(4 + \mathsf{OPT}(0), \mathsf{OPT}(1)) = 4 \\ \mathsf{OPT}(1) = v_1 = 2 \\ \mathsf{OPT}(0) = 0 \end{array}$$

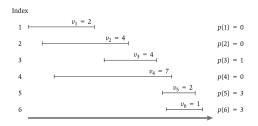


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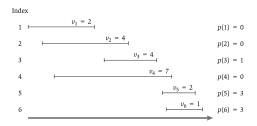


Figure 6.2 An instance of weighted interval scheduling with the functions p(j) defined for each interval *j*.

$$\begin{array}{l} \mathsf{OPT}(6) = \max(v_6 + \mathsf{OPT}(p(6)), \mathsf{OPT}(5)) = \max(1 + \mathsf{OPT}(3), \mathsf{OPT}(5)) = 8\\ \mathsf{OPT}(5) = \max(v_5 + \mathsf{OPT}(p(5)), \mathsf{OPT}(4)) = \max(2 + \mathsf{OPT}(3), \mathsf{OPT}(4)) = 8\\ \mathsf{OPT}(4) = \max(v_4 + \mathsf{OPT}(p(4)), \mathsf{OPT}(3)) = \max(7 + \mathsf{OPT}(0), \mathsf{OPT}(3)) = 7\\ \mathsf{OPT}(3) = \max(v_3 + \mathsf{OPT}(p(3)), \mathsf{OPT}(2)) = \max(4 + \mathsf{OPT}(1), \mathsf{OPT}(2)) = 6\\ \mathsf{OPT}(2) = \max(v_2 + \mathsf{OPT}(p(2)), \mathsf{OPT}(1)) = \max(4 + \mathsf{OPT}(0), \mathsf{OPT}(1)) = 4\\ \mathsf{OPT}(1) = v_1 = 2\\ \mathsf{OPT}(0) = 0 \end{array}$$

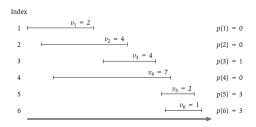


Figure 6.2 An instance of weighted interval scheduling with the functions p(j) defined for each interval *j*.

$$OPT(6) = \max(v_6 + OPT(p(6)), OPT(5)) = \max(1 + OPT(3), OPT(5)) = 8$$

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

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

$$OPT(2) = \max(v_2 + OPT(p(2)), OPT(1)) = \max(4 + OPT(0), OPT(1)) = 4$$

$$OPT(1) = v_1 = 2$$

$$OPT(0) = 0$$

$$Ontimal solution is CPU$$

٥

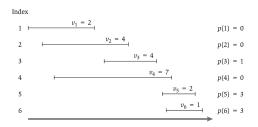


Figure 6.2 An instance of weighted interval scheduling with the functions p(j) defined for each interval *j*.

OPT(6) =
$$\max(v_6 + OPT(p(6)), OPT(5)) = \max(1 + OPT(3), OPT(5)) = 8$$

OPT(5) = $\max(v_5 + OPT(p(5)), OPT(4)) = \max(2 + OPT(3), OPT(4)) = 8$
OPT(4) = $\max(v_4 + OPT(p(4)), OPT(3)) = \max(7 + OPT(0), OPT(3)) = 7$
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OPT(2) = $\max(v_2 + OPT(p(2)), OPT(1)) = \max(4 + OPT(0), OPT(1)) = 4$
OPT(1) = $v_1 = 2$
OPT(0) = 0
Optimal solution is job 5, job 3, and job 1.

```
Compute-Opt(j)
If j=0 then
Return 0
Else
Return max(v<sub>j</sub>+Compute-Opt(p(j)), Compute-Opt(j-1))
Endif
```

Compute-Opt(j) If j = 0 then Return 0 Else Return max(vj+Compute-Opt(p(j)), Compute-Opt(j - 1)) Endif • What is the running time of the algorithm?

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- 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.

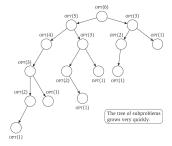


Figure 6.4 An instance of weighted interval scheduling on which the simple Compute-Opt recursion will take exponential time. The values of all intervals in this instance are 1.

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

Memoisation

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

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Running Time of Memoisation

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- 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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- 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}_j in addition to OPT(j).

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- Recall: request j belong to \mathcal{O}_j if and only if $v_j + OPT(p(j)) \ge OPT(j-1)$.
- Can recover \mathcal{O}_j from values of the optimal solutions in $\mathcal{O}(j)$ 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 $v_j + OPT(p(j)) \ge OPT(j-1)$.
- Can recover \mathcal{O}_j from values of the optimal solutions in O(j) time.

```
\label{eq:selected_select} \begin{array}{l} \mbox{Find-Solution}(j) \\ \mbox{If} \ j=0 \ \mbox{then} \\ \mbox{Output nothing} \\ \mbox{Else} \\ \mbox{If} \ v_j + M[p(j)] \geq M[j-1] \ \mbox{then} \\ \mbox{Output} \ j \ \mbox{together with the result of Find-Solution}(p(j)) \\ \mbox{Else} \\ \mbox{Output the result of Find-Solution}(j-1) \\ \mbox{Endif} \\ \mbox{Endif} \end{array}
```

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.

```
\begin{split} & \texttt{Iterative-Compute-Opt} \\ & M[0] = 0 \\ & \texttt{For } j = 1, 2, \dots, n \\ & M[j] = \max(v_j + M[p(j)], M[j-1]) \\ & \texttt{Endfor} \end{split}
```

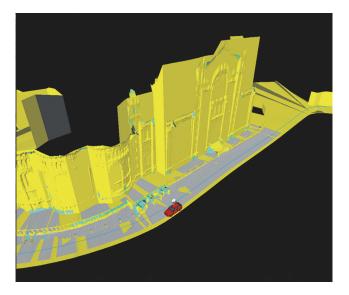
Basic Outline of Dynamic Programming

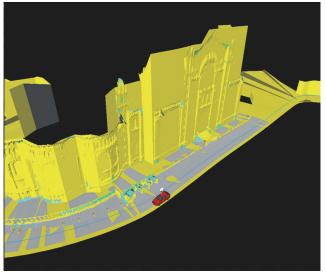
- To solve a problem, we need a collection of sub-problems that satisfy a few properties:
 - There are a polynomial number of sub-problems.
 - The solution to the problem can be computed easily from the solutions to the sub-problems.
 - Solution There is a natural ordering of the sub-problems from "smallest" 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.

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- To solve a problem, we need a collection of sub-problems that satisfy a few properties:
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 - Solution 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.
- Difficulties in designing dynamic programming algorithms:
 - Which sub-problems to define?
 - 2 How can we tie together sub-problems using a recurrence?
 - How do we order the sub-problems (to allow iterative computation of optimal solutions to sub-problems)?



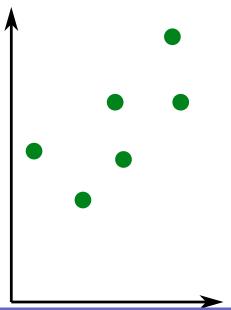




Imagery from street view vehicles is accompanied by laser range data, which is aggregated and simplified by robustly fitting it in a coarse mesh that models the dominant scene surfaces.

October 19, 21, 26, 28, 2021

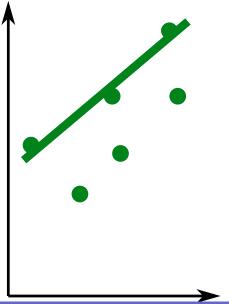
Fitting Lines

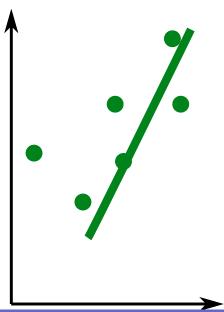


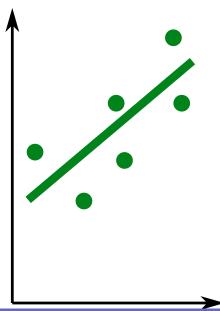
T. M. Murali

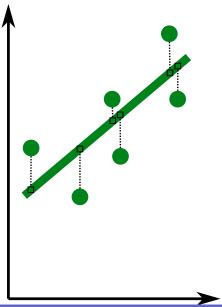
October 19, 21, 26, 28, 2021

Dynamic Programming





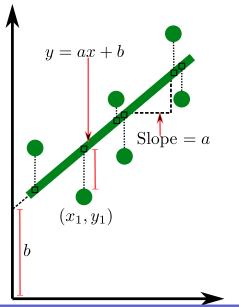




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October 19, 21, 26, 28, 2021

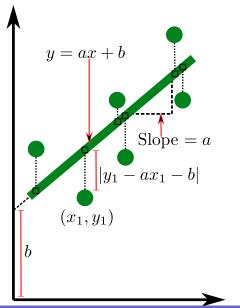
Dynamic Programming

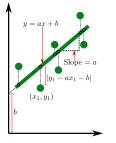


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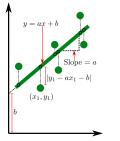
October 19, 21, 26, 28, 2021

Dynamic Programming





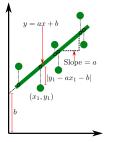
- Given scientific or statistical data plotted on two axes.
- Find the "best" line that "passes" through these points.



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

LEAST SQUARES REGRESSION **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

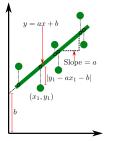
$$\mathsf{Error}(L,P) = \sum_{i=1}^{\infty} (y_i - \mathsf{a} x_i - b)^2.$$



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

LEAST SQUARES REGRESSION **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 $\operatorname{Error}(L, P) = \sum_{i=1}^{n} (y_i - ax_i - b)^2.$

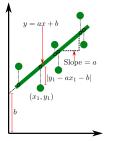
• How many unknown parameters must we find values for? ••••



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

LEAST SQUARES REGRESSION **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 $\operatorname{Error}(L, P) = \sum_{i=1}^{n} (y_i - ax_i - b)^2.$

• How many unknown parameters must we find values for? Two: *a* and *b*.



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

LEAST SQUARES REGRESSION **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

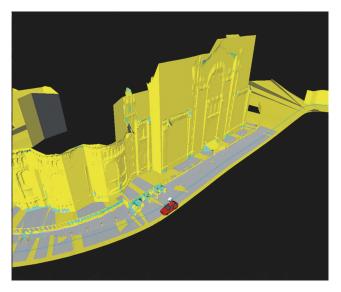
$$\mathsf{Error}(L, P) = \sum_{i=1}^{\infty} (y_i - ax_i - b)^2.$$

• How many unknown parameters must we find values for? Two: a and b.

Solution is achieved by

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

Segmented Least Squares



Segmented Least Squares

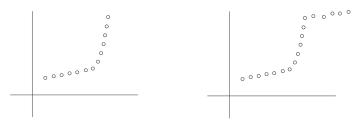
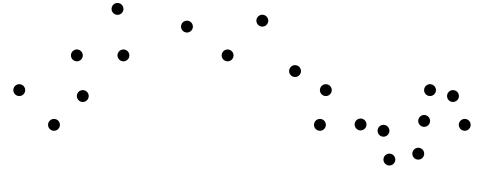
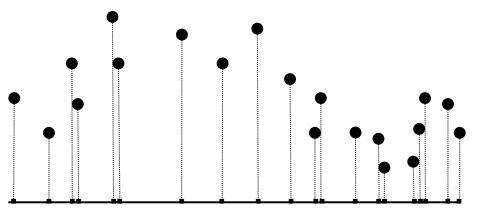


Figure 6.7 A set of points that lie approximately on two lines. Figure 6.8 A set of points that lie approximately on three lines.

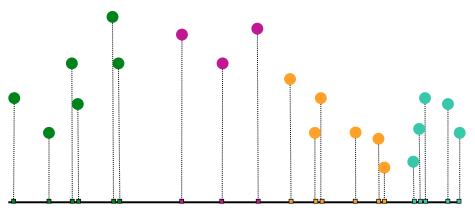
- Want to fit multiple lines through *P*.
- Each line must fit contiguous set of x-coordinates.
- Lines must minimise total error.



Input contains a set of two-dimensional points.

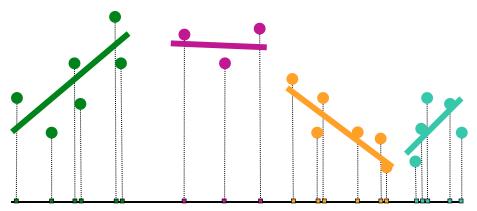


Consider the sorted *x*-coordinates of the points in the input.

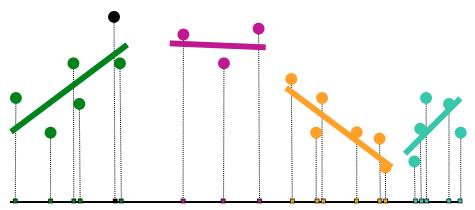


Divide the points into segments; each *segment* contains consecutive points in the sorted order by *x*-coordinate.

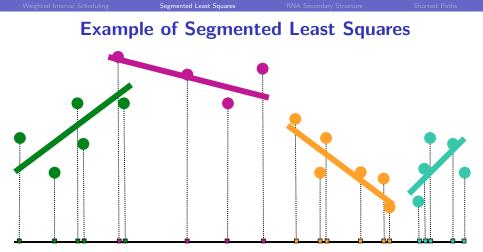
Here we are defining a meaning for "segment" that is specific to this problem.



Fit the best line for each segment.



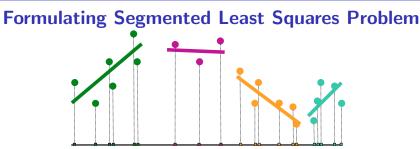
Illegal solution: black point is not in any segment.



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



SEGMENTED LEAST SQUARES **INSTANCE:** Set $P = \{p_i = (x_i, y_i), 1 \le i \le n\}$ of *n* points, $x_1 < x_2 < \cdots < x_n$ **SOLUTION:**



INSTANCE: Set $P = \{p_i = (x_i, y_i), 1 \le i \le n\}$ of *n* points,

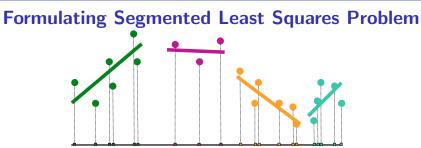
 $x_1 < x_2 < \cdots < x_n$ SOLUTION:

• An integer k,

2 a partition of *P* into *k* segments $\{P_1, P_2, \ldots, P_k\}$, and

§ for each segment P_j , the best-fit line L_j : $y = a_j x + b_j$, $1 \le j \le k$ that minimise the total error

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



INSTANCE: Set $P = \{p_i = (x_i, y_i), 1 \le i \le n\}$ of *n* points,

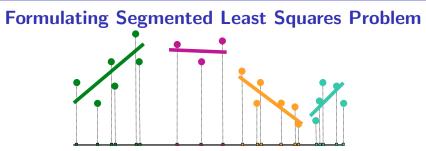
 $x_1 < x_2 < \cdots < x_n$ and a parameter C > 0. **SOLUTION:**

• An integer k,

2 a partition of *P* into *k* segments $\{P_1, P_2, \ldots, P_k\}$, and

§ for each segment P_j , the best-fit line L_j : $y = a_j x + b_j, 1 \le j \le k$ that minimise the total error μ

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



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:**

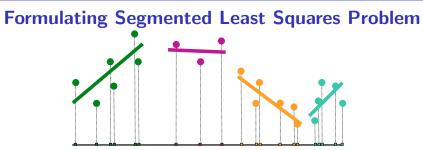
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$$\sum_{j=1} \mathsf{Error}(L_j, P_j) + Ck$$

• How many unknown parameters must we find? 2k, and we must find k too!



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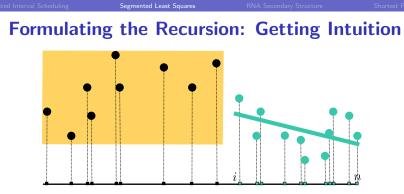
2 a partition of *P* into *k* segments $\{P_1, P_2, \ldots, P_k\}$, and

• for each segment P_j , the best-fit line $L_j : y = a_j x + b_j, 1 \le j \le k$ that minimise the total error p_j .

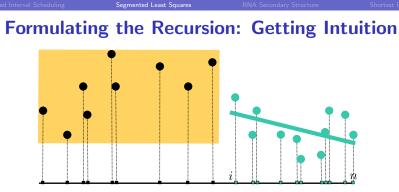
$$\sum_{i=1} \operatorname{Error}(L_j, P_j) + Ck$$

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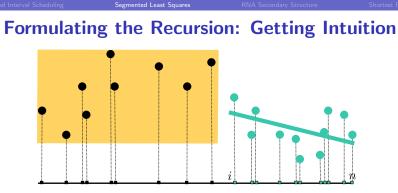
• Assume points in *P* are sorted in increasing order of *x*-coordinate.



• Observation: Where does the last segment in the optimal solution end?

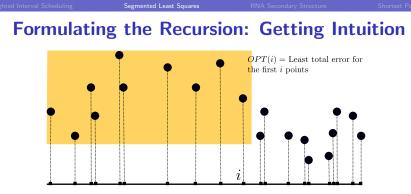


• Observation: Where does the last segment in the optimal solution end? p_n , and this segment starts at some point p_i . We don't know *i* yet!



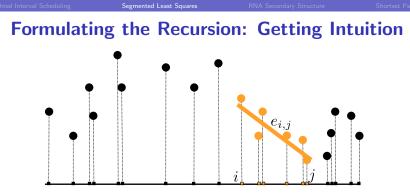
• Observation: Where does the last segment in the optimal solution end? p_n , and this segment starts at some point p_i . We don't know *i* yet!

• If the last segment in the optimal partition is $\{p_i, p_{i+1}, \ldots, p_n\}$, then optimal total error for n points = Error of the best line fitting $\{p_i, p_{i+1}, \ldots, p_n\} + C$ + optimal total error for the first i - 1 points.



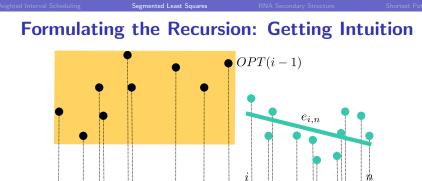
- Observation: Where does the last segment in the optimal solution end? p_n , and this segment starts at some point p_i . We don't know *i* yet!
- Let *OPT*(*i*) be the optimal total error for the points {*p*₁, *p*₂,..., *p_i*}.
- We want to compute OPT(n).

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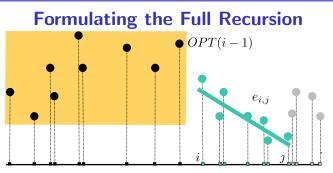
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- Let $e_{i,j}$ denote the minimum error of a (single) line that fits $\{p_i, p_2, \ldots, p_j\}$.
- If the last segment in the optimal partition is $\{p_i, p_{i+1}, \ldots, p_n\}$, then

optimal total error for *n* points = Error of the best line fitting $\{p_i, p_{i+1}, \ldots, p_n\} + C$ + optimal total error for the first *i* - 1 points.

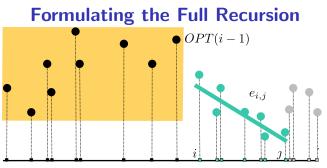


- Observation: Where does the last segment in the optimal solution end? p_n , and this segment starts at some point p_i . We don't know *i* yet!
- Let OPT(i) be the optimal total error for the points $\{p_1, p_2, \ldots, p_i\}$.
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$$OPT(n) = e_{i,n} + C + OPT(i-1)$$

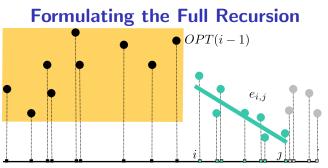


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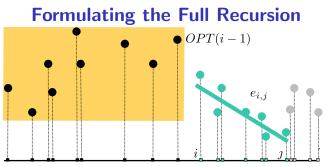
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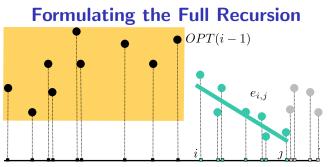


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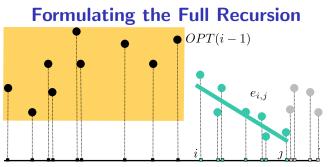


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- Segment $\{p_i, p_{i+1}, \dots, p_j\}$ is part of the optimal solution for this sub-problem if and only if the minimum value of OPT(j) is obtained using index *i*.

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

```
Segmented-Least-Squares(n)

Array M[0...n]

Set M[0] = 0

For all pairs i \le j

Compute the least squares error e_{i,j} for the segment p_i, ..., p_j

Endfor

For j = 1, 2, ..., n

Use the recurrence (6.7) to compute M[j]

Endfor

Return M[n]
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• We can find the segments in the optimal solution by backtracking.

Running Time

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

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• Let T(n) be the running time of this algorithm.

$$T(n) = \sum_{1 \le j \le n} \sum_{1 \le i \le j} O(j-i) =$$

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Compute the least squares error e_{i,j} for the segment p_i, \dots, p_j

Endfor

For j = 1, 2, \dots, n

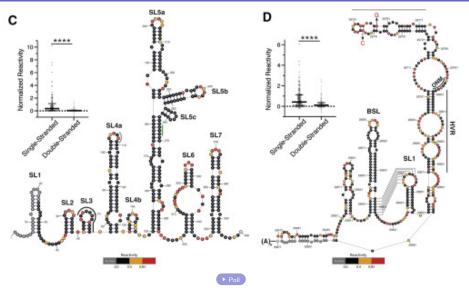
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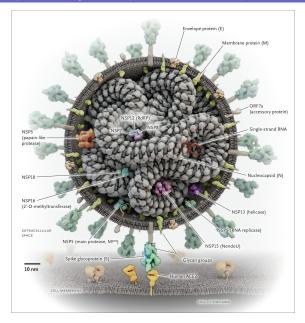
Endfor

Return M[n]
```

- Let T(n) be the running time of this algorithm.
- Running time is $O(n^3)$; can be improved to $O(n^2)$.

$$T(n) = \sum_{1 \le j \le n} \sum_{1 \le i \le j} O(j-i) = O(n^3)$$





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- 2 Adenine always matches with Uracil.
- Oytosine always matches with Guanine.
- There are no kinks in the folded molecule.
- Structures are "knot-free".

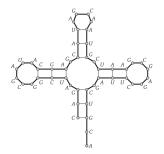


Figure 6.13 An RNA secondary structure. Thick lines connect adjacent elements of the sequence; thin lines indicate pairs of elements that are matched.

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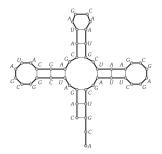


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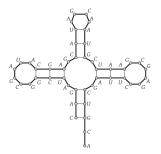


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- Problem: given an RNA molecule, predict its secondary structure.
- Hypothesis: In the cell, RNA molecules form the secondary structure with the lowest total free energy.

Formulating the Problem

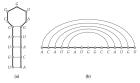


Figure 6.14 Two views of an RNA secondary structure. In the second view, (b), the string has been "stretched" lengthwise, and edges connecting matched pairs appear as noncrossing "bubbles" over the string.

- An RNA molecule is a string $B = b_1 b_2 \dots b_n$; each $b_i \in \{A, C, G, U\}$.
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Formulating the Problem

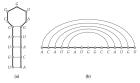
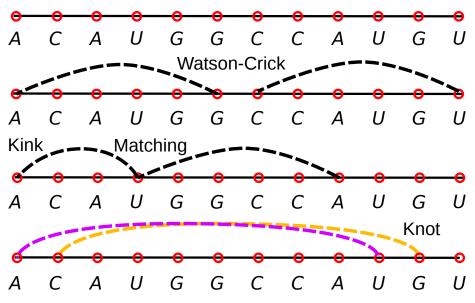


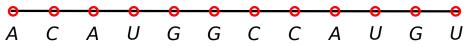
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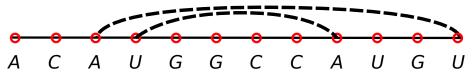
- An RNA molecule is a string $B = b_1 b_2 \dots b_n$; each $b_i \in \{A, C, G, U\}$.
- A secondary structure on B is a set of pairs $S = \{(i, j)\}$, where $1 \le i, j \le n$ and
 - (No kinks.) If $(i,j) \in S$, then i < j 4.
 - (*Watson-Crick*) The elements in each pair in S consist of either $\{A,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

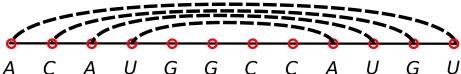
Illegal Secondary Structures

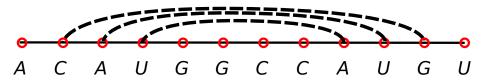


Legal Secondary Structures









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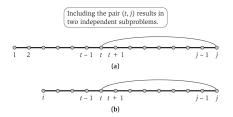


Figure 6.15 Schematic views of the dynamic programming recurrence using (a) one variable, and (b) two variables.

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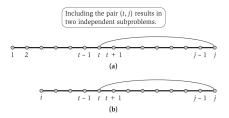


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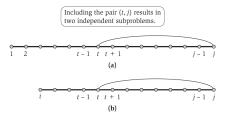


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- Insight: need sub-problems indexed both by start and by end.

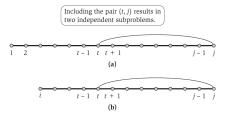


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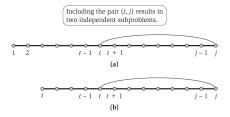


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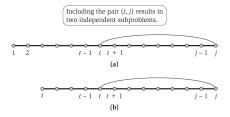


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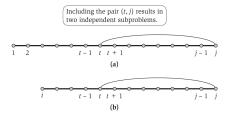


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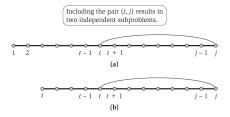


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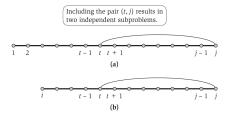


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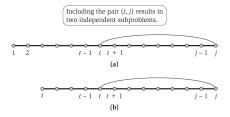


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 - 3) if j pairs with some t < j 4, compute OPT(i, t 1) and OPT(t + 1, j 1).

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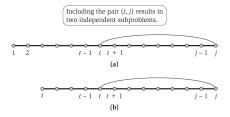


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- if j pairs with some t < j − 4, compute OPT(i, t − 1) and OPT(t + 1, j − 1).
 Since t can range from i to j − 5,

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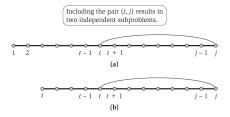
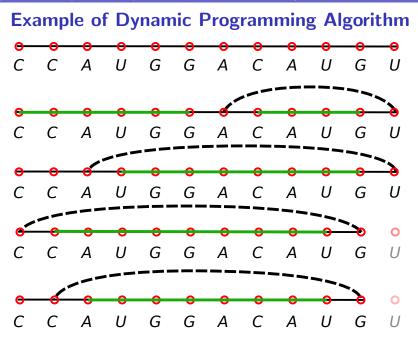


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ight)$$

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



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

• There are **Poll** sub-problems.

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```
Initialise OPT(i,j)=0 for every l,j such that i \ge j-4
for j = 1, 2, ..., n-1, n
for i = 1, 2, ..., j-6, j-5
Compute OPT(i,j) using the recurrence above.
```

- How long does it take to compute OPT(i, j)? Poll
- What is the running time of the algorithm?

Dynamic Programming Algorithm

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

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for $j=1,2,\ldots,n-1,n$
for $i=1,2,\ldots,j-6,j-5$
Compute $OPT(i,j)$ using the recurrence above.

- How long does it take to compute OPT(i, j)? O(j i)
- What is the running time of the algorithm? $O(n^3)$.

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 from source s to destination t with minimum total cost.
 - 2 Does G have a *negative cycle*? Application is to arbritrage opportunities.

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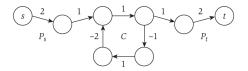


Figure 6.20 In this graph, one can find *s*-*t* paths of arbitrarily negative cost (by going around the cycle *C* many times).

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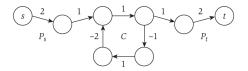


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Run Dijsktra's algorithm.



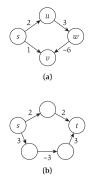


Figure 6.21 (a) With negative edge costs, Dijkstra's Algorithm can give the wrong answer for the Shortest-Path Problem. (b) Adding 3 to the cost of each edge will make all edges nonnegative, but it will change the identity of the shortest s-t path.

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

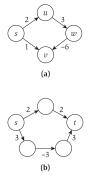


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- Run Dijsktra's algorithm. Computes incorrect answers because it is greedy.
- Add some large constant to each edge. 🕑 Poll

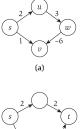




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- Run Dijsktra's algorithm. Computes incorrect answers because it is greedy.
- Add some large constant to each edge. Computes incorrect answers because the minimum cost path changes.

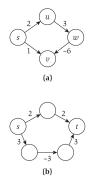


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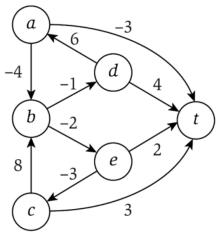
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 - We do not know which nodes will be in shortest s-t path: how we can reach t from each node in V?
- Sub-problems defined by varying the number of edges in the shortest path and by varying the starting node in the shortest path.



- 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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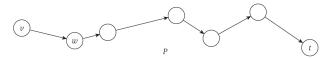


Figure 6.22 The minimum-cost path P from v to t using at most i edges.

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

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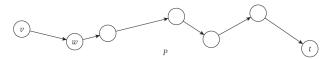


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- Let P be the optimal path whose cost is OPT(i, v).
 - If P actually uses i 1 edges, then OPT(i, v) = OPT(i 1, v).
 - 2 If first node on P is w, then $OPT(i, v) = c_{vw} + OPT(i 1, w)$.

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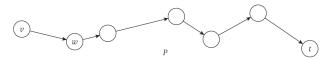
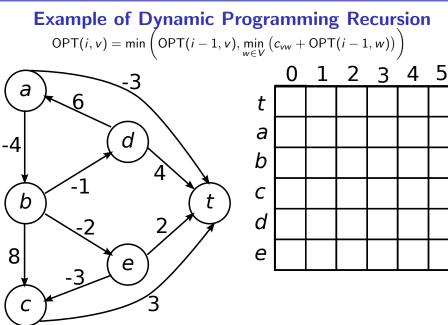
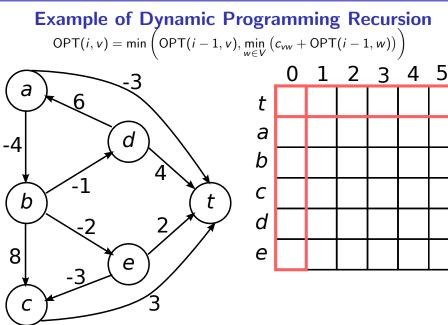


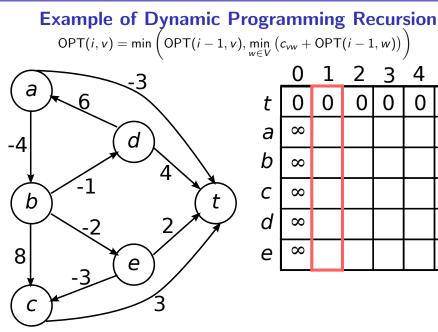
Figure 6.22 The minimum-cost path P from v to t using at most i edges.

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



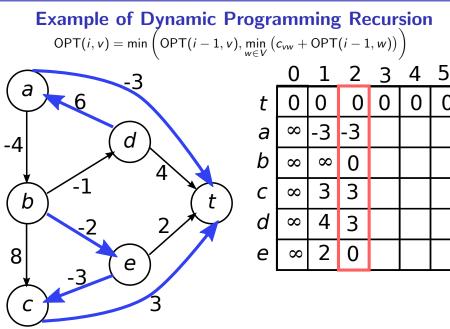


Example of Dynamic Programming Recursion $\mathsf{OPT}(i, v) = \min\left(\mathsf{OPT}(i-1, v), \min_{w \in V} (c_{vw} + \mathsf{OPT}(i-1, w))\right)$ 2 3 4 а ∞ а b ∞ С ∞ b d ∞ ∞ е 8 е



Example of Dynamic Programming Recursion													
$OPT(i, v) = \min\left(OPT(i-1, v), \min_{w \in V} \left(c_{vw} + OPT(i-1, w) \right) ight)$													
-3		0	1	2	3	4							
	t	0	0	0	0	0							
-4 (d)	а	8	-3										
	b	8	8										
b -1 t	С	8	3										
-2 2	d	8	4										
8 e	е	8	2										
-3	•												
(C) 3													

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-3		0	1	2	3	4							
(a) 6	t	0	0	0	0	0							
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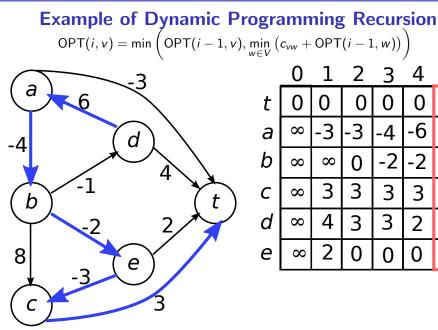
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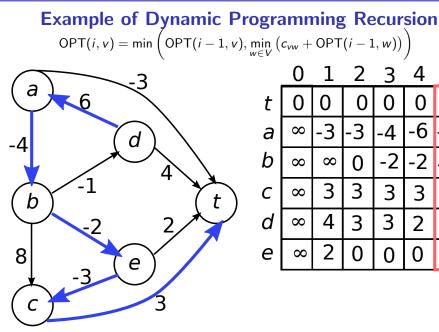
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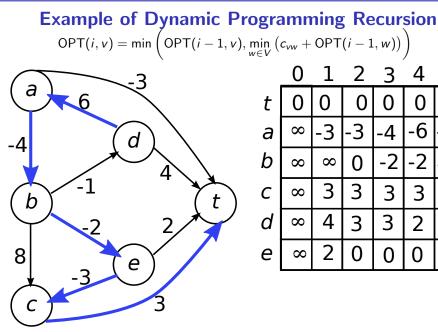
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• Compare the two desired solutions:

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

Bellman-Ford Algorithm

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

```
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

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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.

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- w only needs to range over outgoing neighbours N_v of v.
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• The total running time is O(mn).

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

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 - Maintain two arrays M and M' indexed over V.
 - 2 At the beginning of each iteration, copy M into M'.
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$$M[v] = \min\left(M'[v], \min_{w \in N_v} \left(c_{vw} + M'[w]\right)
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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).

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

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

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- How can we recover the shortest path that has cost M[v]?
- For each node v, compute and update f(v), the first node after v in the current shortest path from v to t.
- Updating f(v):

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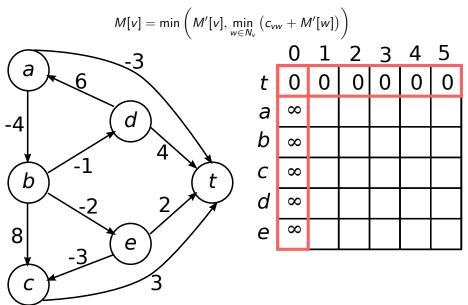
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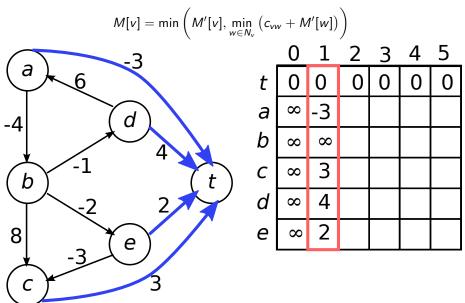
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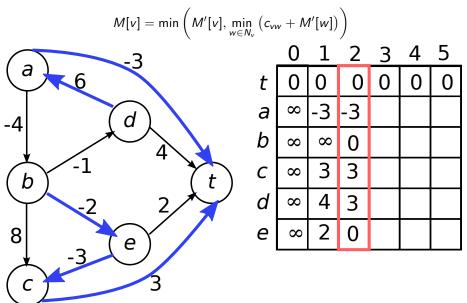
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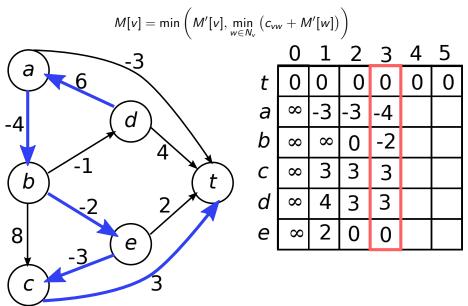
• set
$$M[v] = c_{vx} + M'[x]$$
 and

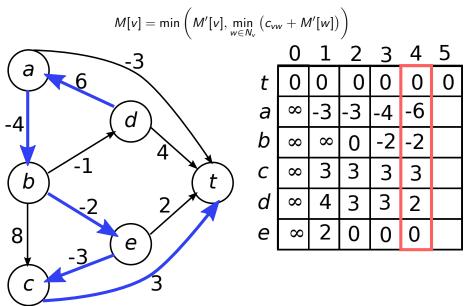
- set f(v) = x.
- At the end, follow f(v) pointers from s to t (and hope for the best).

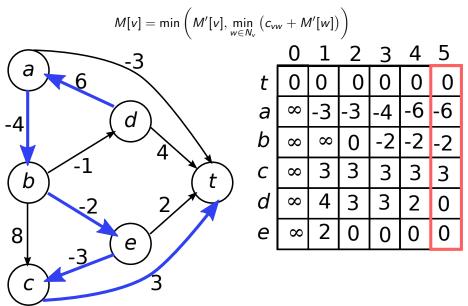


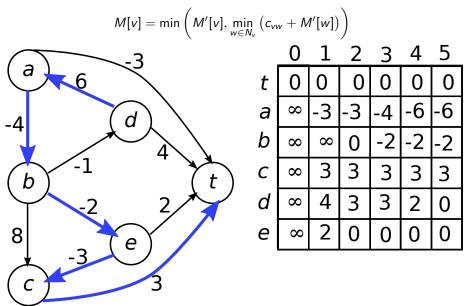








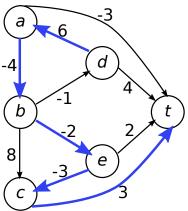




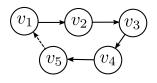
Computing the Shortest Path: Correctness

• Pointer graph P(V, F): each edge in F is (v, f(v)).

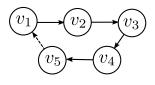
- Can P have cycles?
- Is there a path from s to t in P?
- Can there be multiple paths s to t in P?
- Which of these is the shortest path?



	0	1	2	3	4	5
t	0	0	0	0	0	0
а	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
е	8	2	0	0	0	0



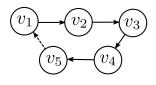
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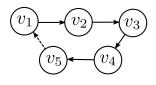
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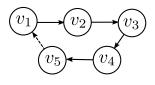
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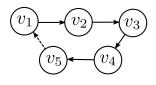
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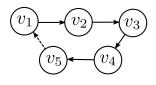
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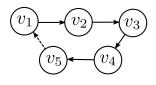
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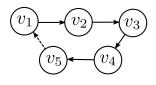
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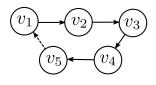
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- Adding all these inequalities, $0 > \sum_{i=1}^{k-1} c_{v_i v_{i+1}} + c_{v_k v_1} = \text{cost of } C$.



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- Corollary: if G has no negative cycles that P does not either.

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

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

Bellman-Ford Algorithm: One Array

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

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

Bellman-Ford Algorithm: Early Termination

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

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- Early termination: If *M* does not change after processing all the nodes, we have computed all the shortest paths to *t*.