Dynamic Programming

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Algorithm Design Techniques

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

History of Dynamic Programming

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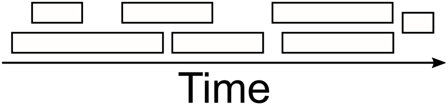
- The Secretary of Defense at that time was hostile to mathematical research.
- Bellman sought an impressive name to avoid confrontation.
  - "it's impossible to use dynamic in a pejorative sense"
  - "something not even a Congressman could object to" (Bellman, R. E., *Eye of the Hurricane, An Autobiography*).

Applications of Dynamic Programming

- Computational biology: Smith-Waterman algorithm for sequence alignment.
- Operations research: Bellman-Ford algorithm for shortest path routing in networks.
- Control theory: Viterbi algorithm for hidden Markov models.
- Computer science (theory, graphics, 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.

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

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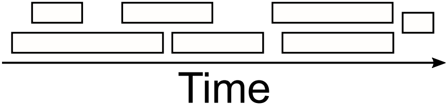

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- For any input set of jobs, algorithm must provably compute the largest set of compatible jobs.
- Greedy algorithm: sort jobs in increasing order of finish times. Add next job to current subset only if it is compatible with previously-selected jobs.

Weighted Interval Scheduling

WEIGHTED INTERVAL SCHEDULING

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

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

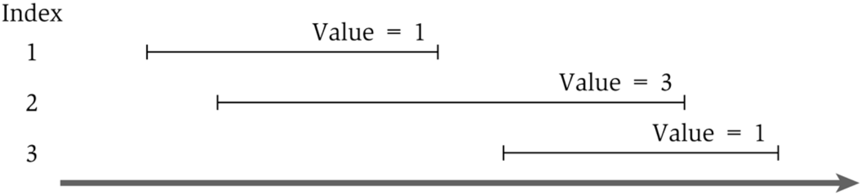

Figure 6.1 A simple instance of weighted interval scheduling.

- Dynamic Programming: Weighted Interval Scheduling: Greedy Algorithm

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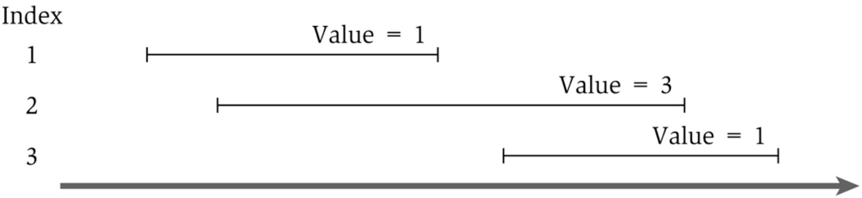
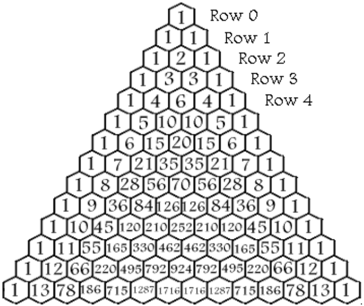


Figure 6.1 A simple instance of weighted interval scheduling.

- ▸ Dynamic Programming: Weighted Interval Scheduling: Greedy Algorithm Greedy algorithm can produce arbitrarily bad results for this problem.

Detour: a Binomial Identity



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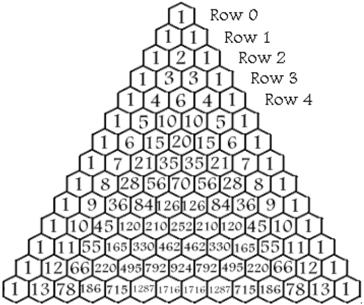

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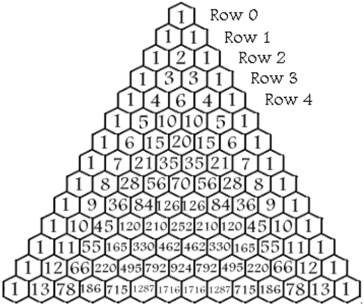

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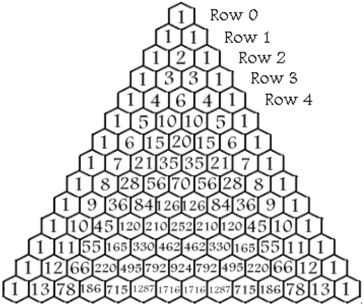

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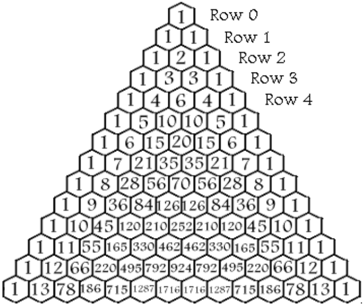

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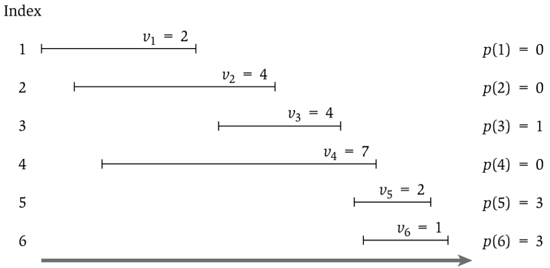
$$\binom{n}{r} = \binom{n-1}{r-1} + \binom{n-1}{r}$$

- Proof: either we include the nth 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. Dynamic Programming: Weighted Interval Scheduling: Compatible jobs



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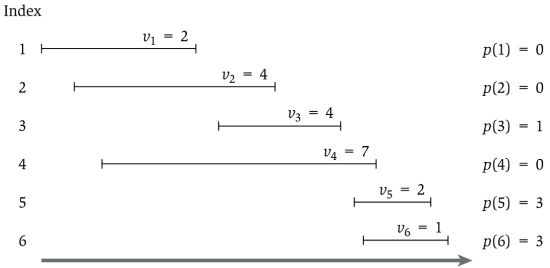
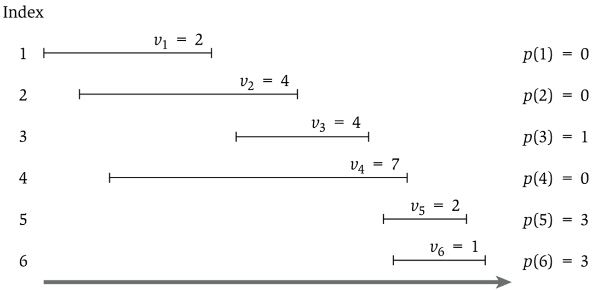
- All jobs that come before job $p(j)$ are also compatible with job j.



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

Sub-problems



- 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 $\mathcal{O}$.

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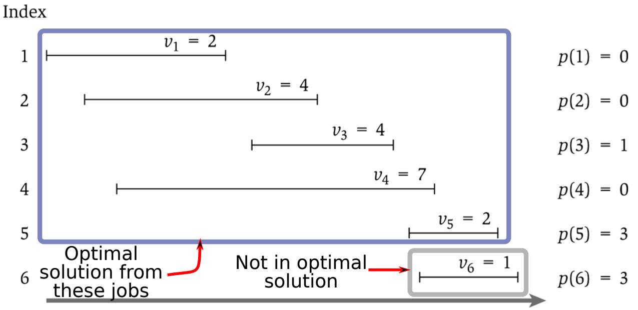
Sub-problems



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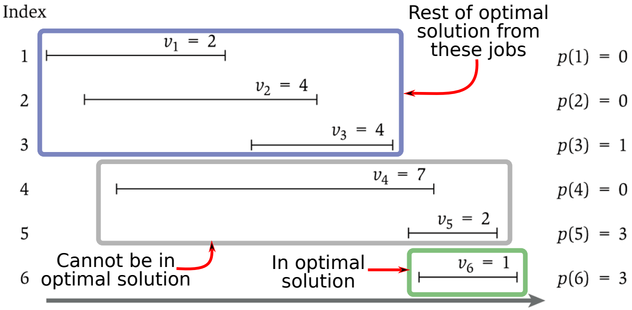

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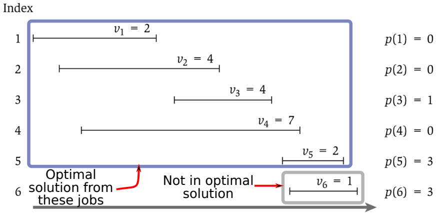
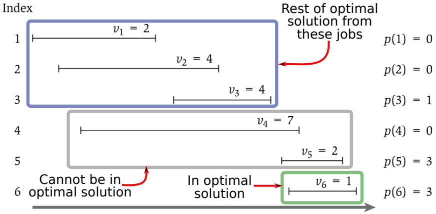
  - Case 2: job n is in $\mathcal{O}$.
    - ★ $\mathcal{O}$ cannot use incompatible jobs $\{p(n)+1, p(n)+2, \ldots, n-1\}$.
    - ★ Remaining jobs in $\mathcal{O}$ must be the optimal solution for jobs $\{1, 2, \ldots, p(n)\}$.

Sub-problems





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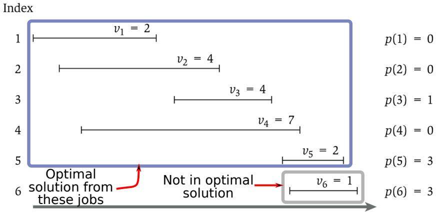

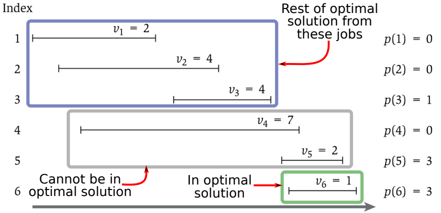

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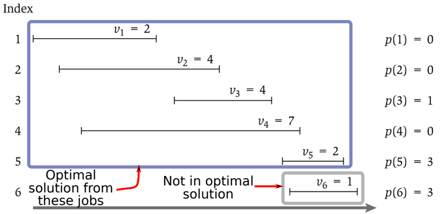
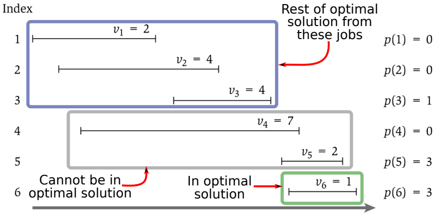
- $\mathcal{O}$ must be the best of these two choices!
- Suggests finding optimal solution for sub-problems consisting of jobs $\{1, 2, \ldots, j-1, j\}$, for all values of j.

Recursion





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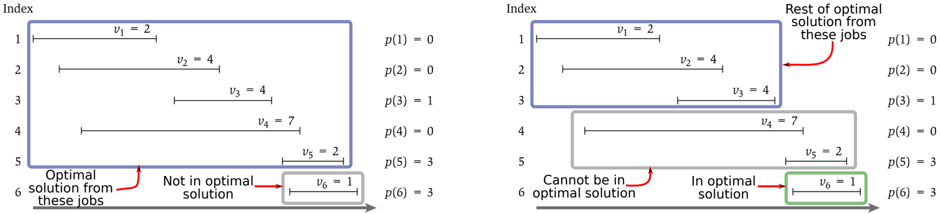

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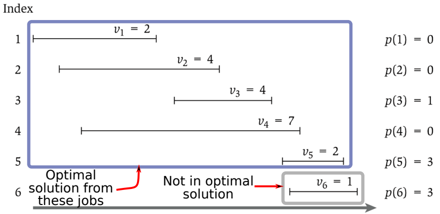

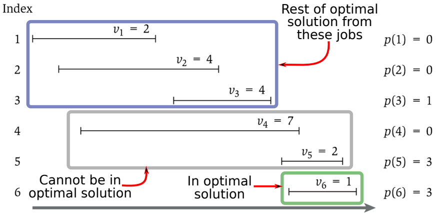

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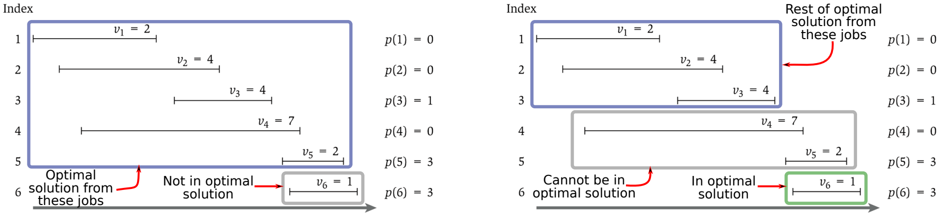

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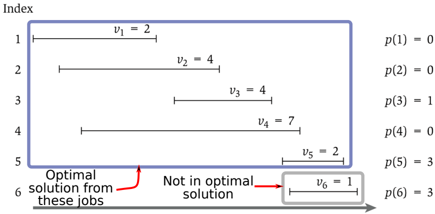

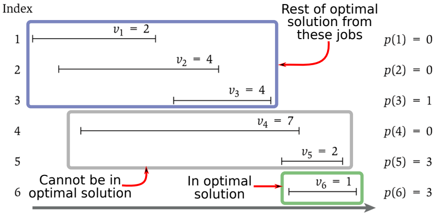

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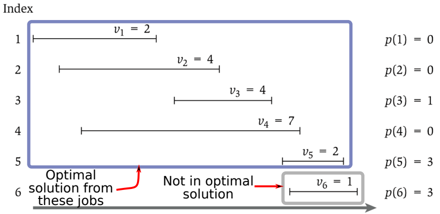

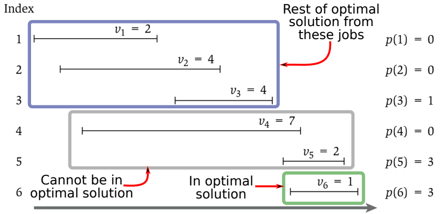

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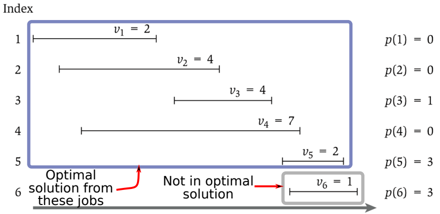

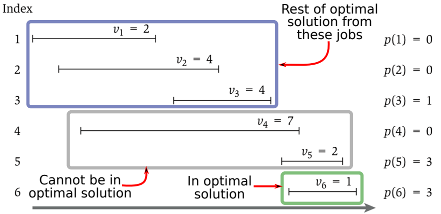

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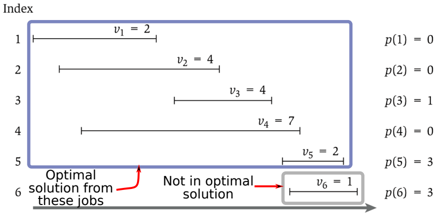

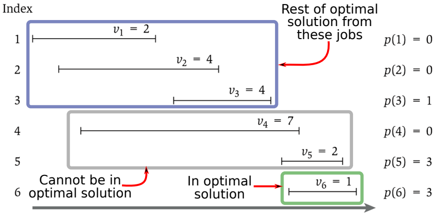

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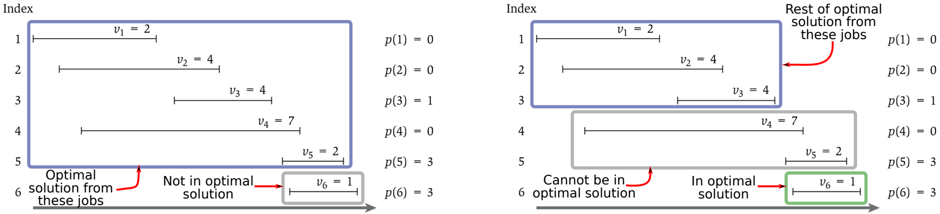
- When does job j belong to $\mathcal{O}_j$? ▸ Dynamic Programming: Weighted Interval Scheduling: Optimal Solution

Recursion



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- When does job j belong to $\mathcal{O}_j$? Dynamic Programming: Weighted Interval Scheduling: Optimal Solution If and only if $v_j + \text{OPT}(p(j)) \geq \text{OPT}(j-1)$.

Recursive Algorithm

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

```
Compute-Opt(j)
  If j = 0 then
    Return 0
  Else
    Return max(v_j+Compute-Opt(p(j)), Compute-Opt(j − 1))
  Endif
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- Correctness of algorithm follows by induction (see textbook for proof).

Example of Recursive Algorithm

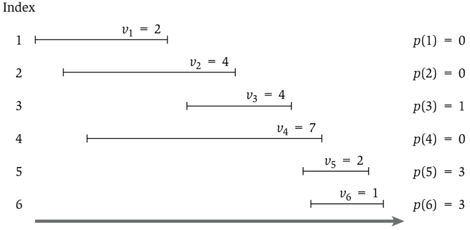

Figure 6.2 An instance of weighted interval scheduling with the functions $p(j)$ defined for each interval j.

$\mathrm{OPT}(6) =$ ▸ Dynamic Programming: Weighted Interval Scheduling: Optimal Solution for Example

$\mathrm{OPT}(5) =$

$\mathrm{OPT}(4) =$

$\mathrm{OPT}(3) =$

$\mathrm{OPT}(2) =$

$\mathrm{OPT}(1) =$

$\mathrm{OPT}(0) = 0$

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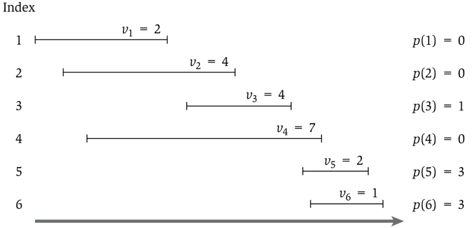

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$\text{OPT}(6) = \max(v_6 + \text{OPT}(p(6)), \text{OPT}(5)) = \max(1 + \text{OPT}(3), \text{OPT}(5))$

$\text{OPT}(5) =$

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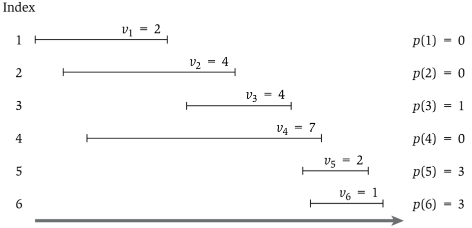

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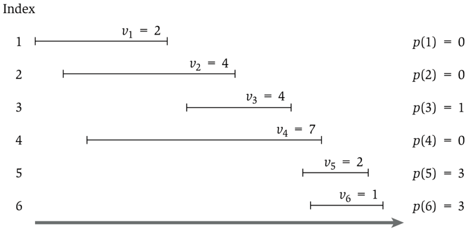
Example of Recursive Algorithm



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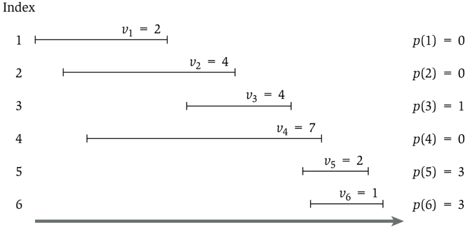

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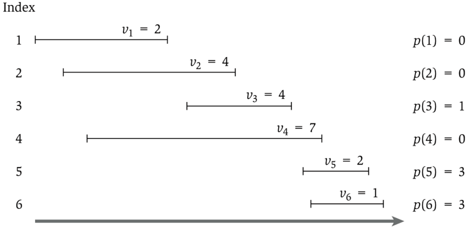

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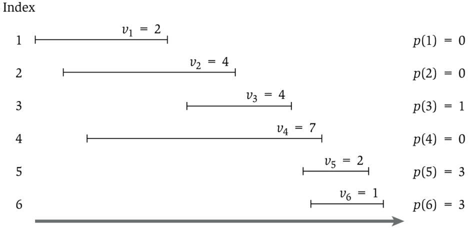

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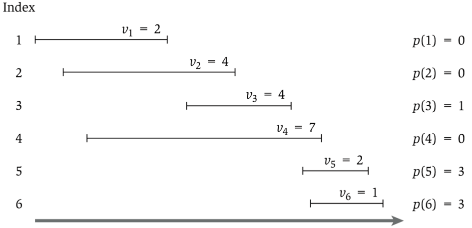
Example of Recursive Algorithm



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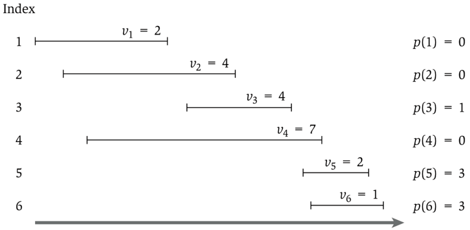

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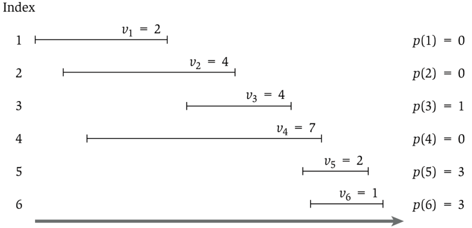

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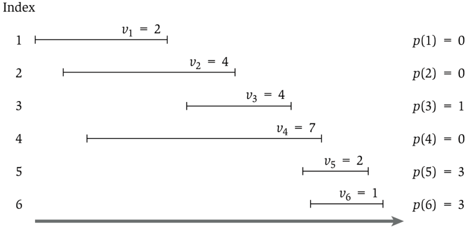

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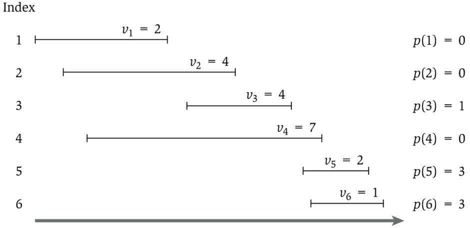

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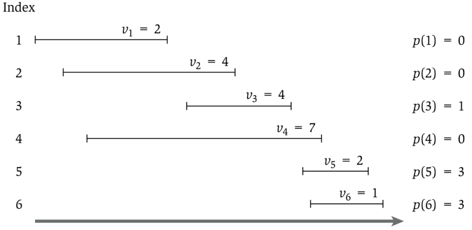

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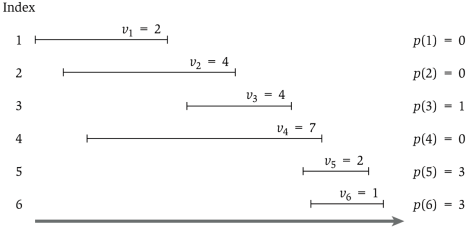
- Optimal solution is

Example of Recursive Algorithm



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\end{aligned}$$

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

Running Time of Recursive Algorithm

```
Compute-Opt(j)
  If j = 0 then
    Return 0
  Else
    Return max(v_j+Compute-Opt(p(j)), Compute-Opt(j − 1))
  Endif
```

Running Time of Recursive Algorithm

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- 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.

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

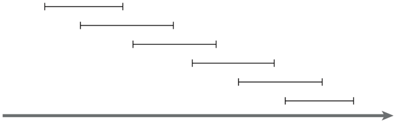

Figure 6.4 An instance of weighted interval scheduling on which the simple Compute-Opt recursion will take exponential time. The values of all intervals in this instance are 1.

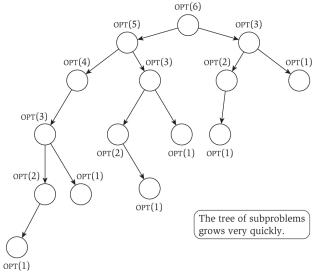

Figure 6.3 The tree of subproblems called by Compute-Opt on the problem instance of Figure 6.2.

Memoisation

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

Memoisation

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

Running Time of Memoisation

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M-Compute-Opt(j)
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- Claim: running time of this algorithm is $O(n)$ (after sorting).

Running Time of Memoisation

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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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- 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)

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

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

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

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

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

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

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- Can recover $\mathcal{O}_j$ 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)] ≥ 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 j = 1, 2, ..., n
    M[j] = max(v_j + M[p(j)], M[j-1])
  Endfor
```

Basic Outline of Dynamic Programming

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

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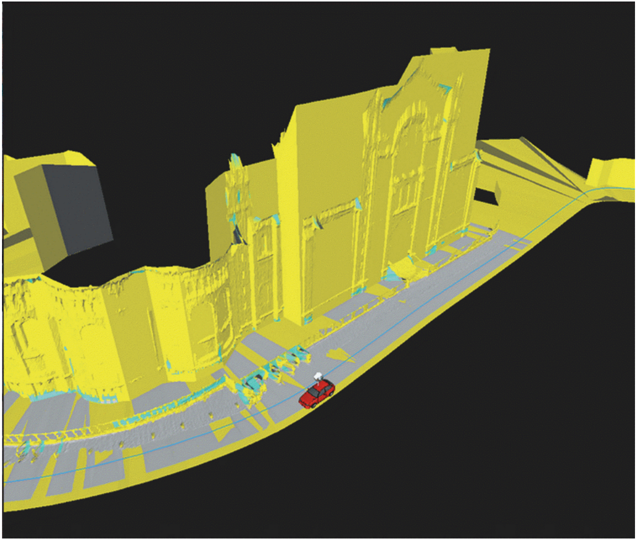
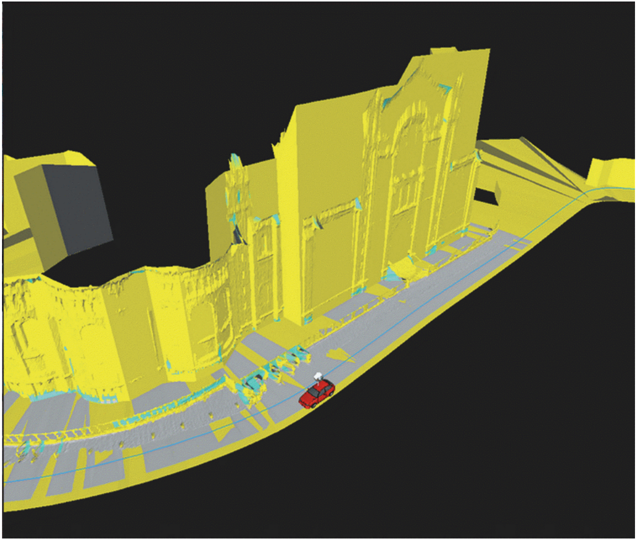
  4. There is an easy-to-compute recurrence that allows us to compute the solution to a sub-problem from the solutions to some smaller sub-problems.
- Difficulties in designing dynamic programming algorithms:
  1. Which sub-problems to define?
  2. How can we tie together sub-problems using a recurrence?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

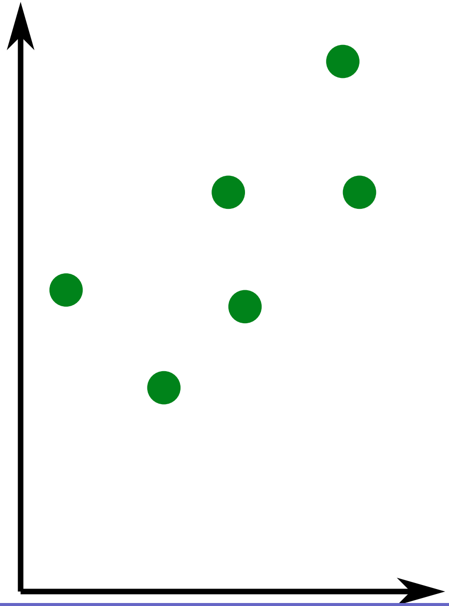

Google maps
Street View
google.com/streetview





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.

Fitting Lines



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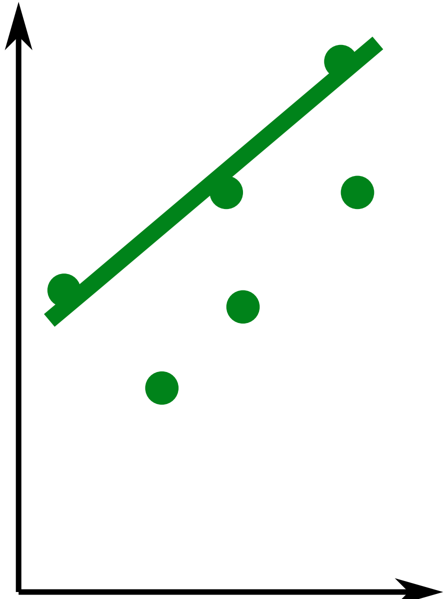

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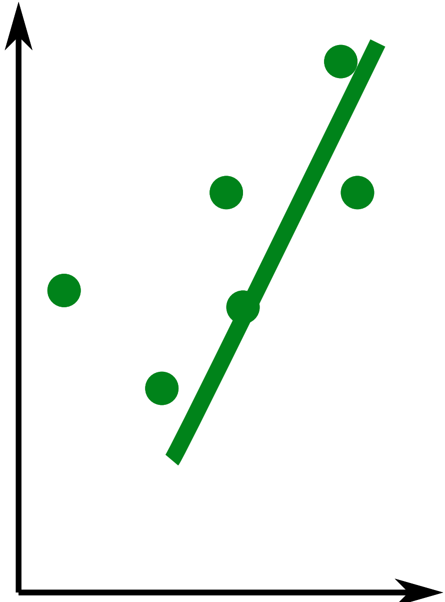

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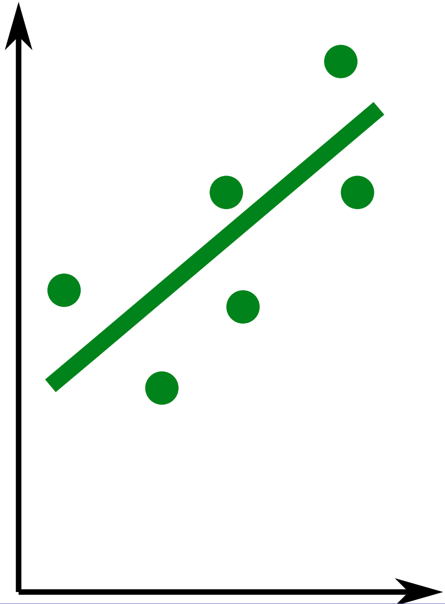
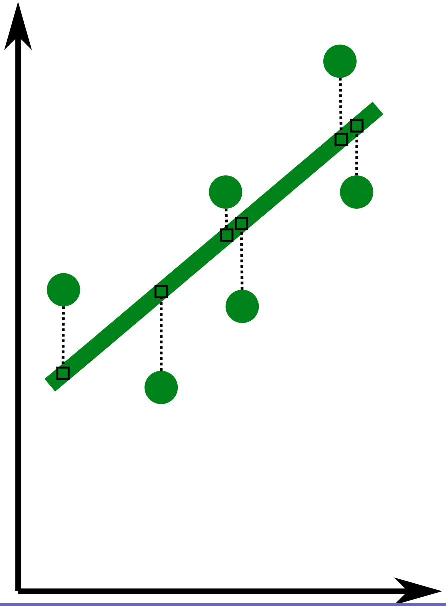
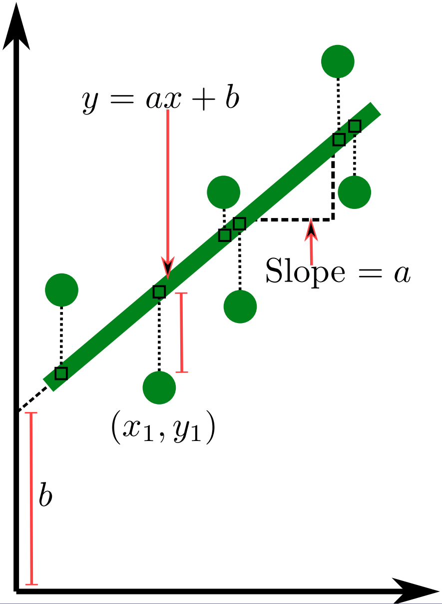


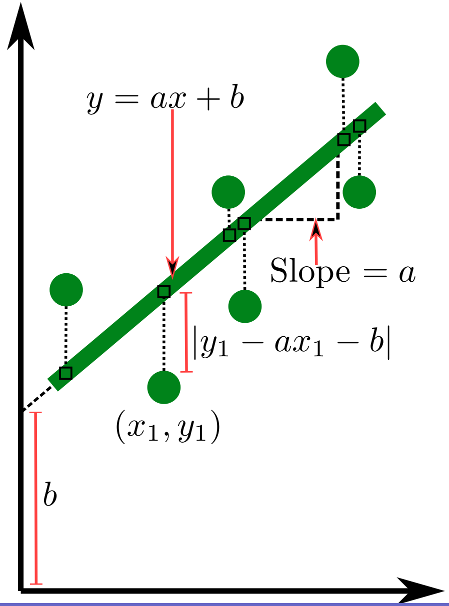
Fitting Lines



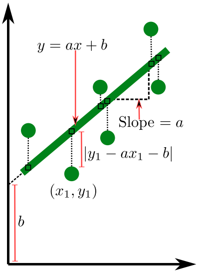
Fitting Lines



Fitting Lines

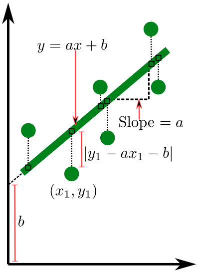


Least Squares Problem



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

Least Squares Problem



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

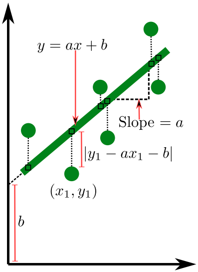
LEAST SQUARES REGRESSION

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

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

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

Least Squares Problem



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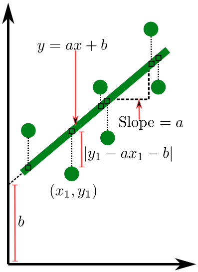
- How many unknown parameters must we find values for?

▸ Dynamic Programming: Segmented Least Squares: Line Fitting

Least Squares Problem



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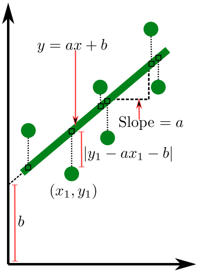
- How many unknown parameters must we find values for? Two: a and b.

Least Squares Problem



- Given scientific or statistical data plotted on two axes.
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LEAST SQUARES REGRESSION

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

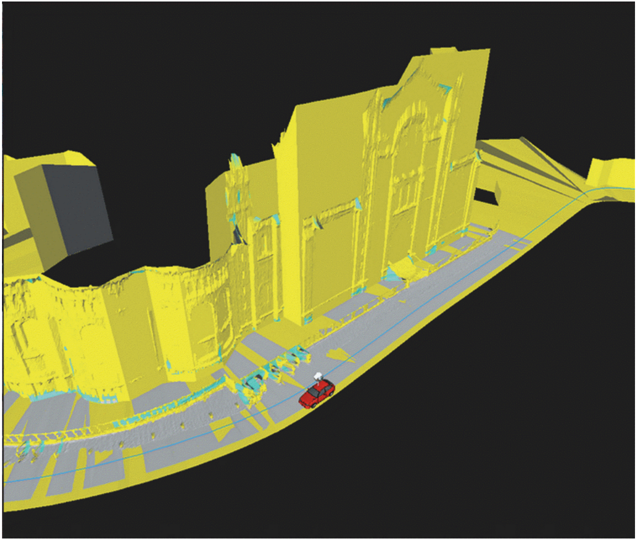
SOLUTION: Line $L : y = ax + b$ that minimises

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

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



Segmented Least Squares

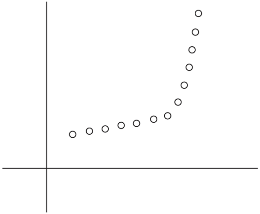


Figure 6.7 A set of points that lie approximately on two lines.

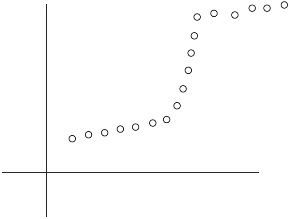
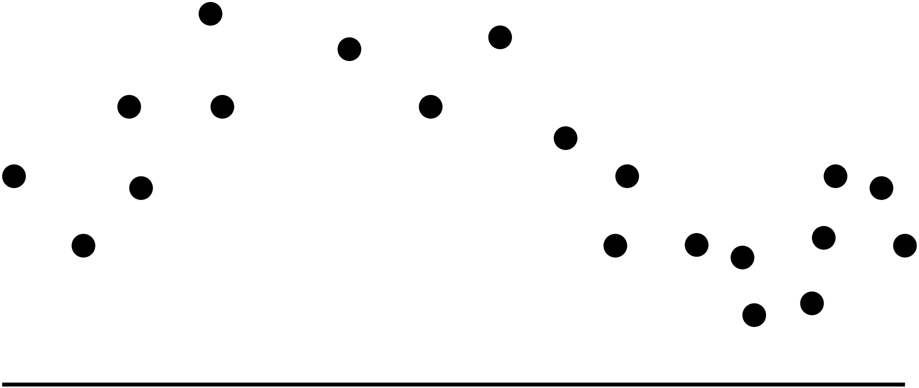


Figure 6.8 A set of points that lie approximately on three lines.

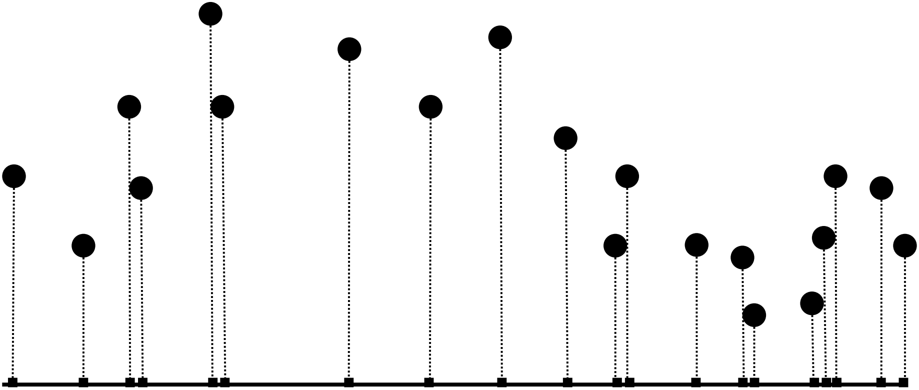
- Want to fit multiple lines through P.
- Each line must fit contiguous set of x-coordinates.
- Lines must minimise total error.

Example of Segmented Least Squares



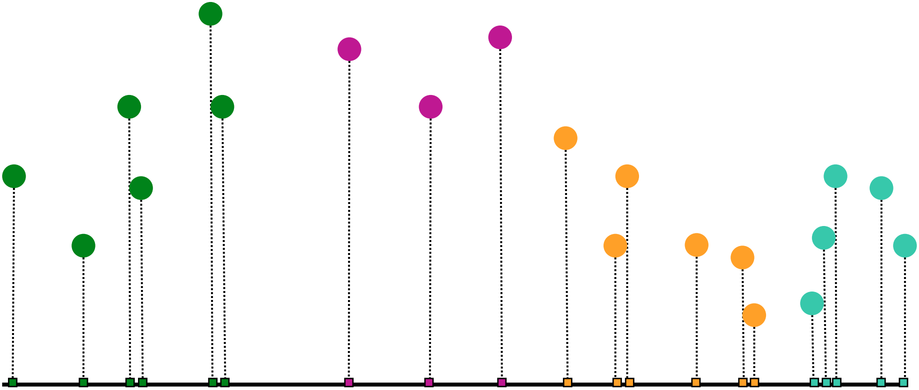
Input contains a set of two-dimensional points.

Example of Segmented Least Squares



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

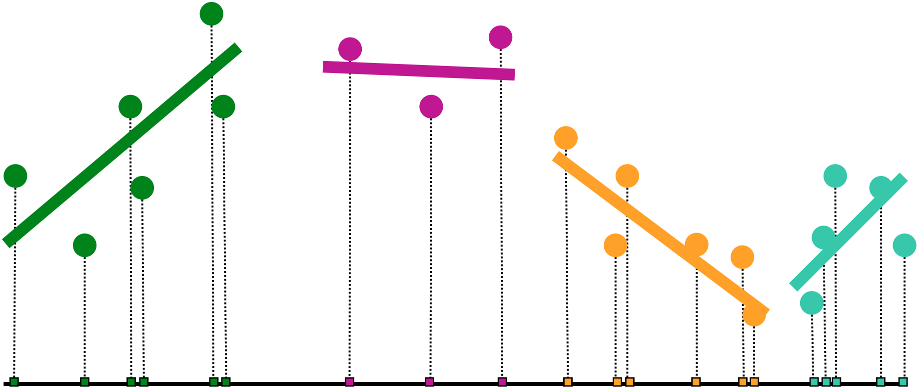
Example of Segmented Least Squares



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

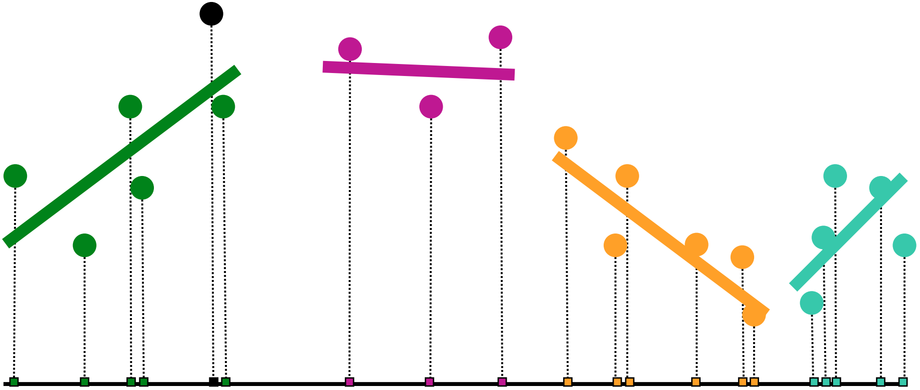
Here we are defining a meaning for "segment" that is specific to this problem.

Example of Segmented Least Squares



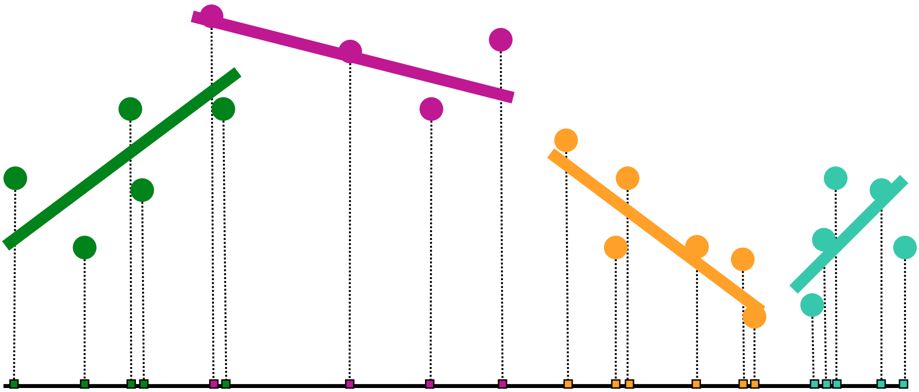
Fit the best line for each segment.

Example of Segmented Least Squares



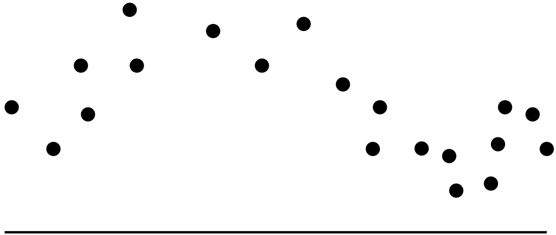
Illegal solution: black point is not in any segment.

Example of Segmented Least Squares



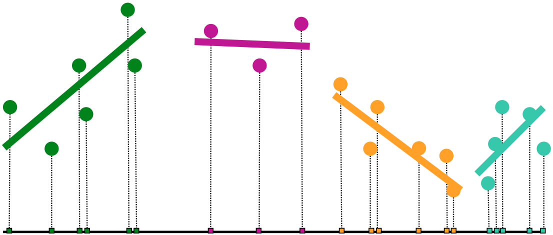
Illegal solution: leftmost purple point has x-coordinate between last two points in green segment.

Formulating Segmented Least Squares Problem



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

Formulating Segmented Least Squares Problem



SEGMENTED LEAST SQUARES

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

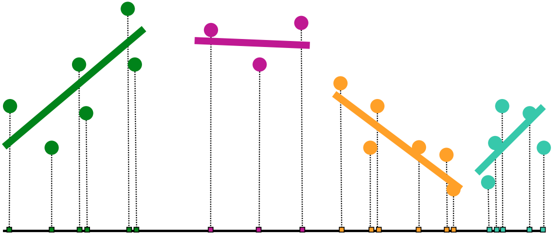
SOLUTION:

1. An integer k,
2. a partition of P into k segments $\{P_1, P_2, \ldots, P_k\}$, and
3. for each segment P_j, the best-fit line $L_j : y = a_j x + b_j, 1 \leq j \leq k$

that minimise the total error

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

Formulating Segmented Least Squares Problem



SEGMENTED LEAST SQUARES

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

SOLUTION:

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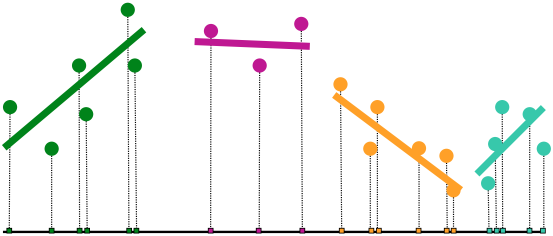
that minimise the total error

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

Formulating Segmented Least Squares Problem



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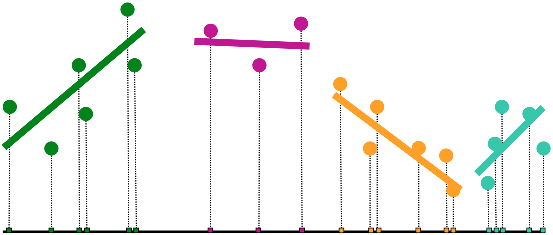
- How many unknown parameters must we find? $2k$, and we must find k too!

Formulating Segmented Least Squares Problem



SEGMENTED LEAST SQUARES

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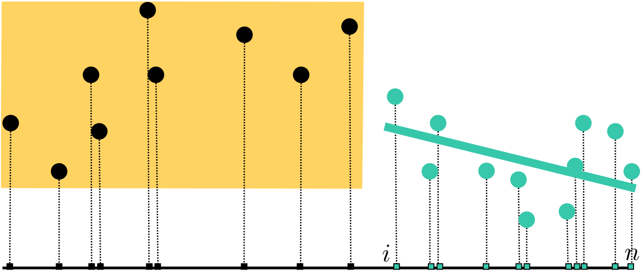
that minimise the total error

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

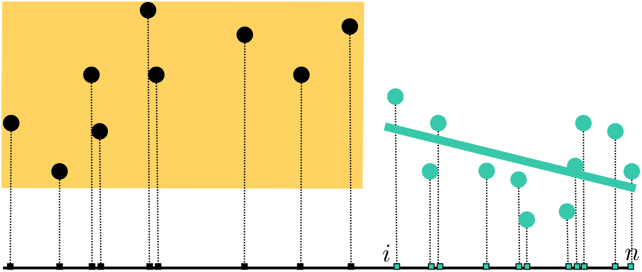
- How many unknown parameters must we find? $2k$, and we must find k too!
- Assume points in P are sorted in increasing order of x-coordinate.

Formulating the Recursion: Getting Intuition



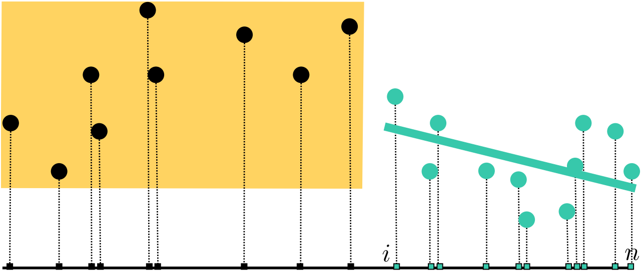
- Observation: Where does the last segment in the optimal solution end?

Formulating the Recursion: Getting Intuition



- 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!

Formulating the Recursion: Getting Intuition

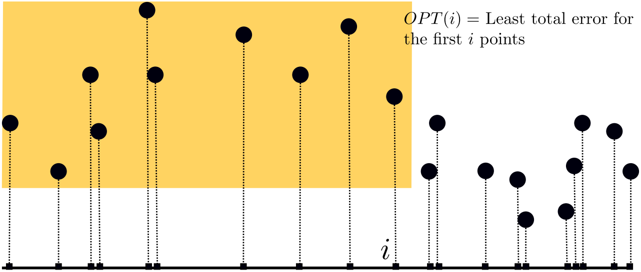


- Observation: Where does the last segment in the optimal solution end? p_n, and this segment starts at some point p_i. We don't know i yet!

- 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.

Formulating the Recursion: Getting Intuition



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- Let $OPT(i)$ be the optimal total error for the points $\{p_1, p_2, \ldots, p_i\}$.
- We want to compute OPT(n).

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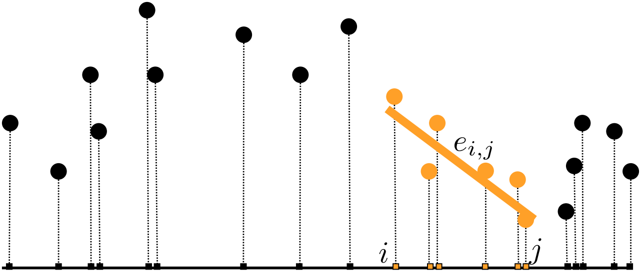

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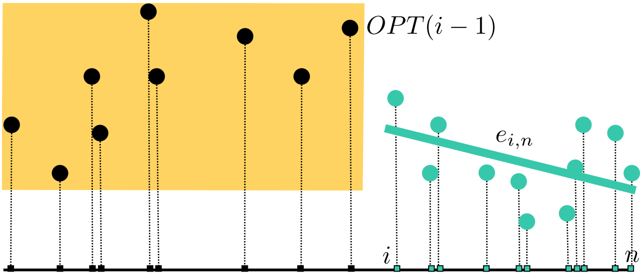
- Let $OPT(i)$ be the optimal total error for the points $\{p_1, p_2, \ldots, p_i\}$.
- We want to compute $\text{OPT}(n)$.
- Let $e_{i,j}$ denote the minimum error of a (single) line that fits $\{p_i, p_2, \ldots, p_j\}$.
- If the last segment in the optimal partition is $\{p_i, p_{i+1}, \ldots, p_n\}$, 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.

Formulating the Recursion: Getting Intuition



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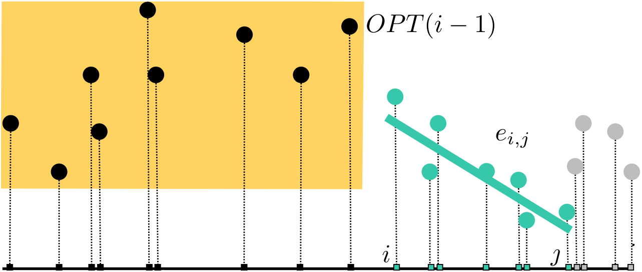
- If the last segment in the optimal partition is $\{p_i, p_{i+1}, \ldots, p_n\}$, then

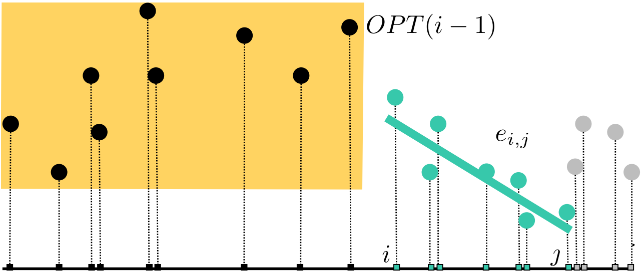
$$\text{OPT}(n) = e_{i,n} + C + \text{OPT}(i-1)$$

Formulating the Full Recursion



- In general, we want to solve sub-problem on the points $\{p_1, p_2, \ldots p_j\}$, i.e., we want to compute $\text{OPT}(j)$, where j lies between 1 and n.

Formulating the Full Recursion



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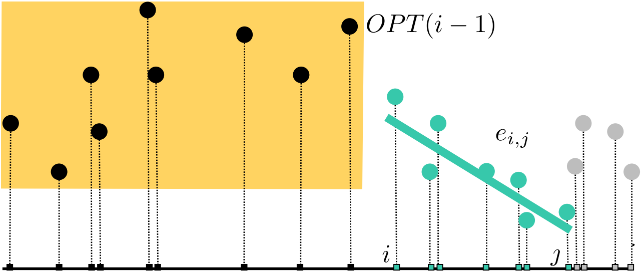
Formulating the Full Recursion



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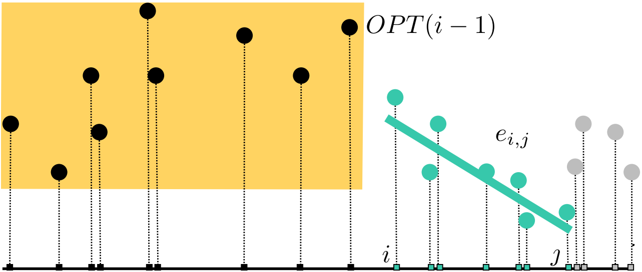
Formulating the Full Recursion



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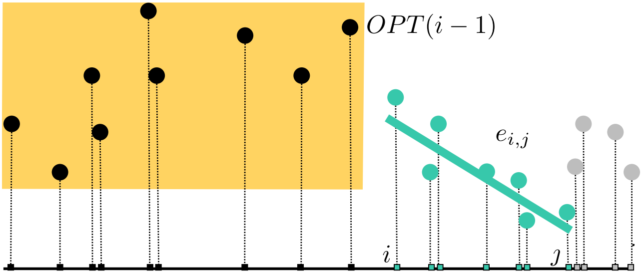
- If the last segment in the optimal partition is $\{p_i, p_{i+1}, \ldots, p_j\}$, then

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

- We don't know i! Dynamic Programming: Segmented Least Squares: First j points

Formulating the Full Recursion



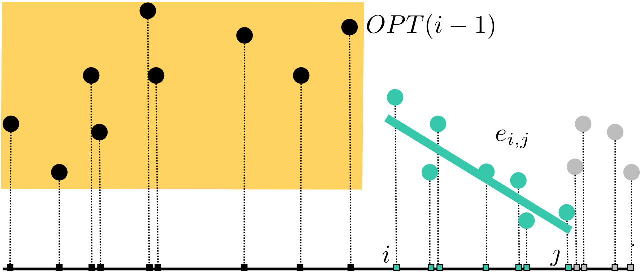
- In general, we want to solve sub-problem on the points $\{p_1, p_2, \ldots p_j\}$, i.e., we want to compute OPT(j), where j lies between 1 and n.
- If the last segment in the optimal partition is $\{p_i, p_{i+1}, \ldots, p_j\}$, then

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

- We don't know i! But i can take only j distinct values: $1, 2, \ldots, j-1, j$. Therefore,

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

Formulating the Full Recursion



- In general, we want to solve sub-problem on the points $\{p_1, p_2, \dots p_j\}$, i.e., we want to compute OPT(j), where j lies between 1 and n.
- If the last segment in the optimal partition is $\{p_i, p_{i+1}, \dots, p_j\}$, then

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

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

Dynamic Programming Algorithm

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

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

Dynamic Programming Algorithm

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

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    Use the recurrence (6.7) to compute M[j]
  Endfor
  Return M[n]
```

- We can find the segments in the optimal solution by backtracking.

Running Time

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

```
Segmented-Least-Squares(n)
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    Use the recurrence (6.7) to compute M[j]
  Endfor
  Return M[n]
```

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

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

Running Time

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

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

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

▸ Dynamic Programming: Segmented Least Squares: Running Time Part 1

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

Running Time

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

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

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

▸ Dynamic Programming: Segmented Least Squares: Running Time Part 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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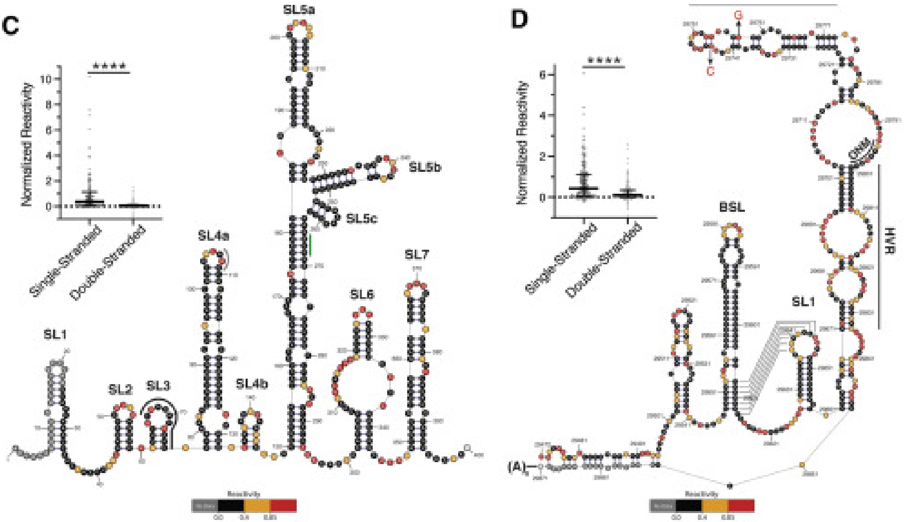
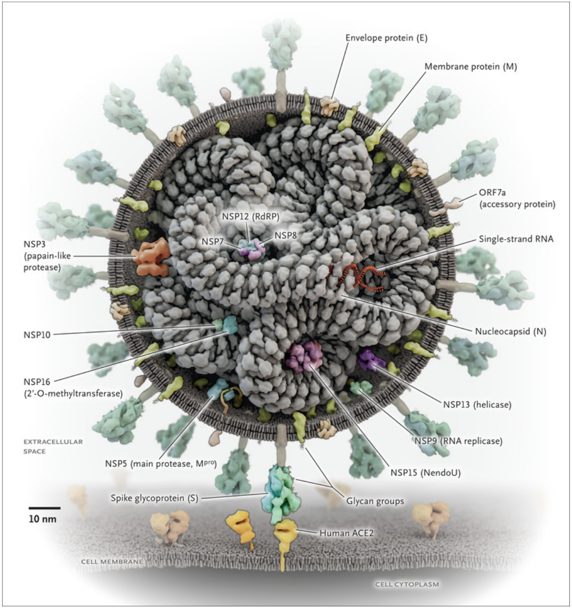
$$T(n) = \sum_{1 \le j \le n} \sum_{1 \le i \le j} O(j-i) = O(n^3)$$

- Running time is $O(n^3)$; can be improved to $O(n^2)$.



Dynamic Programming: Image


Envelope protein (E)
Membrane protein (M)
ORF7a
(accessory protein)
Single-strand RNA
NSP12 (RdRP)
NSP8
NSP7
NSP3
(papain-like
protease)
Nucleocapsid (N)
NSP10
NSP16
(2'-O-methyltransferase)
NSP13 (helicase)
NSP9 (RNA replicase)
EXTRACELLULAR
SPACE
NSP5 (main protease, Mpro)
NSP15 (NendoU)
Spike glycoprotein (S)
Glycan groups
10 nm
Human ACE2
CELL MEMBRANE
CELL CYTOPLASM

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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1. Pairs of bases match up; each base matches with ≤ 1 other base.
2. Adenine always matches with Uracil.
3. Cytosine always matches with Guanine.
4. There are no kinks in the folded molecule.
5. Structures are “knot-free”.

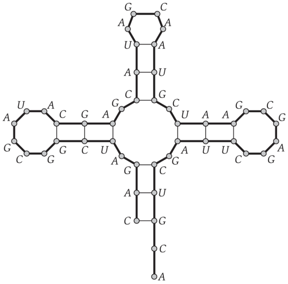

Figure 6.13 An RNA secondary structure. Thick lines connect adjacent elements of the sequence; thin lines indicate pairs of elements that are matched.

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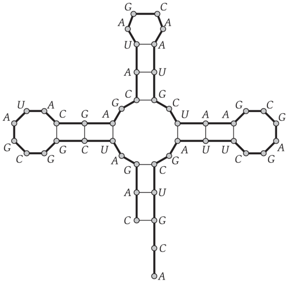

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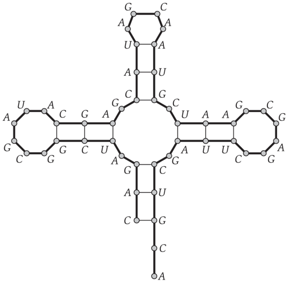

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- Problem: given an RNA molecule, predict its secondary structure.
- Hypothesis: In the cell, RNA molecules form the secondary structure with the lowest total free energy.

Formulating the Problem

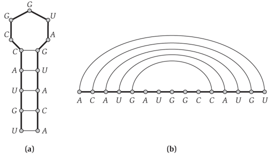
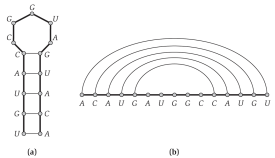


Figure 6.14 Two views of an RNA secondary structure. In the second view, (b), the string has been "stretched" lengthwise, and edges connecting matched pairs appear as noncrossing "bubbles" over the string.

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

Formulating the Problem



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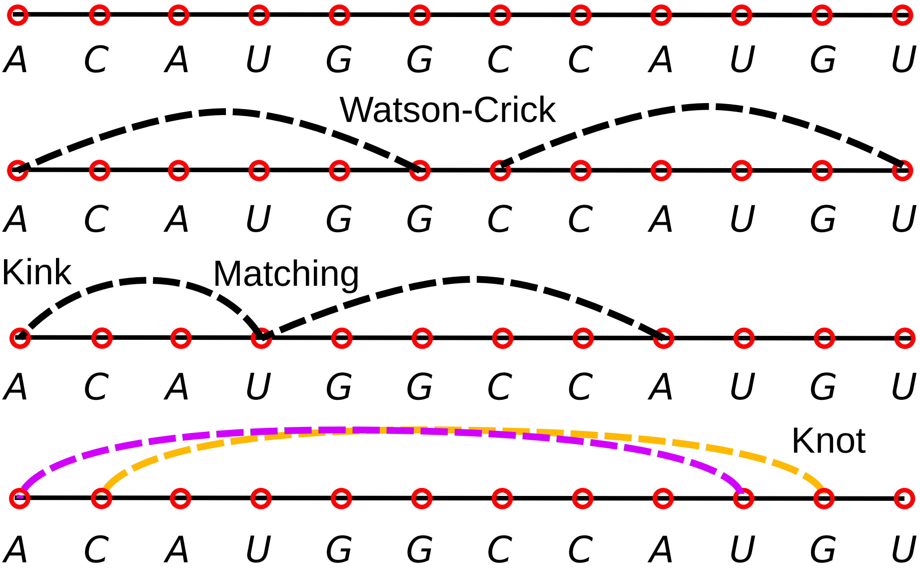
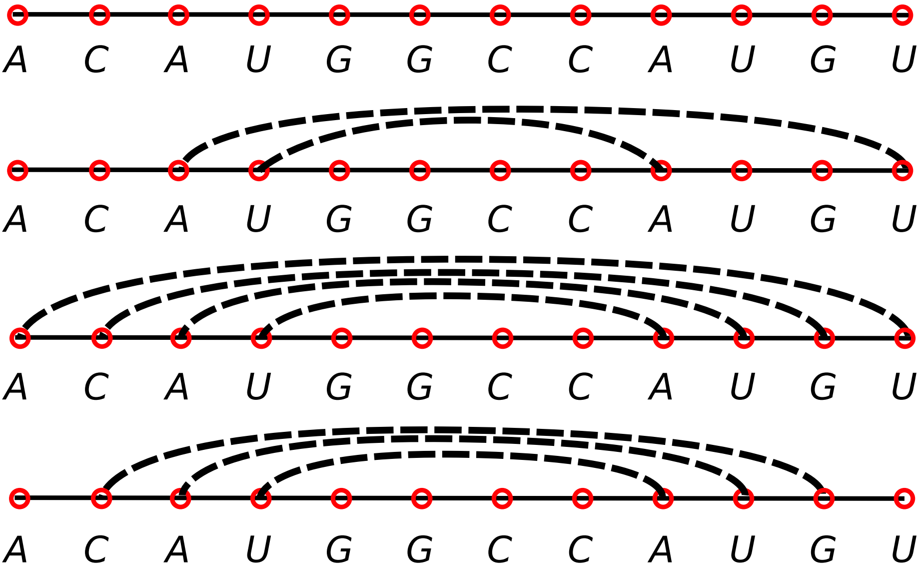
- A *secondary structure on B* is a set of pairs $S = \{(i, j)\}$, where $1 \leq i, j \leq n$ and
  1. *(No kinks.)* If $(i, j) \in S$, then $i < j - 4$.
  2. *(Watson-Crick)* The elements in each pair in S consist of either $\{A, U\}$ or $\{C, G\}$ (in either order).
  3. S is a *matching*: no index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

Illegal Secondary Structures



Legal Secondary Structures



Dynamic Programming Approach

- $OPT(j)$ is the maximum number of base pairs in a secondary structure for $b_1 b_2 \dots b_j$. ▸ Dynamic Programming: RNA Secondary Structure: Base cases 1

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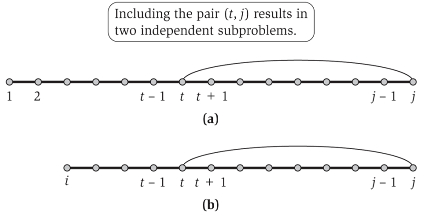

Figure 6.15 Schematic views of the dynamic programming recurrence using (a) one variable, and (b) two variables.

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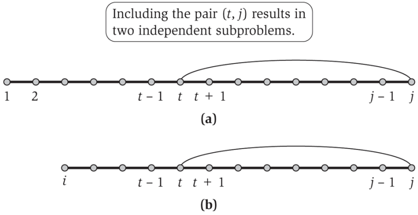

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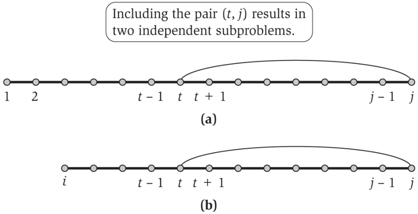

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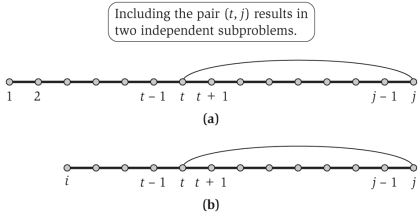
- Insight: need sub-problems indexed both by start and by end.



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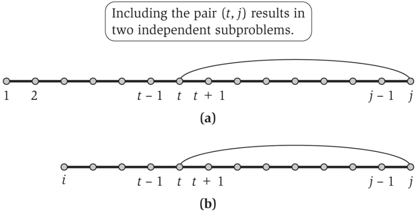
Correct Dynamic Programming Approach



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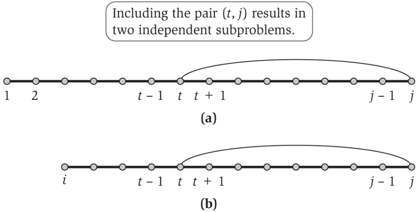

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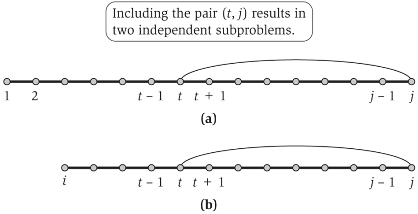

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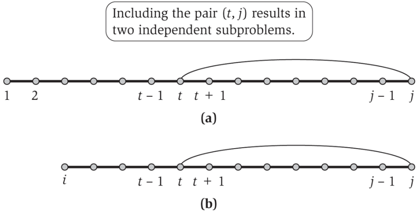
$$\text{OPT}(i, j) = \max \left(\qquad \right)$$

Correct Dynamic Programming Approach



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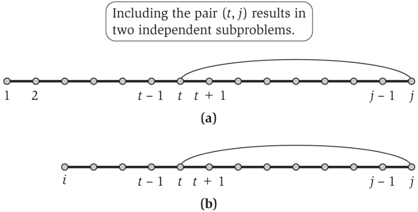

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▸ Dynamic Programming: RNA Secondary Structure: Subproblems 2

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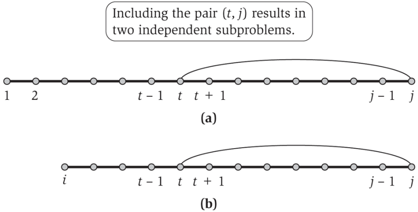
Correct Dynamic Programming Approach



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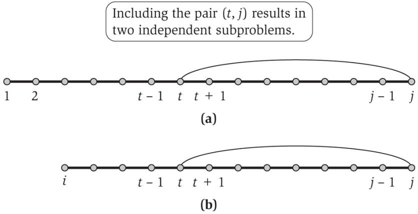
Correct Dynamic Programming Approach



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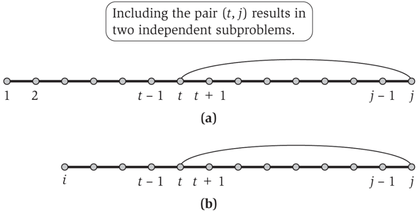
$$\text{OPT}(i,j) = \max\left(\text{OPT}(i,j-1), \max_t \left(1 + \text{OPT}(i,t-1) + \text{OPT}(t+1,j-1)\right)\right)$$

Correct Dynamic Programming Approach



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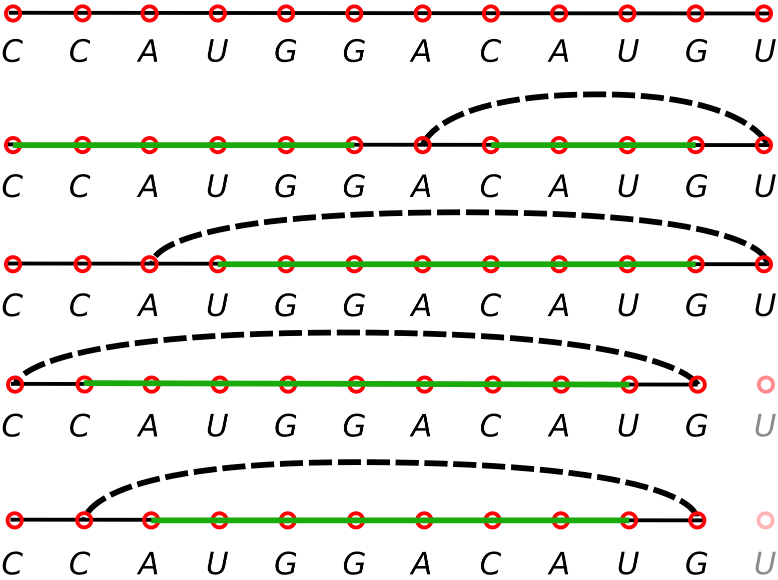
- In the "inner" maximisation, t runs over all indices between i and $j - 5$ that are allowed to pair with j.

Example of Dynamic Programming Algorithm



Dynamic Programming Algorithm

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- There are ▸ Dynamic Programming: RNA Secondary Structure: Number of sub-problems sub-problems.

Dynamic Programming Algorithm

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

Dynamic Programming Algorithm

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- How do we order them from "smallest" to "largest"?
- Computing $\text{OPT}(i,j)$ involves sub-problems of the form $\text{OPT}(l,j-1)$.
- We should compute OPT() values in increasing order of the second argument.

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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 $\text{OPT}(i,j)$?

▸ Dynamic Programming: RNA Secondary Structure: Running time

- What is the running time of the algorithm?   .

Dynamic Programming Algorithm

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```
Initialise OPT(i,j)= 0 for every l,j such that i ≥ 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 $\text{OPT}(i,j)$? $O(j-i)$
- 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 $c : E \rightarrow \mathbb{R}$, i.e., c_{uv} is the cost of the edge $(u, v) \in E$.
- A *negative cycle* is a directed cycle whose edges have a total cost that is negative.
- Two related problems:
  1. If G has no negative cycles, find the *shortest s-t path*: a path from source s to destination t with minimum total cost.
  2. Does G have a *negative cycle*? Application is to arbitrage opportunities.

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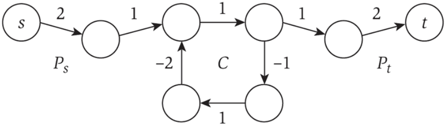

Figure 6.20 In this graph, one can find s-t paths of arbitrarily negative cost (by going around the cycle C many times).

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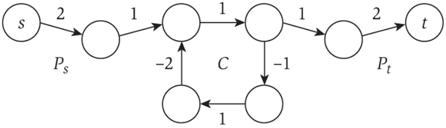

Figure 6.20 In this graph, one can find s-t paths of arbitrarily negative cost (by going around the cycle C many times).

Approaches for Shortest Path Algorithm

1. Run Dijsktra's algorithm.
   - Dynamic Programming: Shortest Paths: Example Graph (a)

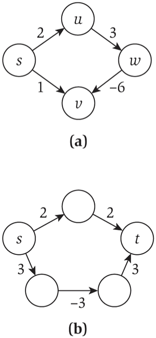

Figure 6.21 (a) With negative edge costs, Dijkstra's Algorithm can give the wrong answer for the Shortest-Path Problem. (b) Adding 3 to the cost of each edge will make all edges nonnegative, but it will change the identity of the shortest *s*-*t* path.

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1. Run Dijsktra's algorithm.
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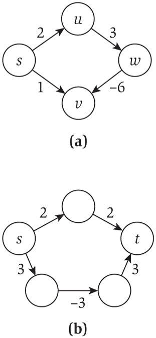

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Approaches for Shortest Path Algorithm

1. Run Dijsktra's algorithm.
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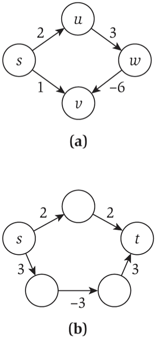
2. Add some large constant to each edge.

   ▸ Dynamic Programming: Shortest Paths: Example Graph (b)



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Approaches for Shortest Path Algorithm

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

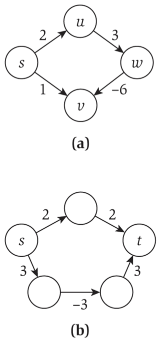

Figure 6.21 (a) With negative edge costs, Dijkstra's Algorithm can give the wrong answer for the Shortest-Path Problem. (b) Adding 3 to the cost of each edge will make all edges nonnegative, but it will change the identity of the shortest *s*-*t* path.

Dynamic Programming Approach

- Assume G has no negative cycles.
- Claim: There is a shortest path from s to t that is *simple* (does not repeat a node) ▸ Dynamic Programming: Shortest Paths: "Simple" Proof

Dynamic Programming Approach

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- How do we define sub-problems?
  - Shortest s-t path has $\leq n-1$ edges: how we can reach t using i edges, for different values of i?
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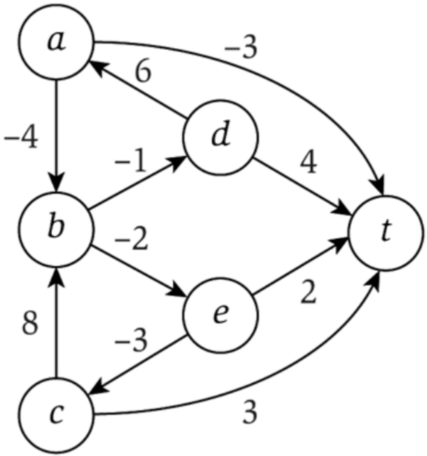
- Sub-problems defined by varying the number of edges in the shortest path and by varying the starting node in the shortest path.



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 $\text{OPT}(n-1, s)$.

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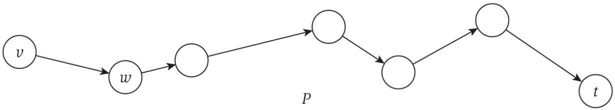

Figure 6.22 The minimum-cost path P from v to t using at most i edges.

- Let P be the optimal path whose cost is $\text{OPT}(i, v)$.

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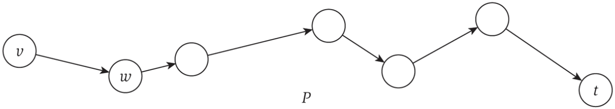

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- Let P be the optimal path whose cost is $\text{OPT}(i, v)$.
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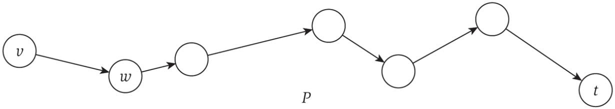

Figure 6.22 The minimum-cost path P from v to t using at most i edges.

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  1. If P actually uses $i-1$ edges, then $\text{OPT}(i, v) = \text{OPT}(i-1, v)$.
  2. If first node on P is w, then $\text{OPT}(i, v) = c_{vw} + \text{OPT}(i-1, w)$.

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

Example of Dynamic Programming Recursion

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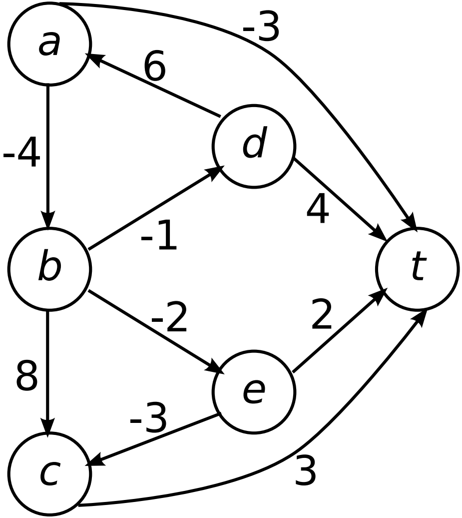

	0	1	2	3	4	5
t						
a						
b						
c						
d						
e						

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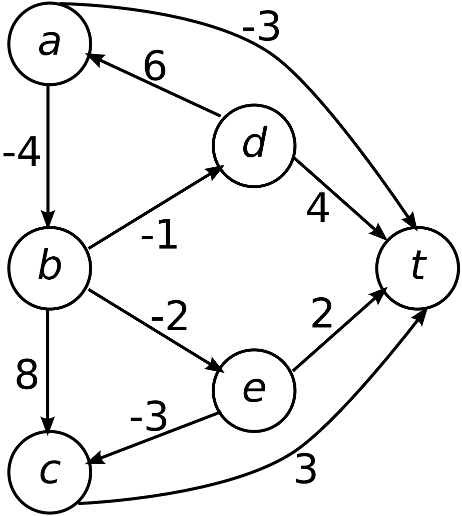

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t						
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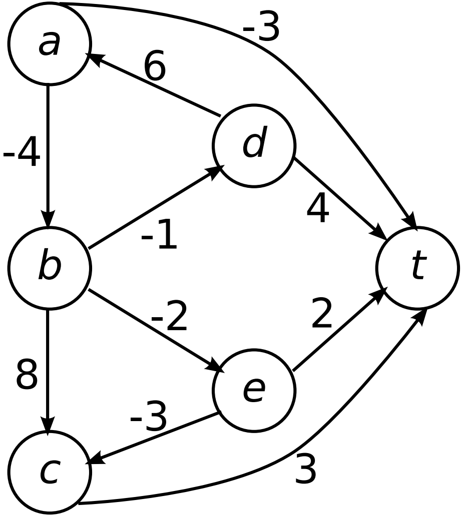

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞					
b	∞					
c	∞					
d	∞					
e	∞					

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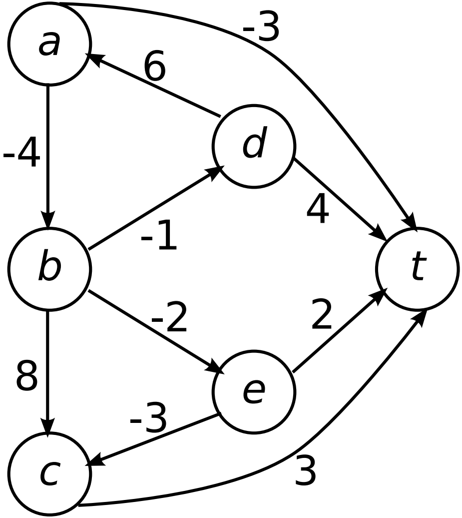

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞					
b	∞					
c	∞					
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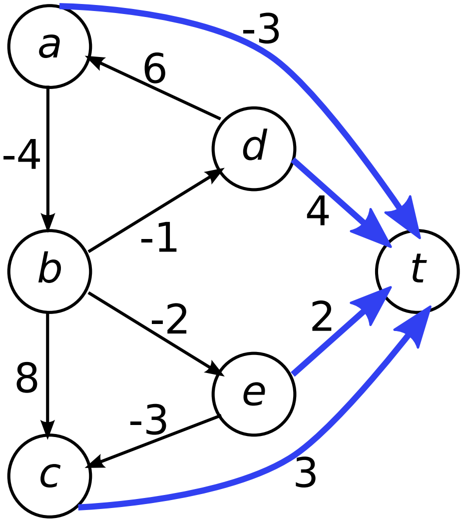

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3				
b	∞	∞				
c	∞	3				
d	∞	4				
e	∞	2				

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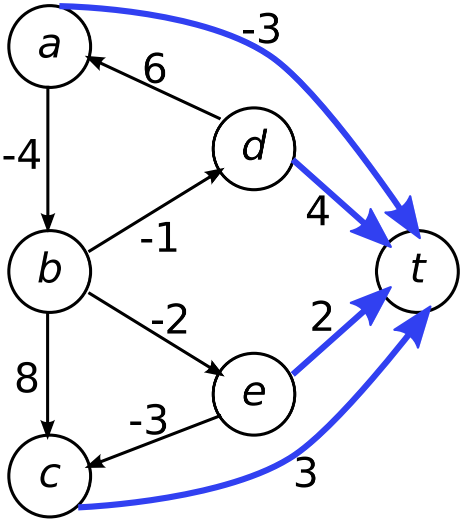

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3				
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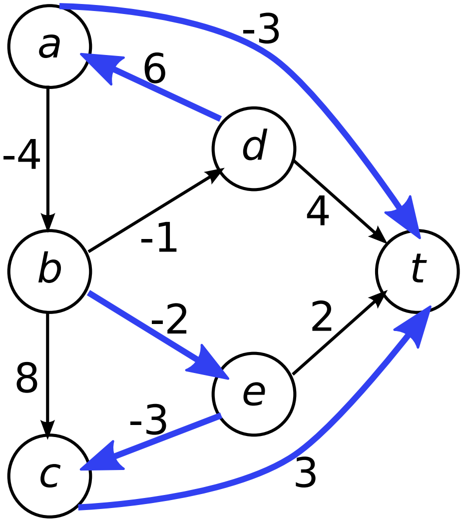

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3			
b	∞	∞	0			
c	∞	3	3			
d	∞	4	3			
e	∞	2	0			

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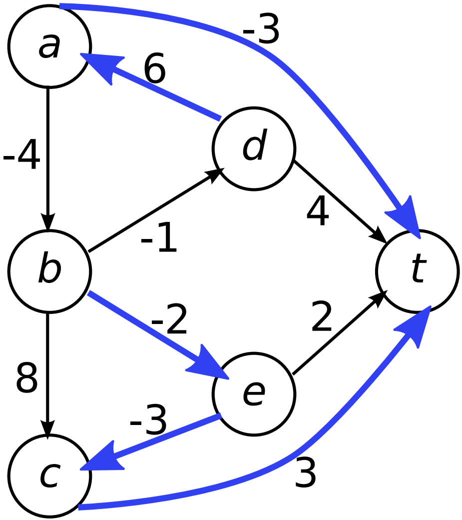

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3			
b	∞	∞	0			
c	∞	3	3			
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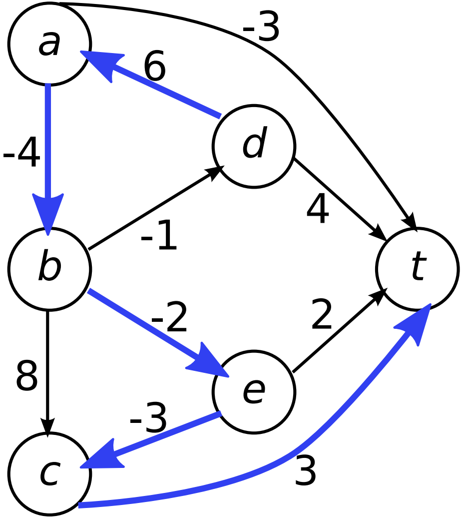

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3	-4		
b	∞	∞	0	-2		
c	∞	3	3	3		
d	∞	4	3	3		
e	∞	2	0	0		

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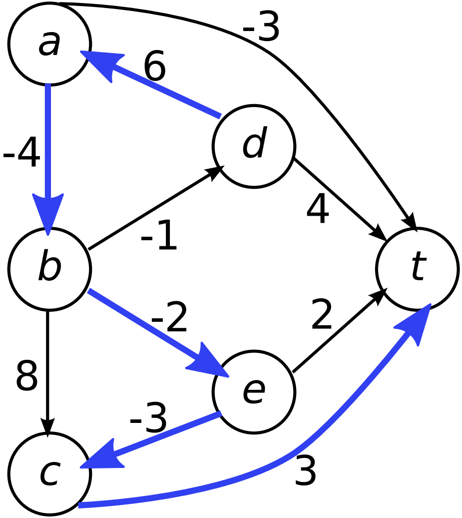

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3	-4		
b	∞	∞	0	-2		
c	∞	3	3	3		
d	∞	4	3	3		
e	∞	2	0	0		

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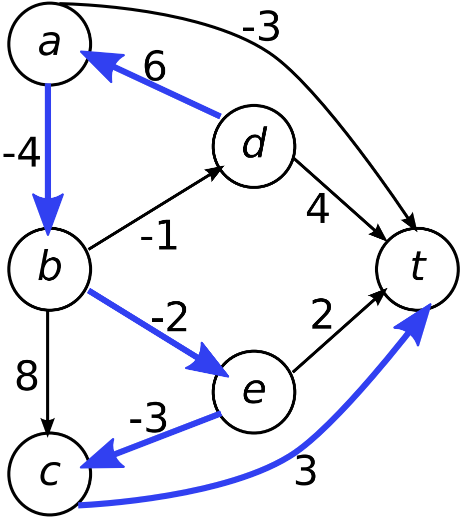

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3	-4	-6	
b	∞	∞	0	-2	-2	
c	∞	3	3	3	3	
d	∞	4	3	3	2	
e	∞	2	0	0	0	

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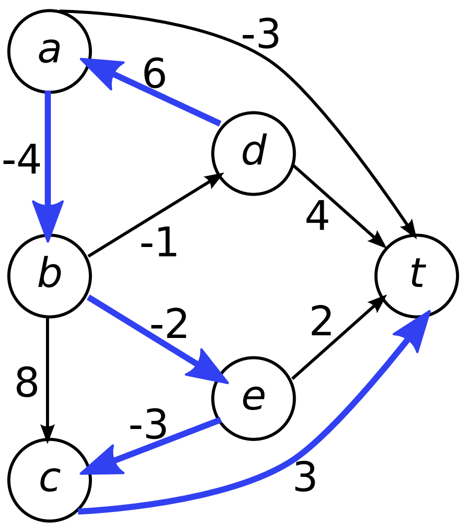

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3	-4	-6	
b	∞	∞	0	-2	-2	
c	∞	3	3	3	3	
d	∞	4	3	3	2	
e	∞	2	0	0	0	

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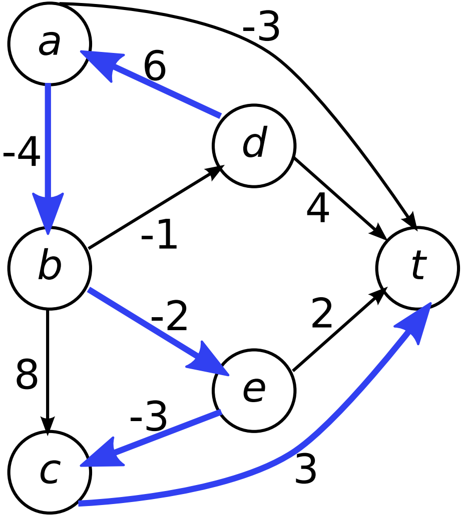

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3	-4	-6	-6
b	∞	∞	0	-2	-2	-2
c	∞	3	3	3	3	3
d	∞	4	3	3	2	0
e	∞	2	0	0	0	0

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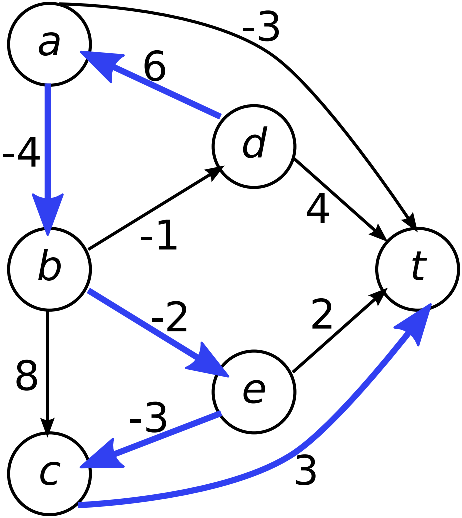

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3	-4	-6	-6
b	∞	∞	0	-2	-2	-2
c	∞	3	3	3	3	3
d	∞	4	3	3	2	0
e	∞	2	0	0	0	0

Alternate Dynamic Programming Formulation

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

Alternate Dynamic Programming Formulation

- *$OPT_{=}(i, v)$*: minimum cost of a v-t path that uses exactly i edges. Goal is to compute

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  - If first node on P is w, then $\text{OPT}_{=}(\text{i, v}) = c_{vw} + \text{OPT}_{=}(\text{i - 1, w})$.

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

- Compare the two desired solutions:

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

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

Bellman-Ford Algorithm

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

```
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] = ∞ for all other v ∈ V
  For i = 1, ..., n − 1
    For v ∈ V in any order
      Compute M[i, v] using the recurrence (6.23)
    Endfor
  Endfor
  Return M[n − 1, s]
```

Bellman-Ford Algorithm

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    For v ∈ V in any order
      Compute M[i,v] using the recurrence (6.23)
    Endfor
  Endfor
  Return M[n-1, s]
```

▸ Dynamic Programming: Shortest Paths: Space and Running Time

- Space used is ??. Running time is ??.

Bellman-Ford Algorithm

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      Compute M[i, v] using the recurrence (6.23)
    Endfor
  Endfor
  Return M[n−1, s]
```

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

An Improved Bound on the Running Time

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

- w only needs to range over outgoing neighbours N_v of v.
- If $n_v = |N_v|$ is the number of outgoing 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 outgoing neighbours N_v of v.
- If $n_v = |N_v|$ is the number of outgoing 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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  1. Maintain two arrays M and M' indexed over V.
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- Claim: at the beginning of iteration i, M stores values of $\mathrm{OPT}(i-1, v)$ for all nodes $v \in V$.
- Space used is $O(n)$.

Computing the Shortest Path: Algorithm

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

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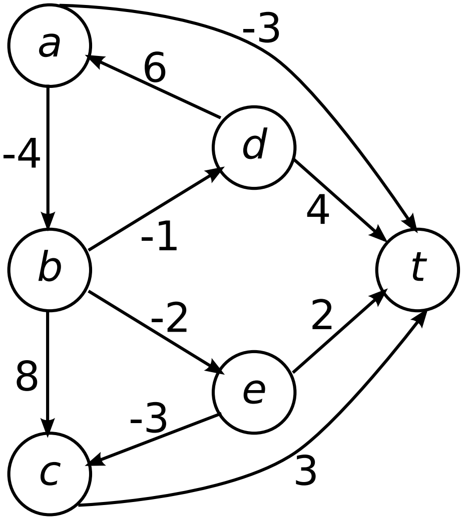
  - set $M[v] = c_{vx} + M'[x]$ and
  - set $f(v) = x$.
- At the end, follow $f(v)$ pointers from s to t (and hope for the best).

Example of Maintaining Pointers

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



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

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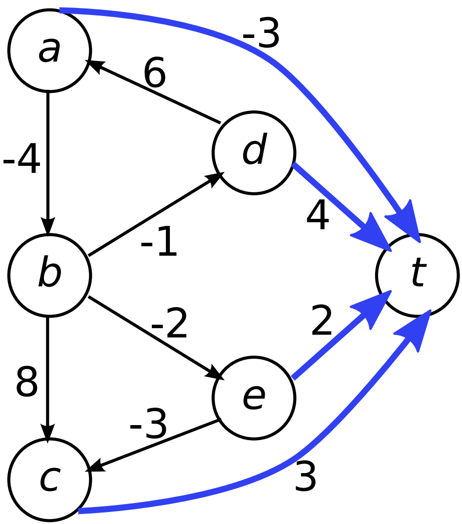

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3				
b	∞	∞				
c	∞	3				
d	∞	4				
e	∞	2				

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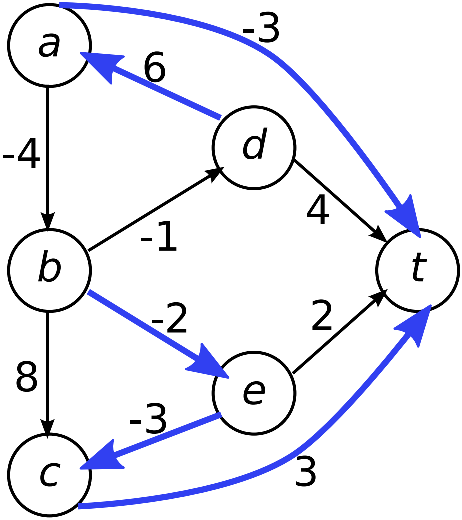

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3			
b	∞	∞	0			
c	∞	3	3			
d	∞	4	3			
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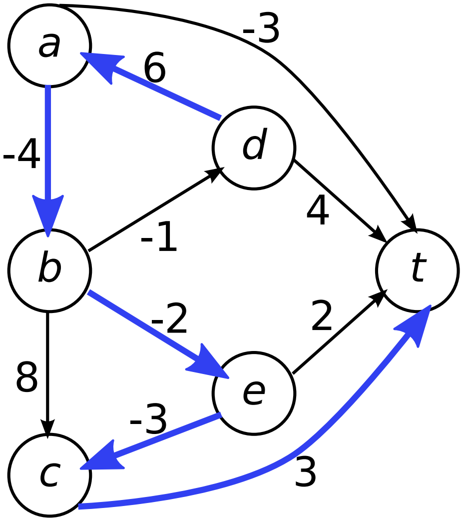

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3	-4		
b	∞	∞	0	-2		
c	∞	3	3	3		
d	∞	4	3	3		
e	∞	2	0	0		

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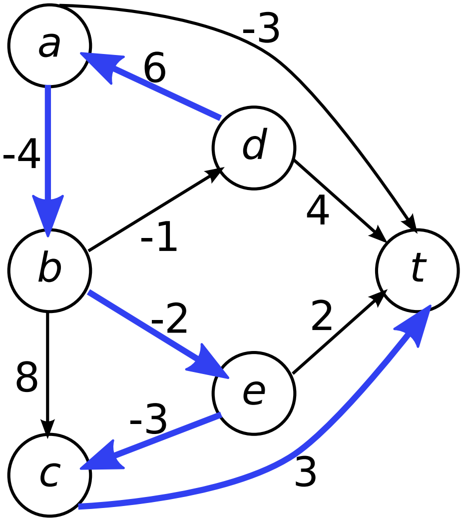

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3	-4	-6	
b	∞	∞	0	-2	-2	
c	∞	3	3	3	3	
d	∞	4	3	3	2	
e	∞	2	0	0	0	

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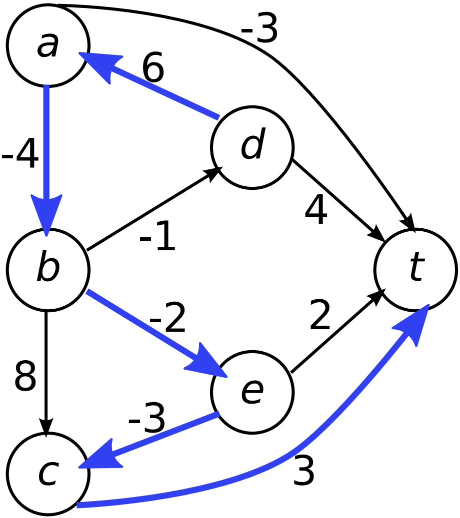

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3	-4	-6	-6
b	∞	∞	0	-2	-2	-2
c	∞	3	3	3	3	3
d	∞	4	3	3	2	0
e	∞	2	0	0	0	0

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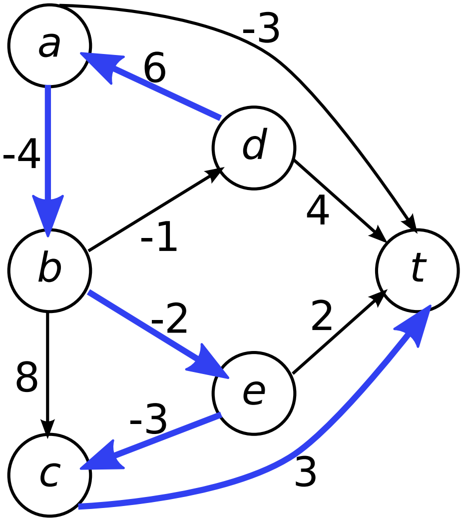

	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3	-4	-6	-6
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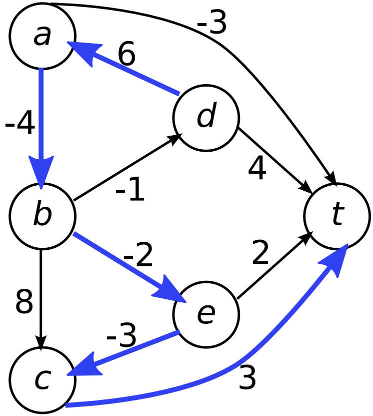
c	∞	3	3	3	3	3
d	∞	4	3	3	2	0
e	∞	2	0	0	0	0

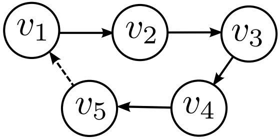
Computing the Shortest Path: Correctness

- *Pointer graph* $P(V, F)$: each edge in F is $(v, f(v))$.
  - Can P have cycles?
  - Is there a path from s to t in P?
  - Can there be multiple paths s to t in P?
  - Which of these is the shortest path?



	0	1	2	3	4	5
t	0	0	0	0	0	0
a	∞	-3	-3	-4	-6	-6
b	∞	∞	0	-2	-2	-2
c	∞	3	3	3	3	3
d	∞	4	3	3	2	0
e	∞	2	0	0	0	0

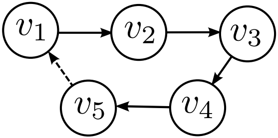
Computing the Shortest Path: Cycles in P



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

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

Computing the Shortest Path: Cycles in P



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  - Suppose we set $f(v) = w$. At this instant, $M[v] = c_{vw} + M'[w]$.

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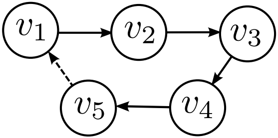

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  - Comparing $M[w]$ and $M'[w]$, Dynamic Programming: Shortest Paths: $M[w]$ and $M'[w]$

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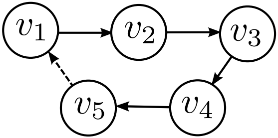

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  - Between this assignment and the assignment of $f(v)$ to some other node, $M[w]$ may itself further decrease. Hence, $M[v] \geq c_{vw} + M[w]$, in general.

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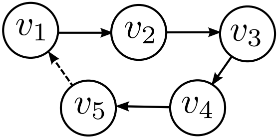

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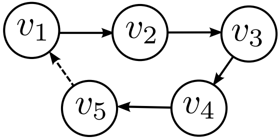
  - What is the situation just before this addition?

Computing the Shortest Path: Cycles in P



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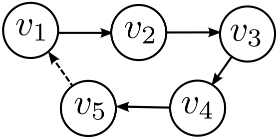

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  - Dynamic Programming: Shortest Paths: Bound on $M[v_k] - M[v_1]$

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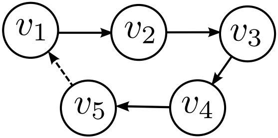

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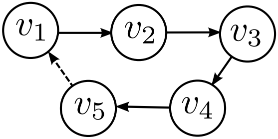

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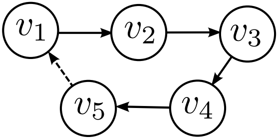
  - Adding all these inequalities, $0 > \sum_{i=1}^{k-1} c_{v_i v_{i+1}} + c_{v_k v_1} =$ cost of C.

Computing the Shortest Path: Cycles in P



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

Computing the Shortest Path: Paths in P

- Let P be the pointer graph upon termination of the algorithm.
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- Claim: P_v terminates at t. ▸ Dynamic Programming: Shortest Paths: Last node of P_v

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- 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.
- Claim: P_v terminates at t.
- 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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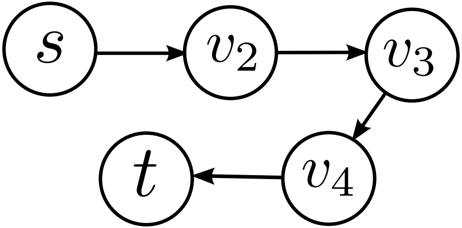

- In general, after i iterations, the path whose length is $M[v]$ may have many more than i edges.

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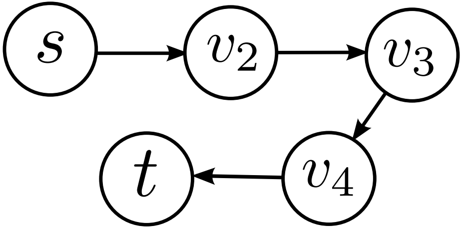

- In general, after i iterations, the path whose length is $M[v]$ may have many more than i edges.
- Early termination: If M does not change after processing all the nodes, we have computed all the shortest paths to t.