Dynamic Programming

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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.

Review: Interval Scheduling

INTERVAL SCHEDULING

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

SOLUTION: The largest subset of mutually compatible jobs.

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

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SOLUTION: The largest subset of mutually compatible jobs.

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

Weighted Interval Scheduling

WEIGHTED INTERVAL SCHEDULING

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

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• Greedy algorithm can produce arbitrarily bad results for this problem.

Approach

- ▶ Sort jobs in increasing order of finish time and relabel: $f_1 \le f_2 \le \ldots \le f_n$.
- Request *i* comes before request *j* if i < j.
- *p(j)* is the largest index *i* < *j* such that job *i* is compatible with job *j*.
 p(j) = 0 if there is no such job *i*.



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

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





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Proof: either we select the *n*th element or not

• Let \mathcal{O} be the optimal solution. Two cases to consider. Case 1 job *n* is not in \mathcal{O} .

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

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When does request j belong to O_j? If and only if 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))
Endif
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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.

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- How many such recursive calls are there in total?

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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?
- ▶ 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).

Sequence Alignment

Shortest Paths in Graphs

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.

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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 O(j) time.

```
\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.

```
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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- Difficulties in designing dynamic programming algorithms:
 - 1. Which sub-problems to define?
 - 2. How can we tie together sub-problems using a recurrence?
 - 3. How do we order the sub-problems (to allow iterative computation of optimal solutions to sub-problems)?



Figure 6.6 A "line of best fit."

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





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LEAST SQUARES **INSTANCE:** Set $P = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$ of *n* points. **SOLUTION:** Line L : y = ax + b that minimises $\operatorname{Error}(L, P) = \sum_{i=1}^{n} (y_i - ax_i - b)^2.$



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Solution is achieved by

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



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



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



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SEGMENTED LEAST SQUARES **INSTANCE:** Set $P = \{p_i = (x_i, y_i), 1 \le i \le n\}$ of *n* points, $x_1 < x_2 < \cdots < x_n$. **SOLUTION:** A integer *k*, a partition of *P* into *k* segments $\{P_1, P_2, \dots, P_k\}$, *k* lines $L_j : y = a_j x + b_j, 1 \le j \le k$ that minimise $\sum_{j=1}^k \operatorname{Error}(L_j, P_j)$

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



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

Formulating the Recursion I

- Observation: p_n is part of some segment in the optimal solution. This segment starts at some point p_i.
- Let OPT(i) be the optimal value for the points $\{p_1, p_2, \ldots, p_i\}$.
- Let $e_{i,j}$ denote the minimum error of any line that fits $\{p_i, p_2, \ldots, p_j\}$.
- ▶ We want to compute OPT(*n*).



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

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

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

Formulating the Recursion II

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

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Since i can take only j distinct values,

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

Segment {p_i, p_{i+1},..., 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

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

```
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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Dynamic Programming Algorithm

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

- ▶ RNA is a basic biological molecule. It is single stranded.
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- Secondary structure often governs the behaviour of an RNA molecule.
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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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- Hypothesis: In the cell, RNA molecules form the secondary structure with the lowest total free energy.



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Formulating the Problem

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



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.

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

Dynamic Programming Approach

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



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

- *OPT(j)* is the maximum number of base pairs in a secondary structure for b₁b₂...b_j. OPT(j) = 0, if j ≤ 5.
- In the optimal secondary structure on $b_1 b_2 \dots b_j$
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- Insight: need sub-problems indexed both by start and by end.



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

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

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

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```

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

Example of Algorithm





Filling in the values for k = 7

Filling in the values for k = 8

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Sequence Similarity

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

Defining Sequence Similarity

o-currance

occurrence

o-curr-ance

occurre-nce

abbbaa--bbbbaab

ababaaabbbbba-b

Defining Sequence Similarity

o-currance

occurrence

o-curr-ance

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abbbaa--bbbbaab ababaaabbbbba-b

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

Edit Distance

o-currance

occurrence

- ▶ Proposed by Needleman and Wunsch in the early 1970s.
- Input: two strings $x = x_1 x_2 x_3 \dots x_m$ and $y = y_1 y_2 \dots y_n$.
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- ▶ A matching of these sets is a set M of ordered pairs such that
 - 1. in each pair (i, j), $1 \le i \le m$ and $1 \le j \le n$ and
 - 2. no index from x (respectively, from y) appears as the first (respectively, second) element in more than one ordered pair.
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RNA Secondary Structure

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- Output: compute an alignment of minimal cost.

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- $(i,j) \in M$ if and only if minimum is achieved by the first term.
- What are the base cases? $OPT(i, 0) = OPT(0, i) = i\delta$.
$\mathsf{OPT}(i,j) = \min\left(\alpha_{x_i y_j} + \mathsf{OPT}(i-1,j-1), \delta + \mathsf{OPT}(i-1,j), \delta + \mathsf{OPT}(i,j-1)\right)$

```
Alignment(X,Y)

Array A[0...m, 0...n]

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

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

For j = 1, ..., n

For i = 1, ..., m

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

Endfor

Endfor

Return A[m,n]
```

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

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\begin{aligned} & \text{Alignment}(X,Y) \\ & \text{Array } A[0\ldots m, 0\ldots n] \\ & \text{Initialize } A[i,0] = i\delta \text{ for each } i \\ & \text{Initialize } A[0,j] = j\delta \text{ for each } j \\ & \text{For } j = 1,\ldots,n \\ & \text{For } i = 1,\ldots,m \\ & \text{Use the recurrence (6.16) to compute } A[i,j] \\ & \text{Endfor} \\ & \text{Endfor} \\ & \text{Return } A[m,n] \end{aligned}
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Running time is O(mn). Space used in O(mn).

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

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

Graph-theoretic View of Sequence Alignment



Figure 6.17 A graph-based picture of sequence alignment.

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

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 - Edges directed upward and to the right have cost δ.
 - ► Edge directed from (i, j) to (i + 1, j + 1) has cost α_{xi+1yj+1}.
- f(i, j): minimum cost of a path in G_{XY} from (0, 0) to (i, j).
- Claim: f(i,j) = OPT(i,j) and diagonal edges in the shortest path are the matched pairs in the alignment.

Motivation

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

Problem Statement

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

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

Approaches for Shortest Path Algorithm

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

Approaches for Shortest Path Algorithm

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



Figure 6.21 (a) With negative edge costs, Dijkstra's Algorithm can give the wrong answer for the Shortest-Path Problem. (b) Adding 3 to the cost of each edge will make all edges nonnegative, but it will change the identity of the shortest *s*¹ path.

- ► Assume *G* has no negative cycles.
- Claim: There is a shortest path from s to t that is simple (does not repeat a node)

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 - Shortest s-t path has ≤ n − 1 edges: how we can reach t using i edges, for different values of i?
 - We do not know which nodes will be in shortest s-t path: how we can reach t from each node in V?

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 - Shortest s-t path has ≤ n − 1 edges: how we can reach t using i edges, for different values of i?
 - We do not know which nodes will be in shortest s-t path: how we can reach t from each node in V?
- Sub-problems defined by varying the number of edges in the shortest path and by varying the starting node in the shortest path.



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• Compare the recurrence above to the previous recurrence:

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Bellman-Ford Algorithm

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

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• The total running time is O(mn).

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 - 1. Maintain two arrays M and N indexed over V.
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- Claim: at the beginning of iteration i, M stores values of OPT(i − 1, v) for all nodes v ∈ V.
- ▶ Space used is *O*(*n*).
Computing the Shortest Path: Algorithm

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

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

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

- How can we recover the shortest path that has cost M[v]?
- ► For each node v, maintain f(v), the first node after v in the current shortest path from v to t.
- ► To maintain f(v), if we ever set M[v] to min_{w∈V} (c_{vw} + N[w]), set f(v) to be the node w that attains this minimum.
- At the end, follow f(v) pointers from s to t.

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?

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

Suppose we set f(v) = w. Between this assignment and the assignment of f(v) to some other node, $M[v] \ge c_{vw} + M[w]$.

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- What is the situation just before this addition?

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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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- Adding all these inequalities, $0 > \sum_{i=1}^{k-1} c_{v_i v_{i+1}} + c_{v_k v_1} = \text{cost of } C$.
- ► Corollary: if *G* has no negative cycles that *P* does not either.

Computing the Shortest Path: Paths in *P*

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

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

Bellman-Ford Algorithm: Early Termination

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

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

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- In general, after i iterations, the path whose length is M[v] may have many more than i edges.
- ► Early termination: If *M* equals *N* after processing all the nodes, we have computed all the shortest paths to *t*.