Algorithm Design and Implementation

Principle of Algorithms IX

Dynamic Programming II

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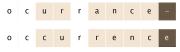
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Sequence Alignment

String similarity

Q. How similar are two strings?

Example. ocurrance and occurrence.



6 mismatches, 1 gap



1 mismatch, 1 gap

0 mismatches, 3 gaps

Edit distance

Edit distance. [Levenshtein 1966, Needleman-Wunsch 1970]

- Gap penalty δ ; mismatch penalty α_{pq} .
- Cost = sum of gap and mismatch penalties.



Applications. Bioinformatics, spell correction, machine translation, speech recognition, information extraction, . . .

Example.

Spokesperson confirms senior government adviser was found Spokesperson said the senior adviser was found

3

BLOSUM matrix for proteins

	Α	R	N	D	C	Q	Ε	G	Н	1	L	K	М	F	Р	S	Т	W	Y	٧
Α	7	-3	-3	-3	-1	-2	-2	0	-3	-3	-3	-1	-2	-4	-1	2	0	-5	-4	-1
R	-3	9	-1	-3	-6	1	-1	-4	0	-5	-4	3	-3	-5	-3	-2	-2	-5	-4	-4
N	-3	-1	9	2	-5	0	-1	-1	1	-6	-6	0	-4	-6	-4	1	0	-7	-4	-5
D	-3	-3	2	10	-7	-1	2	-3	-2	-7	-7	-2	-6	-6	-3	-1	-2	-8	-6	-6
C	-1	-6	-5	-7	13	-5	-7	-6	-7	-2	-3	-6	-3	-4	-6	-2	-2	-5	-5	-2
Q	-2	1	0	-1	-5	9	3	-4	1	-5	-4	2	-1	-5	-3	-1	-1	-4	-3	-4
E	-2	-1	-1	2	-7	3	8	-4	0	-6	-6	1	-4	-6	-2	-1	-2	-6	-5	-4
G	0	-4	-1	-3	-6	-4	-4	9	-4	-7	-7	-3	-5	-6	-5	-1	-3	-6	-6	-6
Н	-3	0	1	-2	-7	1	0	-4	12	-6	-5	-1	-4	-2	-4	-2	-3	-4	3	-5
-1	-3	-5	-6	-7	-2	-5	-6	-7	-6	7	2	-5	2	-1	-5	-4	-2	-5	-3	4
L	-3	-4	-6	-7	-3	-4	-6	-7	-5	2	6	-4	3	0	-5	-4	-3	-4	-2	1
K	-1	3	0	-2	-6	2	1	-3	-1	-5	-4	8	-3	-5	-2	-1	-1	-6	-4	-4
M	-2	-3	-4	-6	-3	-1	-4	-5	-4	2	3	-3	9	0	-4	-3	-1	-3	-3	1
F	-4	-5	-6	-6	-4	-5	-6	-6	-2	-1	0	-5	0	10	-6	-4	-4	0	4	-2
P	-1	-3	-4	-3	-6	-3	-2	-5	-4	-5	-5	-2	-4	-6	12	-2	-3	-7	-6	-4
S	2	-2	1	-1	-2	-1	-1	-1	-2	-4	-4	-1	-3	-4	-2	7	2	-6	-3	-3
T	0	-2	0	-2	-2	-1	-2	-3	-3	-2	-3	-1	-1	-4	-3	2	8	-5	-3	0
W	-5	-5	-7	-8	-5	-4	-6	-6	-4	-5	-4	-6	-3	0	-7	-6	-5	16	3	-5
Υ	-4	-4	-4	-6	-5	-3	-5	-6	3	-3	-2	-4	-3	4	-6	-3	-3	3	11	-3
٧	-1	-4	-5	-6	-2	-4	-4	-6	-5	4	1	-4	1	-2	-4	-3	0	-5	-3	7

Quiz 1

What is edit distance between these two strings?

PALETTE PALATE

Assume gap penalty = 2 and mismatch penalty = 1.

- A. 1
- B. 2
- C. 3
- D. 4
- E. 5

Merging

Goal. Given two strings $x_1x_2...x_m$ and $y_1y_2...y_n$, find a min-cost alignment.

Definition. An alignment M is a set of ordered pairs $x_i - y_j$ such that each character appears in at most one pair and no crossings.

Definition The cost of an alignment M is:

$$cost(M) = \underbrace{\sum_{(x_i, y_j) \in M} \alpha_{x_i y_j}}_{\text{mismatch}} + \underbrace{\sum_{i: x_i \text{ unmached }} \delta + \sum_{j: y_j \text{ unmatched }} \delta}_{\text{gap}}$$



an alignment of CTACCG and TACATG

$$M = \{x_2 - y_1, x_3 - y_2, x_4 - y_3, x_5 - y_4, x_6 - y_6\}$$

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Sequence alignment: problem structure

Def. OPT(i, j): min cost of aligning prefix strings $x_1x_2...x_i$ and $y_1y_2...y_j$. Goal. OPT(m, n).

Case 1. OPT(i, j) matches $x_i - y_j$.

Pay mismatch for $x_i - y_j + \min$ cost of aligning $x_1x_2...x_{i-1}$ and $y_1y_2...y_{j-1}$.

Case 2a. OPT(i,j) leaves x_i unmatched.

Pay gap for x_i + min cost of aligning $x_1x_2...x_{i-1}$ and $y_1y_2...y_j$.

Case 2b. OPT(i,j) leaves y_j unmatched.

Pay gap for y_j + min cost of aligning $x_1x_2...x_i$ and $y_1y_2...y_{j-1}$.

Bellman equation.

$$OPT(i,j) = \left\{ \begin{array}{ll} j\delta & \text{if } i = 0 \\ i\delta & \text{if } j = 0 \\ \min \left\{ \begin{array}{ll} \alpha_{x_iy_j} + OPT(i-1,j-1) \\ \delta + OPT(i-1,j) & \text{otherwise} \\ \delta + OPT(i,j-1) \end{array} \right. \right.$$

Sequence alignment: bottom-up algorithm

```
SequenceAlignment(m, n, x_1, \ldots, x_m, y_1, \ldots, y_n, \delta, \alpha)
for i = 0 to m do
    M[i, 0] \leftarrow i\delta;
end
for i = 0 to n do
    M[0, j] \leftarrow j\delta;
end
for i = 1 to m do
    for i = 1 to n do
        M[i,j] \leftarrow
          \min\{\alpha_{x_i,y_i} + M[i-1, j-1], \delta + M[i-1, j], \delta + M[i, j-1]\};
    end
end
Return M[m, n];
```

Sequence alignment: traceback

		s	1	М	1	L	Α	R	1	Т	Υ
	0 🛶	_ 2	4	6	8	10	12	14	16	18	20
1	2	4	1 🛧	— 3 ←	_ 2	4	6	8	7	9	11
D	4	6	3	3	4	4	6	8	9	9	11
E	6	8	5	5	6	6	6	8	10	11	11
N	8	10	7	7	8	8	8	8	10	12	13
т	10	12	9	9	9	10	10	10	10	9	11
1	12	14	8	10	8	10	12	12	9	11	11
т	14	16	10	10	10	10	12	14	11	8	11
Υ	16	18	12	12	12	12	12	14	13	10	7

Sequence alignment: analysis

Theorem

The DP algorithm computes the edit distance (and an optimal alignment) of two strings of lengths m and n in $\Theta(mn)$ time and space.

Proof.

- · Algorithm computes edit distance.
- Can trace back to extract optimal alignment itself.

Theorem (Backurs-Indyk 2015)

If can compute edit distance of two strings of length n in $O(n^{2-\varepsilon})$ time for some constant $\varepsilon>0$, then can solve SAT with n variables and m clauses in $poly(m)2^{(1-\delta)n}$ time for some constant $\delta>0$.

It is easy to modify the DP algorithm for edit distance to ...

- A. Compute edit distance in O(mn) time and O(m+n) space.
- B. Compute an optimal alignment in O(mn) time and O(m+n) space.
- C. Both A and B.
- D. Neither A nor B.

$$OPT(i,j) = \begin{cases} j\delta & \text{if } i = 0\\ i\delta & \text{if } j = 0 \end{cases}$$

$$\min \begin{cases} \alpha_{x_iy_j} + OPT(i-1,j-1) \\ \delta + OPT(i-1,j) & \text{otherwise} \end{cases}$$

$$\delta + OPT(i,j-1)$$

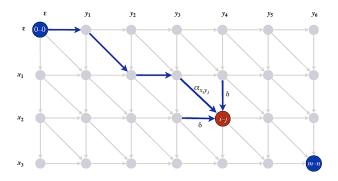
Sequence alignment in linear space

[Hirschberg] There exists an algorithm to find an optimal alignment in O(mn) time and O(m+n) space.

- Clever combination of divide-and-conquer and dynamic programming.
- Inspired by idea of Savitch from complexity theory.

Edit distance graph.

- Let f(i,j) denote length of shortest path from (0,0) to (i,j).
- Lemma: f(i,j) = OPT(i,j) for all i and j.



Edit distance graph.

- Let f(i,j) denote length of shortest path from (0,0) to (i,j).
- Lemma: f(i,j) = OPT(i,j) for all i and j.

Proof. [by strong induction on i + j]

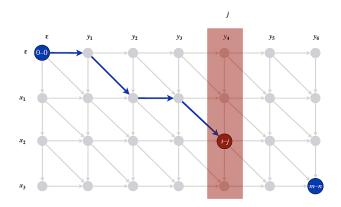
- Base case: f(0,0) = OPT(0,0) = 0.
- Inductive hypothesis: assume true for all (i', j') with i' + j' < i + j.
- Last edge on shortest path to (i,j) is from (i-1,j-1), (i-1,j), or (i,j-1).
- Thus,

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

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

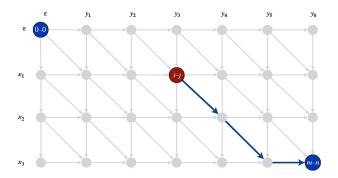
Edit distance graph.

- Let f(i,j) denote length of shortest path from (0,0) to (i,j).
- Lemma: f(i,j) = OPT(i,j) for all i and j.
- Can compute $f(\cdot, j)$ for any j in O(mn) time and O(m) space.



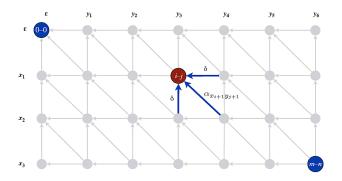
Edit distance graph.

• Let g(i,j) denote length of shortest path from (i,j) to (m,n).



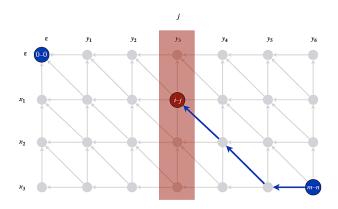
Edit distance graph.

- Let g(i,j) denote length of shortest path from (i,j) to (m,n).
- Can compute g(i, j) by reversing the edge orientations and inverting the roles of (0, 0) and (m, n).

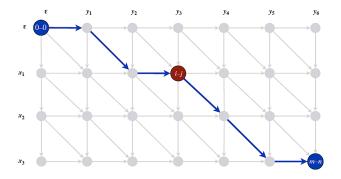


Edit distance graph.

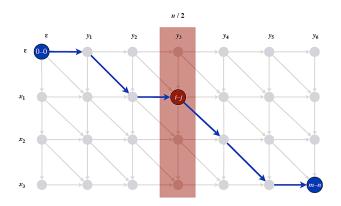
- Let g(i,j) denote length of shortest path from (i,j) to (m,n).
- Can compute $g(\cdot, j)$ for any j in O(mn) time and O(m) space.



Observation 1. The length of a shortest path that uses (i,j) is f(i,j) + g(i,j).

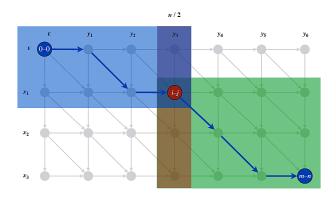


Observation 2. let q be an index that minimizes f(q, n/2) + g(q, n/2). Then, there exists a shortest path from (0, 0) to (m, n) that uses (q, n/2).



Divide. Find index q that minimizes f(q, n/2) + g(q, n/2); save node i-j as part of solution.

Conquer. Recursively compute optimal alignment in each piece.



Hirschberg's algorithm: space analysis

Theorem

Hirschberg's algorithm uses $\Theta(m+n)$ space.

Proof.

- Each recursive call uses $\Theta(m)$ space to compute $f(\cdot, n/2)$ and $g(\cdot, n/2)$.
- Only $\Theta(1)$ space needs to be maintained per recursive call.
- Number of recursive calls $\leq n$.

Quiz 4

What is the worst-case running time of Hirschberg's algorithm?

- A. *O*(*mn*)
- B. $O(mn \log m)$
- C. $O(mn \log n)$
- D. $O(mn \log m \log n)$

Hirschberg's algorithm: running time analysis warmup

Theorem

Let T(m, n) be max running time of Hirschberg's algorithm on strings of lengths at most m and n. Then, $T(m, n) = O(mn \log n)$.

Proof.

• T(m, n) is monotone nondecreasing in both m and n.

•

$$T(m, n) \le 2T(m, n/2) + O(mn)$$

 $\Rightarrow T(m, n) = O(mn \log n)$

Remark. Analysis is not tight because two subproblems are of size (q, n/2) and (m - q, n/2). Next, we prove T(m, n) = O(mn).

Hirschberg's algorithm: running time analysis

Theorem

Let T(m, n) be max running time of Hirschberg's algorithm on strings of lengths at most m and n. Then, T(m, n) = O(mn).

Proof. [by strong induction on m + n]

- O(mn) time to compute $f(\cdot, n/2)$ and $g(\cdot, n/2)$ and find index q.
- T(q, n/2) + T(m q, n/2) time for two recursive calls.
- Choose constant c so that:

$$\begin{split} T(m,2) &\leq cm \\ T(2,n) &\leq cn \\ T(m,n) &\leq cmn + T(q,n/2) + T(m-q,n/2) \end{split}$$

Hirschberg's algorithm: running time analysis

Claim

$$T(m, n) \leq 2cmn$$

- Base cases: m = 2 and n = 2.
- Inductive hypothesis: $T(m, n) \le 2cmn$ for all (m', n') with m' + n' < m + n.

$$T(m, n) \le T(q, n/2) + T(m - q, n/2) + cmn$$

$$\le 2cqn/2 + 2c(m - q)n/2 + cmn$$

$$= cqn + cmn - cqn + cmn$$

$$= 2cmn$$

Longest common subsequence

Problem. Given two strings $x_1x_2...x_m$ and $y_1y_2...y_n$, find a common subsequence that is as long as possible.

Alternative viewpoint. Delete some characters from x; delete some character from y; a common subsequence if it results in the same string.

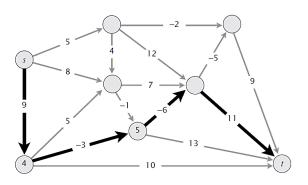
Example. LCS(GGCACCACG, ACGGCGGATACG) = GGCAACG.

Applications. Unix diff, git, bioinformatics.

Bellman-Ford-Moore Algorithm

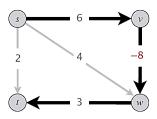
Shortest paths with negative weights

Shortest-path problem. Given a digraph G = (V, E), with arbitrary edge lengths ℓ_{vw} , find shortest path from source node s to destination node t.



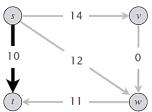
Shortest paths with negative weights: failed attempts

Dijkstra. May not produce shortest paths when edge lengths are negative.



Dijkstra selects the vertices in the orders, t, w, vBut shortest path from s to t is $s \rightarrow v \rightarrow w \rightarrow t$.

Reweighting. Adding a constant to every edge length does not necessarily make Dijkstra's algorithm produce shortest paths.

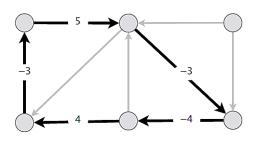


Adding 8 to each edge weight changes the shortest path from $s \rightarrow v \rightarrow w \rightarrow t$ to $s \rightarrow t$.

Negative cycles

Definition

A negative cycle is a directed cycle for which the sum of its edge lengths is negative.



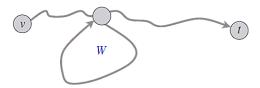
Shortest paths and negative cycles

Lemma 1

If some $v \rightsquigarrow t$ path contains a negative cycle, then there does not exist a shortest $v \rightsquigarrow t$ path.

Proof.

If there exists such a cycle W, then can build a $v \rightsquigarrow t$ path of arbitrarily negative length by detouring around W as many times as desired.



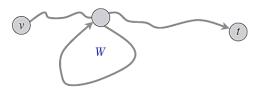
Shortest paths and negative cycles

Lemma 2

If G has no negative cycles, then there exists a shortest $v \rightsquigarrow t$ path that is simple (and has $\leq n-1$ edges).

Proof.

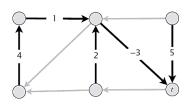
- Among all shortest $v \rightsquigarrow t$ paths, consider one that uses the fewest edges.
- If that path P contains a directed cycle W, can remove the portion of P corresponding to W without increasing its length.

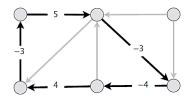


Shortest-paths and negative-cycle problems

Single-destination shortest-paths problem. Given a digraph G = (V, E) with edge lengths ℓ_{vw} (but no negative cycles) and a distinguished node t, find a shortest $v \rightsquigarrow t$ path for every node v.

Negative-cycle problem. Given a digraph G = (V, E) with edge lengths ℓ_{vw} , find a negative cycle (if one exists).





Which subproblems to find shortest $v \rightsquigarrow t$ paths for every node v?

- A. OPT(i, v): length of shortest $v \rightsquigarrow t$ path that uses exactly i edges.
- B. OPT(i, v): length of shortest $v \rightsquigarrow t$ path that uses at most edges.
- C. Neither A nor B.

Shortest paths with negative weights: dynamic programming

Definition. OPT(i, v): length of shortest $v \rightsquigarrow t$ path that uses $\leq i$ edges. Goal OPT(n-1, v) for each v.

Case 1. Shortest $v \rightsquigarrow t$ path uses $\leq i - 1$ edges.

•
$$OPT(i, v) = OPT(i - 1, v)$$

Case 2. Shortest $v \rightsquigarrow t$ path uses exactly i edges.

- if (v, w) is first edge in shortest such $v \rightsquigarrow t$ path, incur a cost of ℓ_{vw} .
- Then, select best $w \rightsquigarrow t$ path using $\leq i 1$ edges.

Bellman equation.

$$OPT(i, v) = \begin{cases} 0 & \text{if } i = 0 \text{ and } v = t \\ \infty & \text{if } i = 0 \text{ and } v \neq t \end{cases}$$

$$\min \left\{ OPT(i-1, v), \min_{(v,w) \in E} \left\{ OPT(i-1, w) + \ell_{vw} \right\} \right\} \quad \text{if } i > 0$$

Shortest paths with negative weights: implementation

```
ShortestPaths(V, E, \ell, t)
for each node (v \in V) do
    M[0, v] \leftarrow \infty:
end
M[0,t] \leftarrow 0;
for i = 1 to n - 1 do
    for each node v \in V do
        M[i, v] \leftarrow M[i-1, v];
        for each edge (v, w) \in E do
            M[i, v] \leftarrow \min \{M[i, v], M[i-1, w] + \ell_{vw}\}:
        end
    end
end
```

Shortest paths with negative weights: implementation

Theorem

Given a digraph G = (V, E) with no negative cycles, the DP algorithm computes the length of a shortest $v \rightsquigarrow t$ path for every node v in $\Theta(mn)$ time and $\Theta(n^2)$ space.

Proof.

- Table requires $\Theta(n^2)$ space.
- Each iteration i takes $\Theta(m)$ time since we examine each edge once.

Finding the shortest paths.

- Approach 1: Maintain successor [i, v] that points to next node on a shortest v → t path using ≤ i edges.
- Approach 2: Compute optimal lengths M[i, v] and consider only edges with $M[i, v] = M[i 1, w] + \ell_{vw}$. Any directed path in this subgraph is a shortest path.

It is easy to modify the DP algorithm for shortest paths to ...

- A. Compute lengths of shortest paths in O(mn) time and O(m+n) space.
- B. Compute shortest paths in O(mn) time and O(m+n) space.
- C. Both A and B.
- D. Neither A nor B.

Shortest paths with negative weights: practical improvements

Space optimization. Maintain two 1D arrays (instead of 2D array).

- d[v]: length of a shortest $v \rightsquigarrow t$ path that we have found so far.
- successor[v]: next node on a $v \rightsquigarrow t$ path.

Performance optimization. If d[w] was not updated in iteration i-1, then no reason to consider edges entering w in iteration i.

Bellman-Ford-Moore: efficient implementation

```
Bellman-Ford-Moore(V, E, c, t)
for each node v \in V do
    d[v] \leftarrow \infty;
    successor[v] \leftarrow null;
end
d \leftarrow 0:
for i = 1 to n - 1 do
    for each node w \in V do
        if d[w] was updated in previous pass then
            for each edge (v, w) \in E do
                if (d[v] > d[w] + \ell_{vw}) then
                   d[v] \leftarrow d[w] + \ell_{ww};
                   successor[v] \leftarrow w;
                end
            end
        end
    end
    if no d[\cdot] value changed in pass i then Break;
end
```

Which properties must hold after pass i of Bellman-Ford-Moore?

- A. d[v]: length of a shortest $v \rightsquigarrow t$ path using $\leq i$ edges.
- B. d[v]: length of a shortest $v \rightsquigarrow t$ path using exactly i edges.
- C. Both A and B.
- D. Neither A nor B.

Theorem

Assuming no negative cycles, Bellman-Ford-Moore computes the lengths of the shortest $v \rightsquigarrow t$ paths in O(mn) time and $\Theta(n)$ extra space.

Remark

Bellman-Ford-Moore is typically faster in practice.

- Edge (v, w) considered in pass i + 1 only if d[w] updated in pass i.
- If shortest path has k edges, then algorithm finds it after $\leq k$ passes.

Assuming no negative cycles, which properties must hold throughout Bellman-Ford-Moore?

- A. Following successor[v] pointers gives a directed $v \rightsquigarrow t$ path.
- B. If following successor[v] pointers gives a directed $v \leadsto t$ path, then the length of that $v \leadsto t$ path is d[v].
- C. Both A and B.
- D. Neither A nor B.

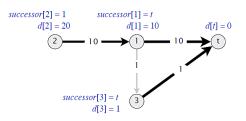
Claim

Throughout Bellman-Ford-Moore, following the successor [v] pointers gives a directed path from v to t of length d[v].

Counterexample. Claim is false!

• Length of successor $v \rightsquigarrow t$ path may be strictly shorter than d[v].

consider nodes in order: t, 1, 2, 3



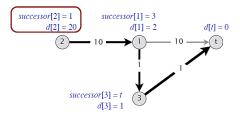
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consider nodes in order: t, 1, 2, 3



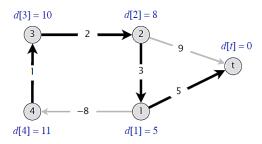
Claim

Throughout Bellman-Ford-Moore, following the successor [v] pointers gives a directed path from v to t of length d[v].

Counterexample. Claim is false!

- Length of successor $v \rightsquigarrow t$ path may be strictly shorter than d[v].
- If negative cycle, successor graph may have directed cycles.

consider nodes in order: t, 1, 2, 3, 4



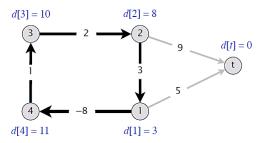
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- If negative cycle, successor graph may have directed cycles.

consider nodes in order: t, 1, 2, 3, 4



Bellman-Ford-Moore: finding the shortest paths

Lemma 6

Any directed cycle W in the successor graph is a negative cycle.

Proof.

- If successor[v] = w, we must have d[v] ≥ d[w] + ℓ_{vw}.
 (LHS and RHS are equal when successor[v] is set; d[w] can only decrease; d[v] decreases only when successor[v] is reset)
- Let $v_1 \rightarrow v_2 \rightarrow \ldots \rightarrow v_k \rightarrow v_1$ be the sequence of nodes in a directed cycle W.
- Assume that (v_k, v_1) is the last edge in W added to the successor graph.
- Just prior to that:

$$\begin{array}{lll} d \left[v_{1} \right] & \geq d \left[v_{2} \right] & + \ell \left(v_{1}, v_{2} \right) \\ d \left[v_{2} \right] & \geq d \left[v_{3} \right] & + \ell \left(v_{2}, v_{3} \right) \\ \vdots & \vdots & \vdots & \vdots \\ d \left[v_{k-1} \right] & \geq d \left[v_{k} \right] & + \ell \left(v_{k-1}, v_{k} \right) \\ d \left[v_{k} \right] & > d \left[v_{1} \right] & + \ell \left(v_{k-1}, v_{1} \right) \end{array}$$

• Adding inequalities yields $\ell(v_1, v_2) + \ell(v_2, v_3) + ... + \ell(v_{k-1}, v_k) + \ell(v_k, v_1) < 0$

Bellman-Ford-Moore: finding the shortest paths

Theorem

Assuming no negative cycles, Bellman-Ford-Moore finds shortest $v \rightsquigarrow t$ paths for every node v in O(mn) time and $\Theta(n)$ extra space.

Proof.

- The successor graph cannot have a directed cycle. [Lemma 6]
- ullet Thus, following the successor pointers from v yields a directed path to t.
- Let $v = v_1 \rightarrow v_2 \rightarrow \ldots \rightarrow v_k = t$ be the nodes along this path P.
- Upon termination, if successor[v] = w, we must have $d[v] = d[w] + \ell_{vw}$. (LHS and RHS are equal when successor[v] is set; $d[\cdot]$ did not change)
- Thus, $d[v_1] = d[v_2] + \ell(v_1, v_2)$ $d[v_2] = d[v_3] + \ell(v_2, v_3)$ $\vdots \qquad \vdots \qquad \vdots$ $d[v_{k-1}] = d[v_k] + \ell(v_{k-1}, v_k)$
- Adding equations yields $d[v] = d + \ell(v_1, v_2) + \ell(v_2, v_3) + \ldots + \ell(v_{k-1}, v_k)$

Single-source shortest paths with negative weights

year	worst case	discovered by
1955	$O(n^4)$	Shimbel
1956	$O\left(mn^2W\right)$	Ford
1958	O(mn)	Bellman, Moore
1983	$O\left(n^{3/4}m\log W\right)$	Gabow
1989	$O\left(mn^{1/2}\log(nW)\right)$	Gabow-Tarjan
1993	$O\left(mn^{1/2}\log W\right)$	Goldberg
2005	$O\left(n^{2.38}W\right)$	Sankowsi, Yuster-Zwick
2016	$\tilde{O}\left(n^{107}\log W\right)$	Cohen-Madry-Sankowski-Vladu
20xx	???	

series single-source shortest paths with weights between $-\mathcal{W}$ and \mathcal{W}