南方科技大学
SOUTHERN UNIVERSITY OF SCIENCE AND TECHNOLOGY

06 Dynamic Programming

CS216 Algorithm Design and Analysis (H)

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Algorithmic Paradigms

- **Greedy.** Process the input in some order, and myopically making irrevocable decisions to optimize some underlying criterion.

- **Divide-and-conquer.** Break up a problem into independent subproblems, solve each subproblem, and combine solution to subproblems to form solution to original problem.

fancy name for caching intermediate results for later use

- **Dynamic programming.** Break up a problem into a series of overlapping subproblems, combine solutions to smaller subproblems to form solution to large subproblem.

Dynamic Programming History

- **Richard Bellman.** Pioneered the systematic study of dynamic programming in 1950s.

- **Etymology of "dynamic programming" (DP).**
  - Dynamic programming = planning over time.
  - Secretary of Defense had pathological fear to mathematical research.
  - Bellman sought a "dynamic" adjective to avoid conflict.

> "...it's impossible to use the word dynamic in a pejorative sense... Thus, I thought dynamic programming was a good name. It was something not even a Congressman could object to."

Reference: Bellman, R. E. *Eye of the Hurricane, An Autobiography.*

Dynamic Programming Applications

- **Application areas:**
  - Bioinformatics
  - Control theory
  - Information theory
  - Operations research
  - Computer science: theory, graphics, AI, compilers, systems, ….
- **Some famous DP algorithms:**
  - Unix diff for comparing two files.
  - Viterbi algorithm for hidden Markov models.
  - Needleman-Wunsch/Smith-Waterman algorithm for sequence alignment.
  - Bellman-Ford-Moore algorithm for shortest path routing in networks.

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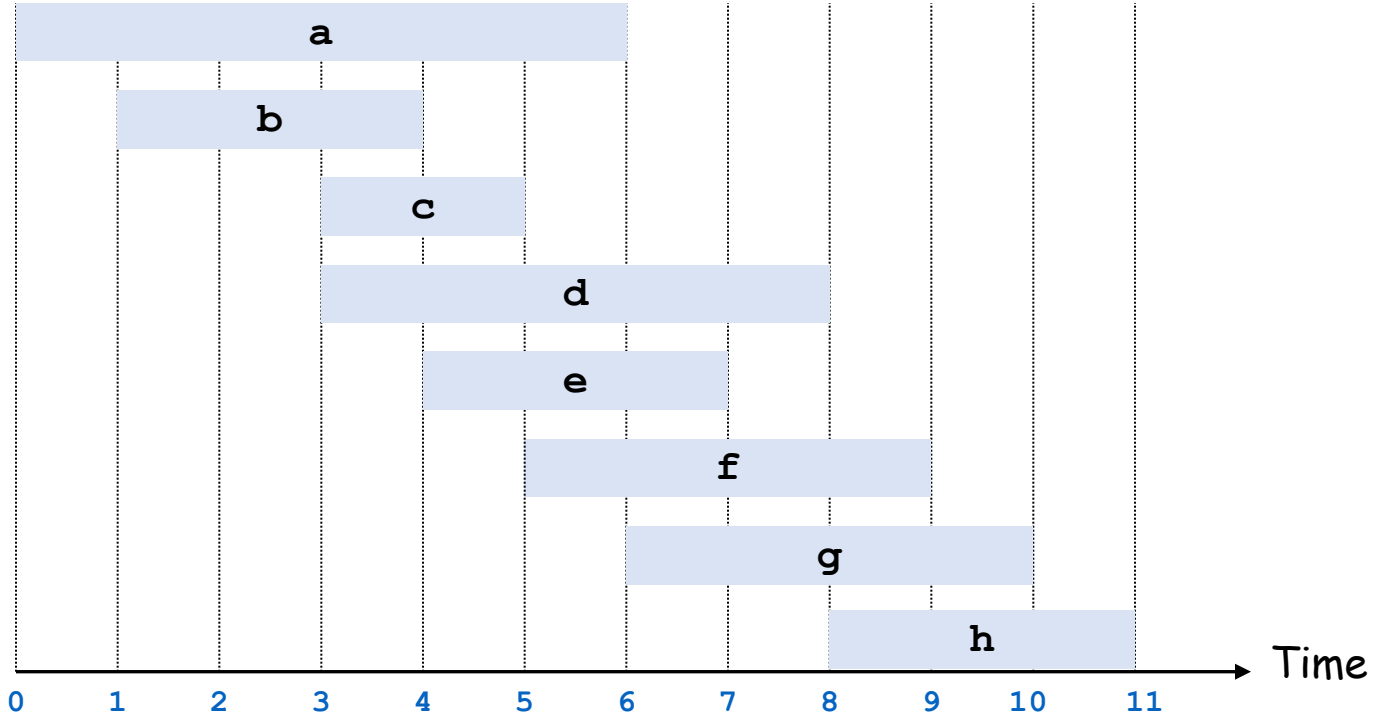
1. Weighted Interval Scheduling

Weighted Interval Scheduling

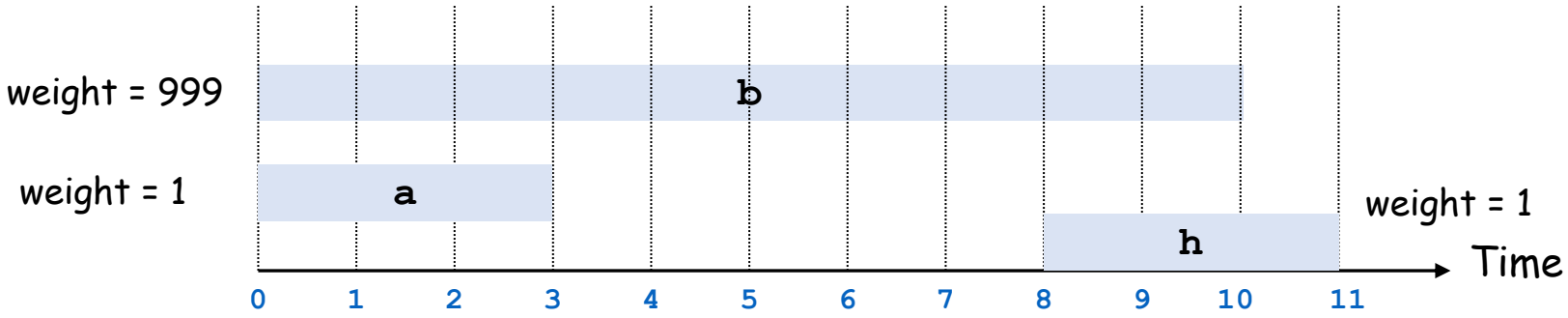
- **Weighted interval scheduling problem:**
  - Job j starts at s_j, finishes at f_j, and has weight/profit/value w_j .
  - Two jobs are compatible if they don't overlap.
  - Goal: find maximum-weight subset of mutually compatible jobs.



Recall: Unweighted Interval Scheduling

- **Recall.** Greedy algorithm works if all weights are *1*.
  - Consider jobs in ascending order of finish time.
  - Add job to subset if it is compatible with previously chosen jobs.

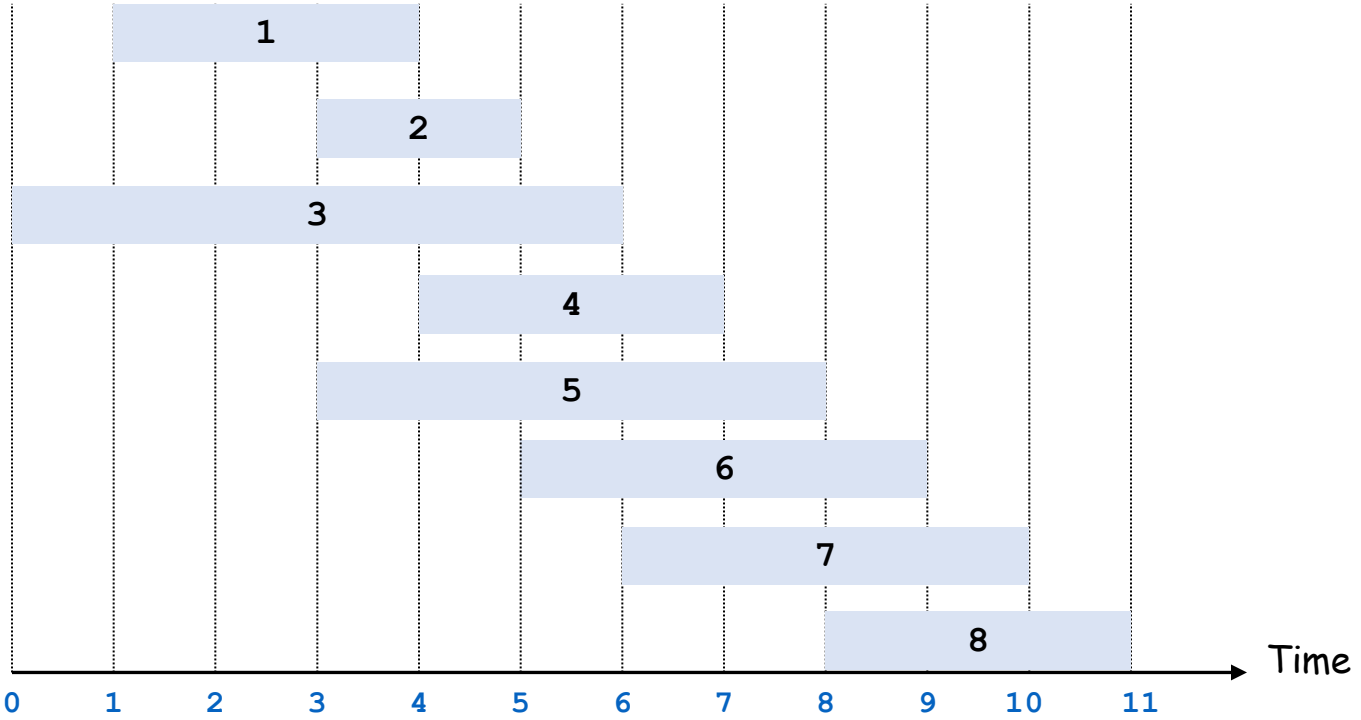
- **Observation.** Greedy algorithm fails spectacularly for weighted version.



Weighted Interval Scheduling

- **Convention.** Order jobs by finish time: $f_1 \leq f_2 \leq \ldots \leq f_n$.
- **Def.** *p(j)* = largest index *i (0 ≤ i < j)* such that job *i* is compatible with job *j*.
- **Example.** *p(8) = 5, p(7) = 3, p(2) = 0.*

p(j) is rightmost interval that ends before j begins



Dynamic Programming: Binary Choice

- **Def.** *OPT(j)* = max weight of any subset of mutually compatible jobs for subproblem consisting only of jobs *1, 2, ..., j*.
- **Goal.** *OPT(n)* = max weight of any subset of mutually compatible jobs.

- **Bellman equation:**

$$OPT(j) = \begin{cases} 0 & \text{if } j = 0 \\ \max\{ OPT(j-1),\ w_j + OPT(p(j)) \} & \text{if } j > 0 \end{cases}$$

- **Pf.** (by cases)
  - Case 1: *OPT(j)* does not select job *j*.
    - ✓Must be optimal solution to problem consisting of remaining jobs *1, 2, ..., j – 1*.
  - Case 2: *OPT(j)* selects job *j*.
    - ✓Collect weight w_j. (Then can't use incompatible jobs *p(j) + 1, p(j) + 2, ..., j – 1*.)
    - ✓Must include optimal solution to problem consisting of remaining compatible jobs *1, 2, ..., p(j)*.

Weighted Interval Scheduling: Brute Force

- **Brute-force algorithm:**

```
Input: n, s1,…,sn , f1,…,fn , w1,…,wn

Sort jobs by finish times and renumber so that f1 ≤ f2 ≤ ... ≤ fn
Compute p(1), p(2), …, p(n) via binary search

return Compute-Opt(n)
```

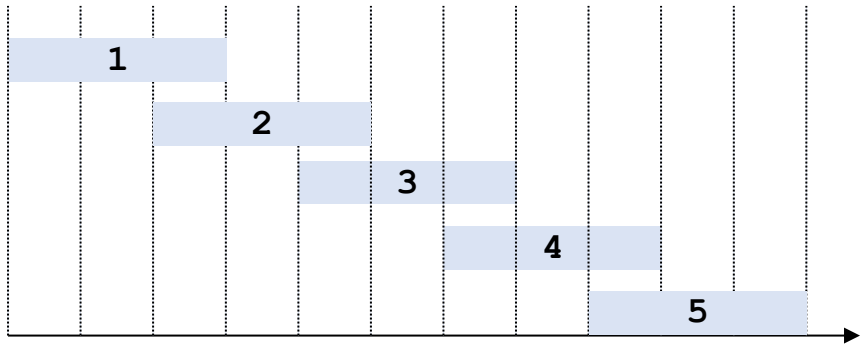
```
Compute-Opt(j) {
   if (j = 0)
      return 0
   else
      return max{ Compute-Opt(j - 1), wj + Compute-Opt(p(j)) }
}
```

recursion could be very expensive (shown next)

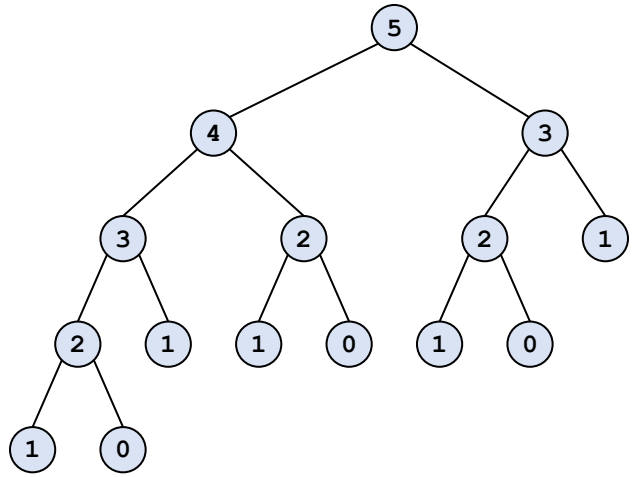
Weighted Interval Scheduling: Brute Force

- **Observation.** Recursive algorithm could be spectacularly slow due to overlapping subproblems ⇒ exponential-time algorithm.

- **Example.** For family of "layered" instances, the number of recursive calls grows like Fibonacci sequence.



p(1) = 0, p(j) = j - 2



depth ≈ n, number of recursive calls ≈ 2^n

Weighted Interval Scheduling: Algorithm

- **Top-down DP algorithm (memorization).** Cache results of subproblem *j* in *M[j]* to avoid solving the same subproblem more than once.

```
Input: n, s1,…,sn , f1,…,fn , w1,…,wn

Sort jobs by finish times and renumber so that f1 ≤ f2 ≤ ... ≤ fn.
Compute p(1), p(2), …, p(n) via binary search

M[0] = 0   ← M[] is global array

return M-Compute-Opt(n)
```

```
M-Compute-Opt(j) {                          ← recur only when M[j] is unknown
   if (M[j] is uninitialized)
      M[j] = max{ M-Compute-Opt(j - 1), wj + M-Compute-Opt(p(j)) }
   return M[j]
}
```

Weighted Interval Scheduling: Running Time

- **Theorem.** Top-down DP algorithm takes *O(n log n)* time.
- **Pf.** (direct proof)
  - Sort by finish time: *O(n log n)*.
  - Compute *p(·)* for each *j*: *O(n log n)* via binary search.
  - M-Compute-Opt(j): each invocation takes *O(1)* time and either
    1) returns an existing value *M[j]*; or
    2) initializes *M[j]* and makes two recursive calls
  - At most *n* uninitialized *M[]* entries ⇒ at most *2n* recursive calls.
  - Overall running time of M-Compute-Opt(n) is *O(n)*. ▪

Weighted Interval Scheduling: Finding a Solution

- **Q.** DP computes optimal value *M[n]*. How to find an optimal solution?
- **A.** Do backtrack post-processing by calling Find-Solution(n).

```
Find-Solution(j) {
    if (j = 0)
        return empty set
    else if (M[j] > M[j - 1])
        return {j} U Find-Solution(p(j))
    else
        return Find-Solution(j - 1)
}
```

$M[j] = \max\{ M[j - 1], w_j + M[p(j)] \}$

- **Running time.** Number of recursive calls $\leq n \Rightarrow O(n)$
- **Note.** Such a trace-back technique also applies to other DP algorithms to find an optimal solution to other problems.

Weighted Interval Scheduling: Bottom-Up

- **Bottom-up DP algorithm.** Unwind recursion.

```
Input: n, s1,…,sn , f1,…,fn , v1,…,vn

Sort jobs by finish times and renumber so that f1 ≤ f2 ≤ ... ≤ fn.
Compute p(1), p(2), …, p(n) via binary search

M[0] = 0
for j = 1 to n
    M[j] = max{ M[j - 1], vj + M[p(j)] }

return M[n]
```

previously computed M[] values

- **Running time.** Bottom-up DP takes *O(n log n)* time.

A Quote that Suits Dynamic Programming

Those who cannot remember the past are condemned to repeat it.

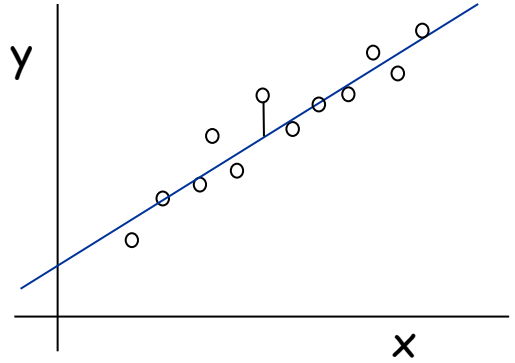
--- George Santayana

2. Segmented Least Squares

Least Squares

- **Least squares.** Foundational problem in statistics.
  - Given n points in the plane: $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$.
  - Find a line $y = ax + b$ that minimizes the sum of the squared errors (SSE).

$$SSE = \sum_{i=1}^{n} (y_i - ax_i - b)^2$$



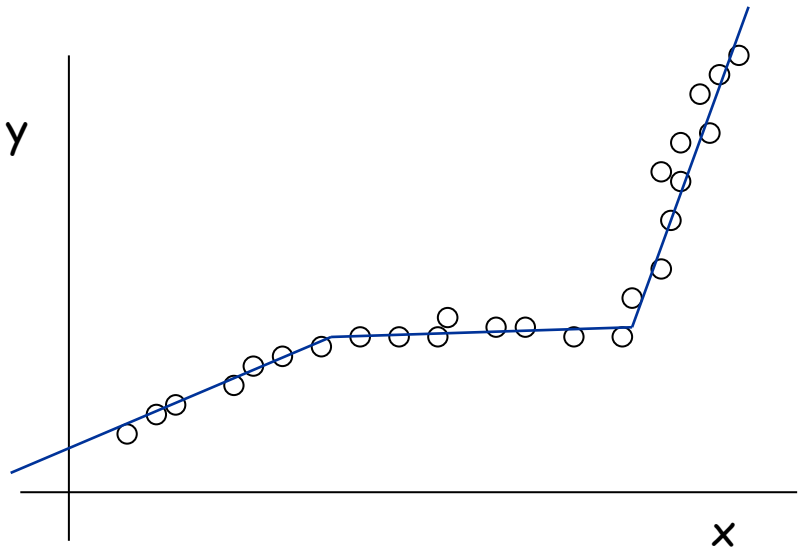
- **Solution.** Calculus ⇒ min SSE is achieved when

$$a = \frac{n \sum_i x_i y_i - (\sum_i x_i)(\sum_i y_i)}{n \sum_i x_i^2 - (\sum_i x_i)^2}, \quad b = \frac{\sum_i y_i - a \sum_i x_i}{n}$$

Segmented Least Squares

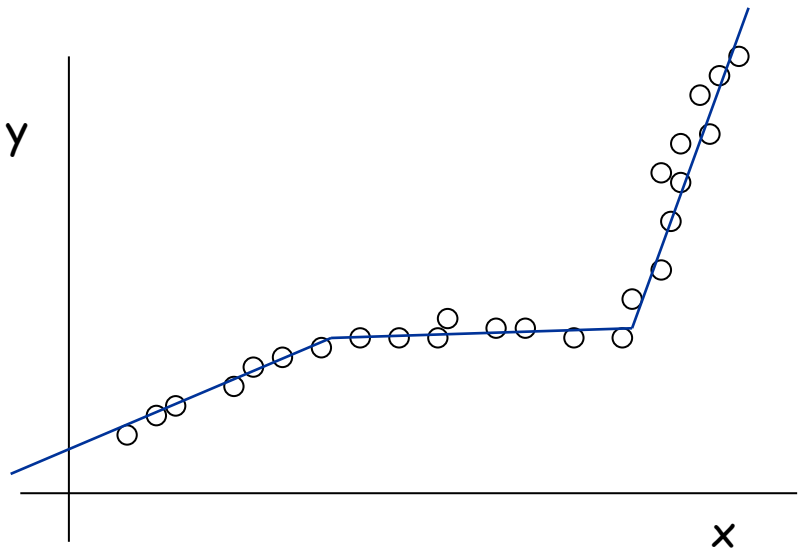
- **Segmented least squares problem:**
  - Points lie roughly on a sequence of several line segments.
  - Given n points in the plane $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ with $x_1 < x_2 < \ldots < x_n$, find a sequence of lines that minimizes cost $f(x)$ (x denotes the problem input).
- **Q.** What's a reasonable choice for $f(x)$ to balance accuracy and parsimony?

goodness of fit number of lines



Segmented Least Squares

- **Segmented least squares problem:**
  - Points lie roughly on a sequence of several line segments.
  - Given n points in the plane $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ with $x_1 < x_2 < \ldots < x_n$, find a sequence of lines that minimizes cost $f(x) = E + cL$ (for some constant $c > 0$).
    - ✓ E = sum of the sums of the squared errors (SSEs) in each segment
    - ✓ L = number of lines



Dynamic Programming: Multiway Choice

- **Notation:**
  - $OPT(j)$ = minimum $f(x)$ cost for points $p_1, p_2, \ldots, p_j$
  - e_{ij} = minimum SSE for points $p_i, p_{i+1}, \ldots, p_j$
- **Goal.** $OPT(n)$
- **To compute $OPT(j)$:**
  - Last segment uses points $p_i, p_{i+1}, \ldots, p_j$ for some $i \le j$.
  - Minimum cost = $e_{ij} + c + OPT(i-1)$.
- **Bellman equation:**

$$OPT(j) = \begin{cases} 0 & \text{if } j = 0 \\ \min\limits_{1 \le i \le j} \{ e_{ij} + c + OPT(i-1) \} & \text{if } j > 0 \end{cases}$$

Segmented Least Squares: Algorithm

- **Bottom-up DP algorithm:**

```
Input: n, p1,…,pn , c
```

$$a_{ij} = \frac{n\sum_k x_k y_k - (\sum_k x_k)(\sum_k y_k)}{n\sum_k x_k^2 - (\sum_k x_k)^2}, \quad b_{ij} = \frac{\sum_k y_k - a_{ij}\sum_k x_k}{n}$$

$$SSE = \sum_{i=1}^{n} (y_i - ax_i - b)^2$$

n = j - i + 1

```
M[0] = 0
for j = 1 to n
   for i = 1 to j
      Compute the minimum SSE eij for the segment pi,…, pj

for j = 1 to n
   M[j] = min 1 ≤ i ≤ j { eij + c + M[i - 1] }

return M[n]
```

previously computed value

$O(n^3)$

$O(n^2)$

- **Running time.** $O(n^3)$ **Space.** $O(n^2)$
- **Q.** Can we improve the time complexity to $O(n^2)$?

Segmented Least Squares: Algorithm

- **Bottom-up DP algorithm:**

```
Input: n, p1,…,pn , c

M[0] = 0
for j = 1 to n
   for i = 1 to j
      Compute the minimum SSE eij for the segment pi,…, pj

for j = 1 to n
   M[j] = min 1 ≤ i ≤ j { eij + c + M[i - 1] }

return M[n]
```

$$a_{ij} = \frac{n\sum_k x_k y_k - (\sum_k x_k)(\sum_k y_k)}{n\sum_k x_k^2 - (\sum_k x_k)^2}, \quad b_{ij} = \frac{\sum_k y_k - a_{ij}\sum_k x_k}{n}$$

$$SSE = \sum_{i=1}^{n} (y_i - ax_i - b)^2$$

n = j - i + 1

previously computed value

~~$O(n^3)$~~ $O(n^2)$

$O(n^2)$

- **Remark.** Can be improved to $O(n^2)$ time.
  - For each i, precompute cumulative sums:
  - Compute a_{ij}, b_{ij}, e_{ij} in $O(1)$ time.

$$\sum_{k=1}^{i} x_k, \quad \sum_{k=1}^{i} y_k, \quad \sum_{k=1}^{i} x_k^2, \quad \sum_{k=1}^{i} x_k y_k$$

3. Knapsack Problem

Knapsack Problem

- **Knapsack problem:**
  - Given n objects and a "knapsack".
  - Item i has value $v_i > 0$ and weighs $w_i > 0$ kilograms. (assume all weights are integral)
  - Knapsack has capacity of W kilograms.
  - Goal: fill knapsack to maximize total value of items taken.
- **Example.** What is the optimal subset for $W = 11$?
  - $\{3, 4\}$ with maximum value 40
- **Greedy approaches that fail to work:**
  - Repeatedly add item with maximum v_i.
  - Repeatedly add item with maximum w_i.
  - Repeatedly add item with maximum ratio v_i / w_i.

#	value	weight
1	1	1
2	6	2
3	18	5
4	22	6
5	28	7

Dynamic Programming: A First Attempt

- **Def.** *OPT(i)* = maximum value within weight capacity *W* using items *1, …, i*.
- **Goal.** *OPT(n)*
- **To compute *OPT(i)*:**
  - Case 1: *OPT(i)* does not select item *i*.
    - ✓Select best of *{1, 2, …, i – 1}*
  - Case 2: *OPT(i)* selects item *i*.
    - ✓Which other items should be excluded?
    - ✓How to relate to smaller subproblems *OPT(j) (j < i)* ?
- **Conclusion.** Need more sub-problems!

Dynamic Programming: Adding a Variable

- **Def.** *OPT(i, w)* = maximum value within weight limit *w* using items *1, …, i*.
- **Goal.** *OPT(n, W)* ← weights are integers from 0 to W
- **To compute *OPT(i, w)*:**
  - Case 1: *OPT(i, w)* does not select item *i*.
    - ✓Select best of *{1, 2, …, i – 1}* within weight limit *w*
  - Case 2: *OPT(i)* selects item *i*.
    - ✓Collect value v_i
    - ✓Select best of *{1, 2, …, i – 1}* within weight limit $w - w_i$
- **Bellman equation:**

$$OPT(i, w) = \begin{cases} 0 & \text{if } i = 0 \\ OPT(i-1, w) & \text{if } w_i > w \\ \max\{\, OPT(i-1, w),\ v_i + OPT(i-1, w - w_i)\,\} & \text{otherwise} \end{cases}$$

Knapsack Problem: Algorithm

- **Bottom-up DP algorithm:**

```
Input: n, W, w1,…,wn, v1,…,vn

for w = 0 to W
   M[0, w] = 0

for i = 1 to n
   for w = 1 to W
      if (wi > w)
         M[i, w] = M[i - 1, w]
      else
         M[i, w] = max { M[i - 1, w], vi + M[i - 1, w - wi ] }

return M[n, W]
```

- **Running time.** *O(nW)*

Knapsack DP Algorithm: Demo

W + 1 →

n + 1 ↓

W = 11	0	1	2	3	4	5	6	7	8	9	10	11
ϕ	0	0	0	0	0	0	0	0	0	0	0	0
{ 1 }	0	$1_{\{1\}}$	$1_{\{1\}}$	$1_{\{1\}}$	$1_{\{1\}}$	$1_{\{1\}}$	$1_{\{1\}}$	$1_{\{1\}}$	$1_{\{1\}}$	$1_{\{1\}}$	$1_{\{1\}}$	$1_{\{1\}}$
{ 1, 2 }	0	$1_{\{1\}}$	$6_{\{2\}}$	$7_{\{1,2\}}$	$7_{\{1,2\}}$	$7_{\{1,2\}}$	$7_{\{1,2\}}$	$7_{\{1,2\}}$	$7_{\{1,2\}}$	$7_{\{1,2\}}$	$7_{\{1,2\}}$	$7_{\{1,2\}}$
{ 1, 2, 3 }	0	$1_{\{1\}}$	$6_{\{2\}}$	$7_{\{1,2\}}$	$7_{\{1,2\}}$	$18_{\{3\}}$	$19_{\{1,3\}}$	$24_{\{2,3\}}$	$25_{\{1,2,3\}}$	$25_{\{1,2,3\}}$	$25_{\{1,2,3\}}$	$25_{\{1,2,3\}}$
{ 1, 2, 3, 4 }	0	$1_{\{1\}}$	$6_{\{2\}}$	$7_{\{1,2\}}$	$7_{\{1,2\}}$	$18_{\{3\}}$	$22_{\{4\}}$	$24_{\{2,3\}}$	$28_{\{2,4\}}$	$29_{\{1,2,4\}}$	$29_{\{1,2,4\}}$	$40_{\{3,4\}}$
{ 1, 2, 3, 4, 5 }	0	$1_{\{1\}}$	$6_{\{2\}}$	$7_{\{1,2\}}$	$7_{\{1,2\}}$	$18_{\{3\}}$	$22_{\{4\}}$	$28_{\{5\}}$	$29_{\{1,5\}}$	$34_{\{2,5\}}$	$34_{\{2,5\}}$	$40_{\{3,4\}}$

Item	Value	Weight
1	1	1
2	6	2
3	18	5
4	22	6
5	28	7

optimal subset: {3, 4} value = 18 + 22 = 40

$$OPT(i,w) = \begin{cases} 0 & \text{if } i = 0 \\ OPT(i-1,w) & \text{if } w_i > w \\ \max\{\, OPT(i-1,w),\ v_i + OPT(i-1,w-w_i)\,\} & \text{otherwise} \end{cases}$$

Knapsack DP Algorithm: Space Complexity

- **Bottom-up DP algorithm:**

```
Input: n, W, w1,…,wn, v1,…,vn

for w = 0 to W
   M[0, w] = 0

for i = 1 to n
   for w = 1 to W
      if (wi > w)
         M[i, w] = M[i - 1, w]
      else
         M[i, w] = max { M[i - 1, w], vi + M[i - 1, w - wi ] }

return M[n, W]
```

only M[i - 1, .] is used!

- **Space.** *O(nW)* ← can we reduce space? 10^{10} operations (~1000s) vs 10^{10} bytes (~10G)

Knapsack DP Algorithm: Space Complexity

- **Bottom-up DP algorithm:**

```
Input: n, W, w1,…,wn, v1,…,vn

for w = 0 to W
   M[w] = 0          ← 1-D scrolling array

for i = 1 to n
   for w = W to 1    ← updating in reverse order
      if (wi > w)
         M[w] = M[w]          ← these M[.] values are from (i - 1)-th iteration!
      else
         M[w] = max { M[w], vi + M[w - wi ] }

return M[W]
```

- **Space.** *O(W)*

Knapsack Problem: Closing Remarks

- DP algorithm depends crucially on assumption that weights are integral.
- Running time *O(nW)* is not polynomial in input size! "pseudo-polynomial"
- The decision version of the knapsack problem is hard: **NP**-complete. [Section 8 of textbook]
  - Can a value ≥ *V* be achieved under a restriction of a certain capacity *W*?
- There exists a polynomial-time algorithm that produces an approximate solution to the knapsack problem that has value ≤ *0.01%* of optimum. [Section 11.8 of textbook]

Exercise: Coin Changing

- **Observation.** Greedy algorithm is not optimal for US postal denominations: *1, 10, 21, 34, 70, 100, 350, 1225, 1500*
- **Example.** *140¢*
  - Greedy: *100, 34, 1, 1, 1, 1, 1, 1.*
  - Optimal: *70, 70.*

- **Q.** How to solve this problem using DP?
- **Problem.** Given n denominations $\{d_1, d_2, \ldots, d_n\}$ and a target value V, find the fewest stamps needed to make change for V (or report impossible).

Coin Changing: Dynamic Programming

- **Def.** *OPT(v)* = minimum number of stamps to make change for value *v*.
- **Goal.** *OPT(V)*
- **To compute *OPT(v)*:**
  - Case *i*: *OPT(v)* selects the stamp with value d_i
    - ✓ *OPT(v)* continues to select fewest stamps to make change for $v - d_i$
  - What if $v - d_i < 0$?
    - ✓ set $OPT(v - d_i)$ = arbitrarily large number (i.e., the impossible case)
- **Bellman equation:**

$$OPT(v) = \begin{cases} \infty & \text{if } v < 0 \\ 0 & \text{if } v = 0 \\ \min\limits_{1 \le i \le n} \{ 1 + OPT(v - d_i) \} & \text{if } v > 0 \end{cases}$$

- **Running time.** *O(nV)*

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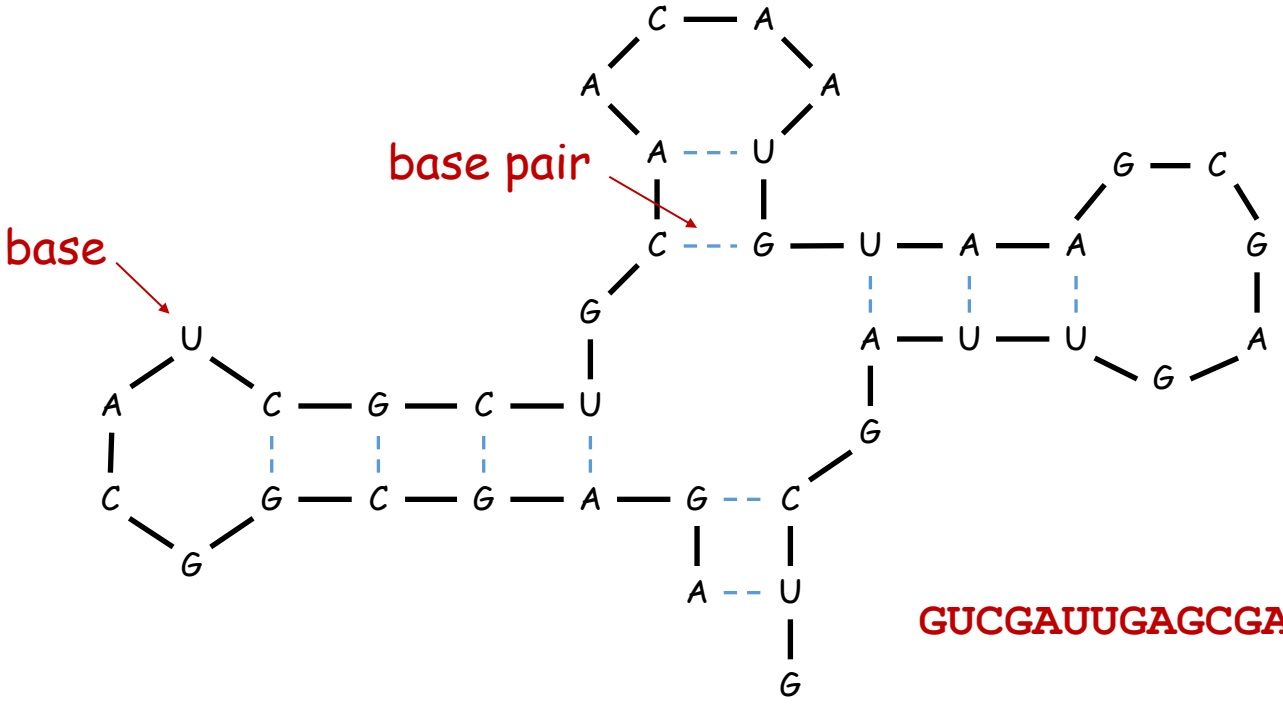
4. RNA Secondary Structure

RNA Secondary Structure

- **RNA.** String $B = b_1 b_2 \ldots b_n$ over alphabet $\{A, C, G, U\}$.
- **Secondary structure.** RNA is single-stranded so it tends to loop back and form base pairs with itself. This structure is essential for understanding behavior of molecule.

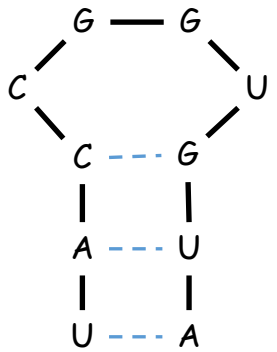


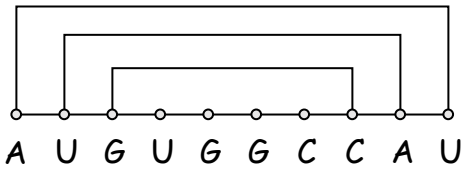
GUCGAUUGAGCGAAUGUAACAACGUGGCUACGGCGAGA

RNA Secondary Structure

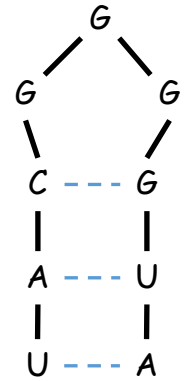
- **Secondary structure.** A set of pairs $S = \{(b_i, b_j)\}$ that satisfy:
  - [Watson-Crick] S is a matching and each pair in S is a Watson-Crick complement: A-U, U-A, C-G, or G-C.
  - [No sharp turns] The ends of each pair are separated by > 4 intervening bases. If $(b_i, b_j) \in S$, then $i < j - 4$.
  - [Non-crossing] If (b_i, b_j) and (b_k, b_l) are two pairs in S, we cannot have $i < k < j < l$.

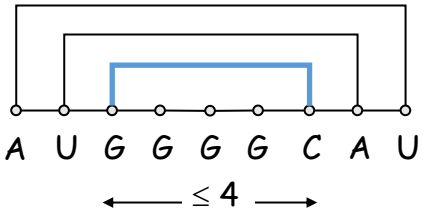
Watson-Crick base pair



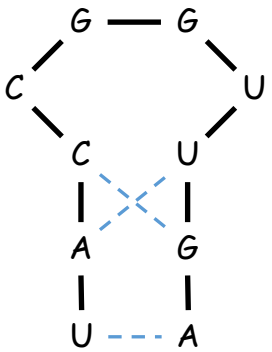


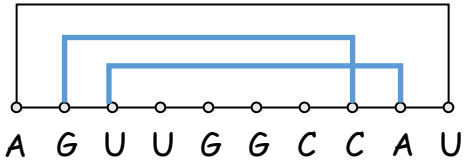
sharp turn





crossing





RNA Secondary Structure

- **Secondary structure.** A set of pairs $S = \{(b_i, b_j)\}$ that satisfy:
  - [Watson-Crick] S is a matching and each pair in S is a Watson-Crick complement: A-U, U-A, C-G, or G-C.
  - [No sharp turns] The ends of each pair are separated by > 4 intervening bases. If $(b_i, b_j) \in S$, then $i < j - 4$.
  - [Non-crossing] If (b_i, b_j) and (b_k, b_l) are two pairs in S, we cannot have $i < k < j < l$.

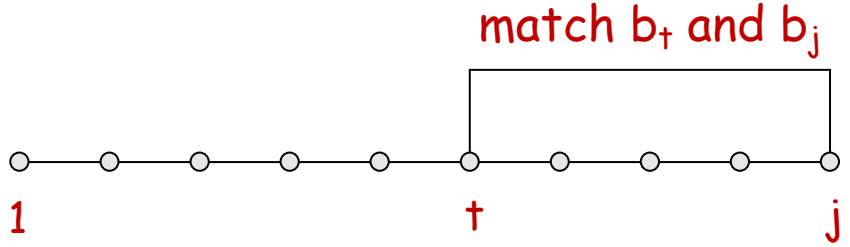
- **Free-energy hypothesis.** RNA molecule will form the secondary structure with the minimum total free energy.

approximate by number of base pairs
more base pairs ⇒ lower free energy

- **Goal.** Given an RNA molecule $B = b_1 b_2 \ldots b_n$, find a secondary structure S that maximizes the number of base pairs.

Dynamic Programming: A First Attempt

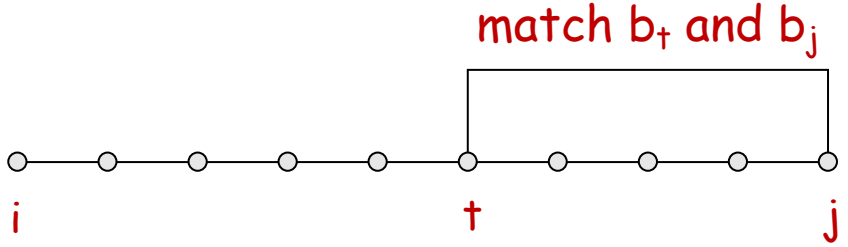
- **Def.** *OPT(j)* = maximum number of base pairs in a secondary structure of the substring $b_1 b_2 \ldots b_j$.
- **Goal.** *OPT(n)*
- **Choices.** Match base b_t $(1 \le t < j)$ and b_j.



- **Difficulty.** Results in two sub-problems (but one of wrong form).
  - Find secondary structure in: $b_1 b_2 \ldots b_{t-1}$. ⟵ OPT(t - 1)
  - Find secondary structure in: $b_{t+1} b_{t+2} \ldots b_{j-1}$. ⟵ need more subproblems

Dynamic Programming over Intervals

- **Def.** *OPT(i, j)* = maximum number of base pairs in a secondary structure of the substring $b_i b_{i+1} \ldots b_j$.
- **Goal.** *OPT(1, n)*
- **Choices.** Match base b_t $(i \le t < j)$ and b_j.

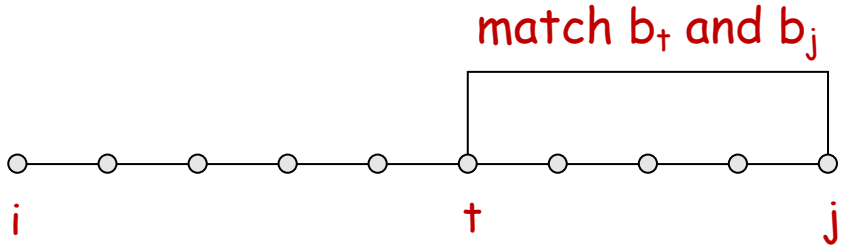


- **To compute *OPT(i, j)*:**
  - Case 1: If $i \ge j - 4$, $OPT(i, j) = 0$ by no-sharp-turns condition.
  - Case 2: If base b_j is not involved in a pair, $OPT(i, j) = OPT(i, j - 1)$.
  - Case 3: If base b_j is paired with b_t for some $i \le t < j - 4$, then:
    - ✓ non-crossing constraint decouples resulting sub-problems
    - ✓ $OPT(i, j) = 1 + \max_t \{OPT(i, t - 1) + OPT(t + 1, j - 1)\}$

take max over t such that $i \le t < j - 4$ and b_t and b_j are Watson-Crick complements

Dynamic Programming over Intervals

- **Def.** *OPT(i, j)* = maximum number of base pairs in a secondary structure of the substring $b_i b_{i+1} \ldots b_j$.
- **Goal.** *OPT(1, n)*
- **Choices.** Match base b_t $(i \le t < j)$ and b_j.
- **Bellman equation:**



compute in which order?

$$\mathrm{OPT}(i,j) = \begin{cases} 0, & \text{if } i \ge j-4 \\ \mathrm{OPT}(i,j-1), & b_j \text{ cannot be paired} \\ 1 + \max_t \{OPT(i,t-1) + OPT(t+1,j-1)\}, & b_j \text{ can be paired} \end{cases}$$

take max over t such that $i \le t < j - 4$ and b_t and b_j are Watson-Crick complements

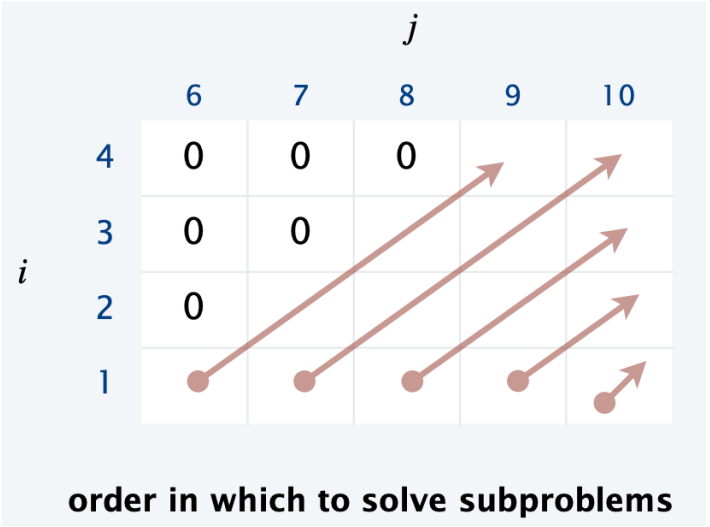
Dynamic Programming over Intervals

- **Bottom-up DP algorithm:**

```
Input: n, b1,…,bn

for k = 5, 6, …, n - 1
   for i = 1, 2, …, n - k
      j = i + k
      Compute M[i, j] using formula

return M[1, n]
```

all needed M[] values already computed

shortest intervals first



order in which to solve subproblems

$$\mathrm{OPT}(i,j) = \begin{cases} 0, & \text{if } i \geq j-4 \\ \mathrm{OPT}(i,j-1), & b_j \text{ cannot be paired} \\ 1 + \max_t \{OPT(i,t-1) + OPT(t+1,j-1)\}, & b_j \text{ can be paired} \end{cases}$$

- **Running time.** $O(n^3)$ **Space.** $O(n^2)$

RNA-Secondary-Structure DP Algorithm: Demo

RNA sequence *ACCGGUAGU*

4	0	0	0	
3	0	0		
2	0			
$i = 1$				
	$j = 6$	7	8	9

Initial values

4	0	0	0	0
3	0	0	1	
2	0	0		
$i = 1$	1			
	$j = 6$	7	8	9

Filling in the values for $k = 5$

4	0	0	0	0
3	0	0	1	1
2	0	0	1	
$i = 1$	1	1		
	$j = 6$	7	8	9

Filling in the values for $k = 6$

4	0	0	0	0
3	0	0	1	1
2	0	0	1	1
$i = 1$	1	1	1	
	$j = 6$	7	8	9

Filling in the values for $k = 7$

4	0	0	0	0
3	0	0	1	1
2	0	0	1	1
$i = 1$	1	1	1	2
	$j = 6$	7	8	9

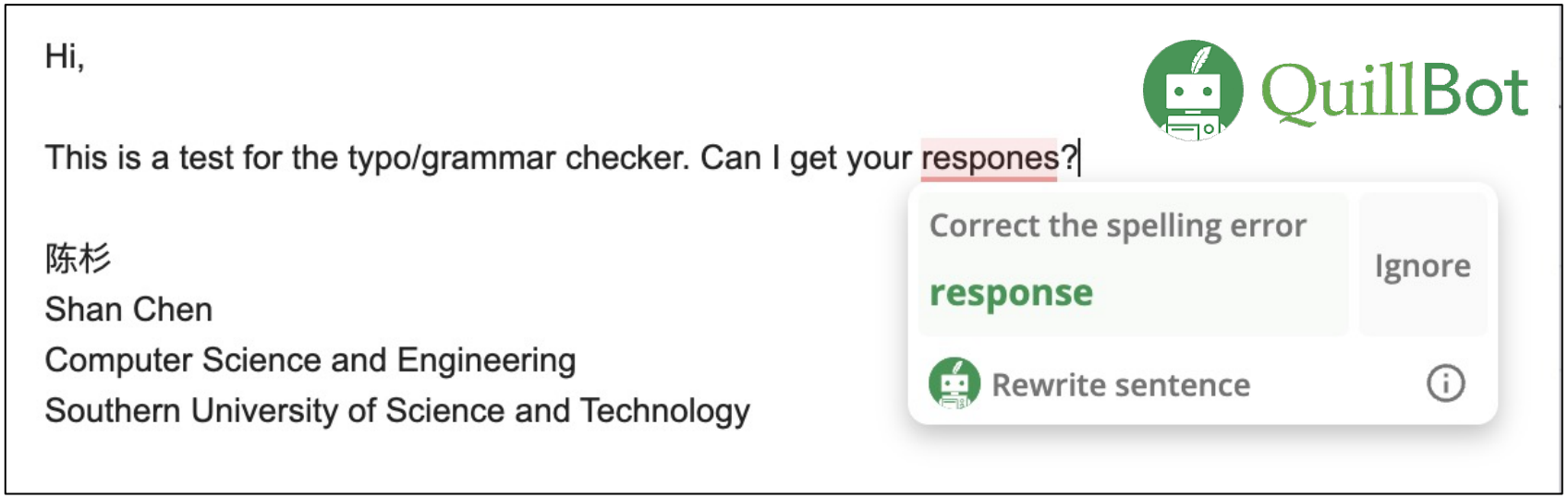
Filling in the values for $k = 8$

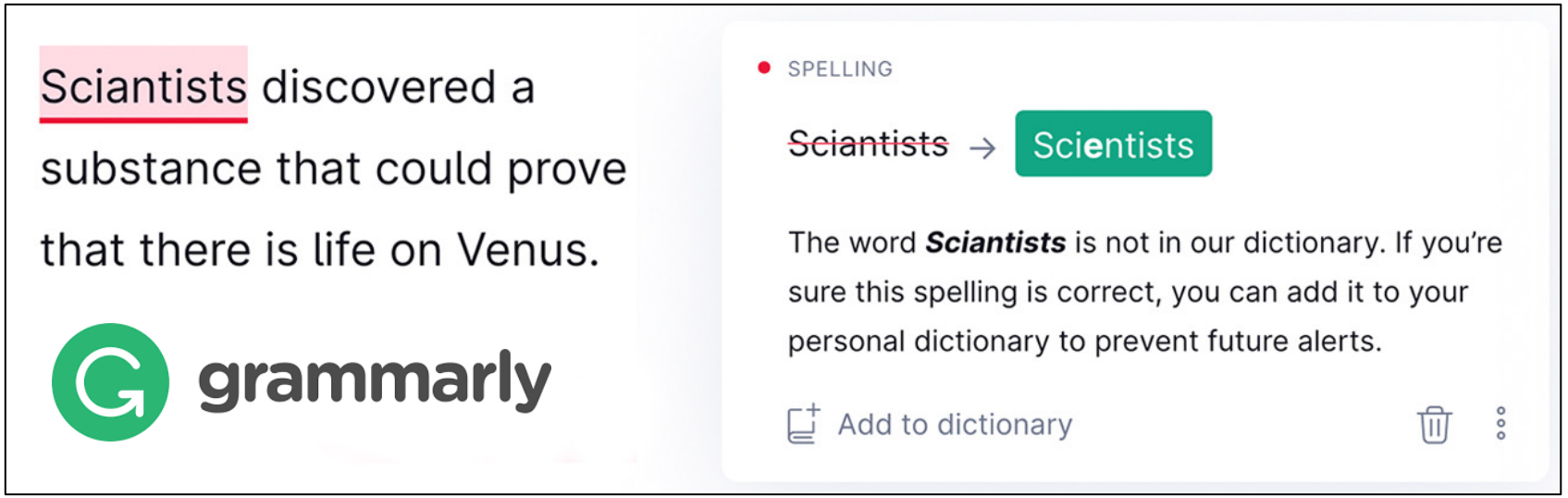
Dynamic Programming: Quick Summary

- **Outline:**
  - Define a collection of subproblems. ← typically only a polynomial number of subproblems
  - Solution to original problem can be computed from subproblems.
  - Naturally order subproblems from "smallest" to "largest" such that a solution to a subproblem can be determined from solutions to smaller subproblems.
- **Techniques:**
  - Binary choice: weighted interval scheduling
  - Multiway choice: segmented least squares
  - Adding a new variable: knapsack problem
  - Intervals: RNA secondary structure
- **Top-down vs. bottom-up DP.** Opinions differ.
  - E.g., simpler logic/implementation vs better performance/parallelization

5. Sequence Alignment

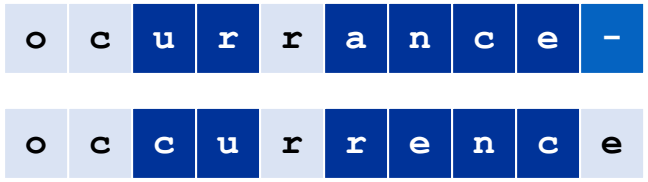
Spell Correction



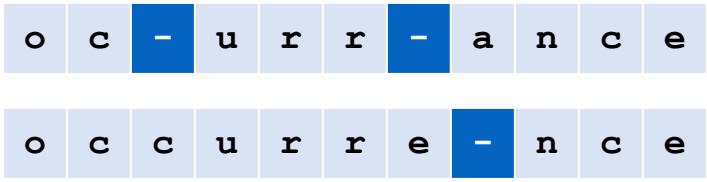


String Similarity

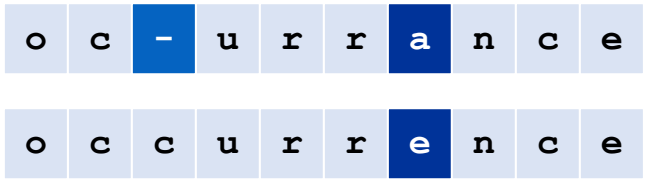
- **Q.** How similar are two strings?
- **Example.** ocurrance and occurrence.



6 mismatches, 1 gap



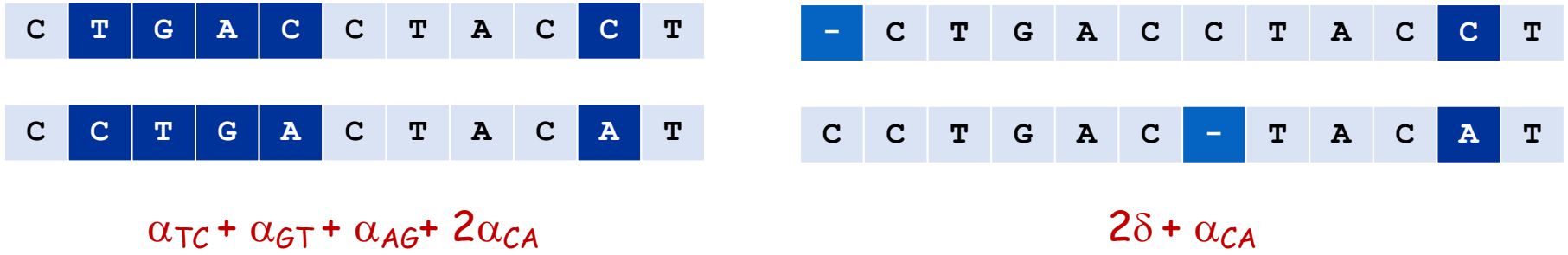
0 mismatches, 3 gaps



1 mismatch, 1 gap

Edit Distance

- **Edit distance.** [Levenshtein 1966, Needleman-Wunsch 1970]
  - Gap penalty δ; mismatch penalty α_{pq}. (Typically, $\alpha_{pp} = 0$.)
  - Cost = sum of gap and mismatch penalties.
  - Edit distance is the minimum cost.



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

BLOSUM62 Score Matrix for Aligning Proteins

	C	S	T	A	G	P	D	E	Q	N	H	R	K	M	I	L	V	W	Y	F	
C	9																				C
S	-1	4																			S
T	-1	1	5																		T
A	0	1	0	4																	A
G	-3	0	-2	0	6																G
P	-3	-1	-1	-1	-2	7															P
D	-3	0	-1	-2	-1	-1	6														D
E	-4	0	-1	-1	-2	-1	2	5													E
Q	-3	0	-1	-1	-2	-1	0	2	5												Q
N	-3	1	0	-2	0	-2	1	0	0	6											N
H	-3	-1	-2	-2	-2	-2	-1	0	0	1	8										H
R	-3	-1	-1	-1	-2	-2	-2	0	1	0	0	5									R
K	-3	0	-1	-1	-2	-1	-1	1	1	0	-1	2	5								K
M	-1	-1	-1	-1	-3	-2	-3	-2	0	-2	-2	-1	-1	5							M
I	-1	-2	-1	-1	-4	-3	-3	-3	-3	-3	-3	-3	-3	1	4						I
L	-1	-2	-1	-1	-4	-3	-4	-3	-2	-3	-3	-2	-2	2	2	4					L
V	-1	-2	0	0	-3	-2	-3	-2	-2	-3	-3	-3	-2	1	3	1	4				V
W	-2	-3	-2	-3	-2	-4	-4	-3	-2	-4	-2	-3	-3	-1	-3	-2	-3	11			W
Y	-2	-2	-2	-2	-3	-3	-3	-2	-1	-2	2	-2	-2	-1	-1	-1	-1	2	7		Y
F	-2	-2	-2	-2	-3	-4	-3	-3	-3	-3	-1	-3	-3	0	0	0	-1	1	3	6	F
	C	S	T	A	G	P	D	E	Q	N	H	R	K	M	I	L	V	W	Y	F	

Reference: https://en.wikipedia.org/wiki/BLOSUM

Sequence Alignment

- **Goal.** Given two strings $x_1 x_2 \ldots x_m$ and $y_1 y_2 \ldots y_n$ find a min-cost alignment.
- **Def.** An alignment M is a set of ordered pairs x_i-y_j such that each item occurs in at most one pair and there are no crossings.

x_i-y_j and $x_{i'}$-$y_{j'}$ cross if $i < i'$ but $j > j'$

- **Example.** CTACCG vs TACATG (gap penalty $\delta = 2$; mismatch penalty $\alpha_{pq} = 1$)
- **Solution.** $M = x_2$-y_1, x_3-y_2, x_4-y_3, x_5-y_4, x_6-y_6.

x_1	x_2	x_3	x_4	x_5		x_6
C	T	A	C	C	-	G

-	T	A	C	A	T	G
y_1	y_2	y_3	y_4	y_5	y_6	

Sequence Alignment: Dynamic Programming

- **Def.** *OPT(i, j)* = min cost of aligning prefix strings $x_1x_2 \ldots x_i$ and $y_1y_2 \ldots y_j$
- **Goal.** *OPT(m, n)*

- **To compute *OPT(i, j)*:**
  - Case 1: *OPT(i, j)* matches x_i-y_j.
    - ✓Pay mismatch for x_i-y_j + min cost of aligning $x_1x_2 \ldots x_{i-1}$ and $y_1y_2 \ldots y_{j-1}$.
  - Case 2a: *OPT(i, j)* leaves x_i unmatched.
    - ✓Pay gap for x_i + min cost of aligning $x_1x_2 \ldots x_{i-1}$ and $y_1y_2 \ldots y_j$.
  - Case 2b: *OPT(i, j)* leaves y_j unmatched.
    - ✓Pay gap for y_j + min cost of aligning $x_1x_2 \ldots x_i$ and $y_1y_2 \ldots y_{j-1}$.

Sequence Alignment: Dynamic Programming

- **Def.** *OPT(i, j)* = min cost of aligning prefix strings $x_1x_2 \ldots x_i$ and $y_1y_2 \ldots y_j$
- **Goal.** *OPT(m, n)*

- **Bellman equation:** [Needleman-Wunsch]

$$OPT(i,j) = \begin{cases} j\delta, & \text{if } i = 0 \\ i\delta, & \text{if } j = 0 \\ \min \begin{cases} \alpha_{x_i y_j} + OPT(i-1, j-1) \\ \delta + OPT(i-1, j) \\ \delta + OPT(i, j-1) \end{cases} & \text{otherwise} \end{cases}$$

Sequence Alignment: Algorithm

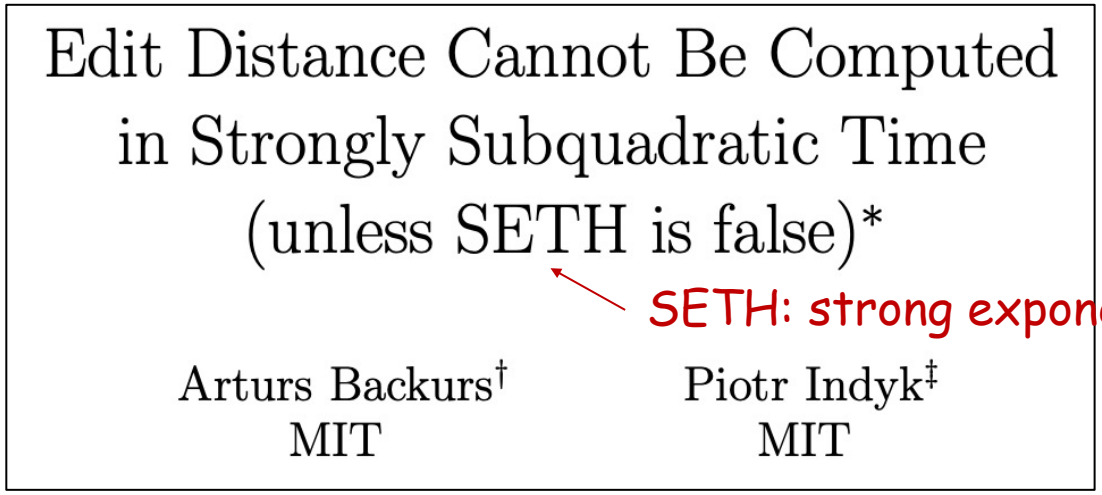
- **Bottom-up DP algorithm:**

```
Sequence-Alignment(m, n, x1x2...xm, y1y2...yn, δ, α) {
   for i = 0 to m
      M[i, 0] = iδ
   for j = 0 to n
      M[0, j] = jδ

   for i = 1 to m
      for j = 1 to n
         M[i, j] = min{ α[xi, yj] + M[i - 1, j - 1],
                        δ + M[i - 1, j],
                        δ + M[i, j - 1] }
   return M[m, n]
}
```

- **Running time.** *O(mn)*

Sequence Alignment: Impossibility Result

- **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 $\delta > 0$.



- **Takeaway.** It is very difficult (if not impossible) to improve the $O(mn)$ running time of computing the edit distance of two strings.

Sequence Alignment: Algorithm

- **Bottom-up DP algorithm:**

```
Sequence-Alignment(m, n, x1x2...xm, y1y2...yn, δ, α) {
   for i = 0 to m
      M[i, 0] = iδ
   for j = 0 to n
      M[0, j] = jδ

   for i = 1 to m
      for j = 1 to n
         M[i, j] = min{ α[xi, yj] + M[i - 1, j - 1],
                        δ + M[i - 1, j],
                        δ + M[i, j - 1] }

   return M[m, n]
}
```

M[i, j] depends only on M[·, j - 1] and M[i - 1, ·]

- **Running time.** *O(mn)* **Space.** *O(min{m, n})* ← only OPT(m, n) is computed cannot find an optimal alignment

Sequence Alignment: Finding a Solution

- **Q.** How to find an optimal alignment?
- **A.** Apply a trace-back algorithm.
- **Example trace-back:**
  - PALETTE
  - PAL–ATE
- **Q.** How much space is required?
- **A.** *O(mn)*: store the *m x n* M[·, ·] matrix

m, n ≤ 10 for English words
m, n ≈ 10^5 for biology applications

		P	A	L	A	T	E
	0	2	4	6	8	10	12
P	2	0	2	4	6	8	10
A	4	2	0	2	4	6	8
L	6	4	2	0	2	4	6
E	8	6	4	2	1	3	4
T	10	8	6	4	3	1	3
T	12	10	8	6	5	3	2
E	14	12	10	8	7	5	3

- **Q.** Can we reduce the required space for sequence alignment?

Sequence Alignment in Linear Space

- **Theorem.** [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.

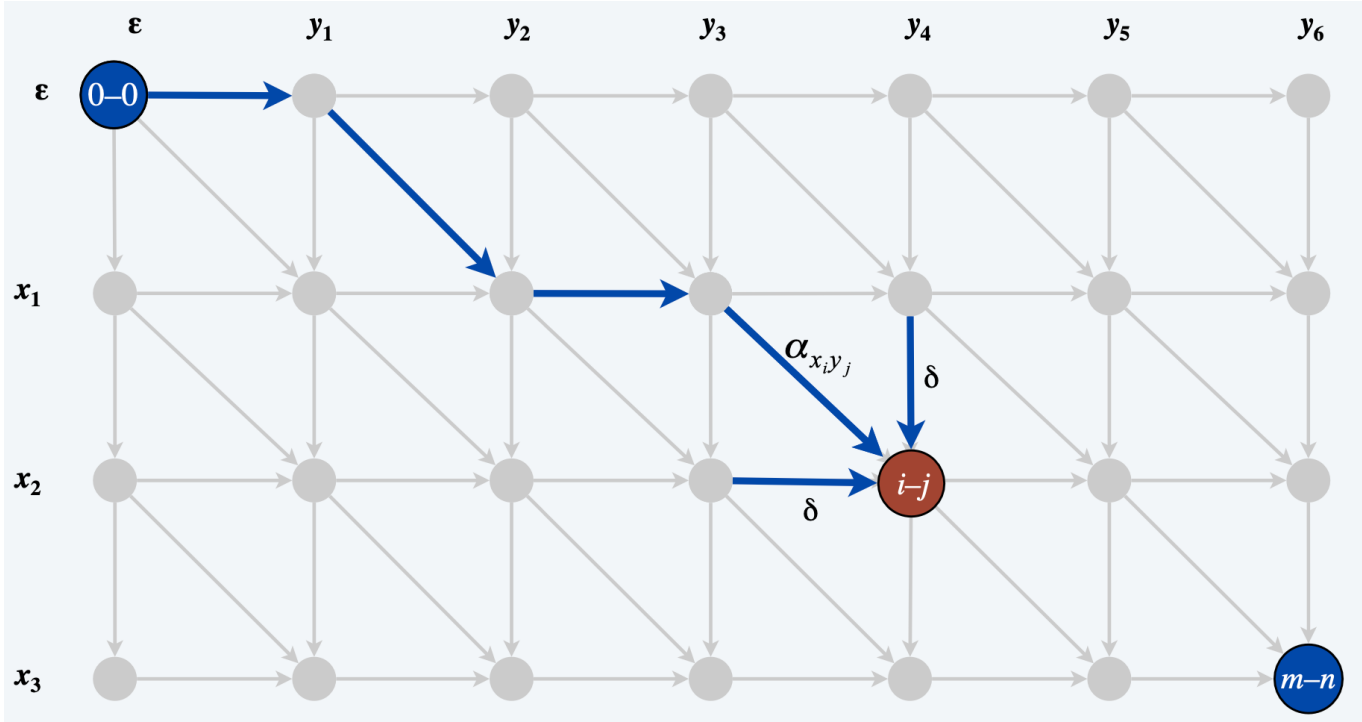
Programming Techniques — G. Manacher Editor

A Linear Space Algorithm for Computing Maximal Common Subsequences

D.S. Hirschberg
Princeton University

Edit Distance Graph

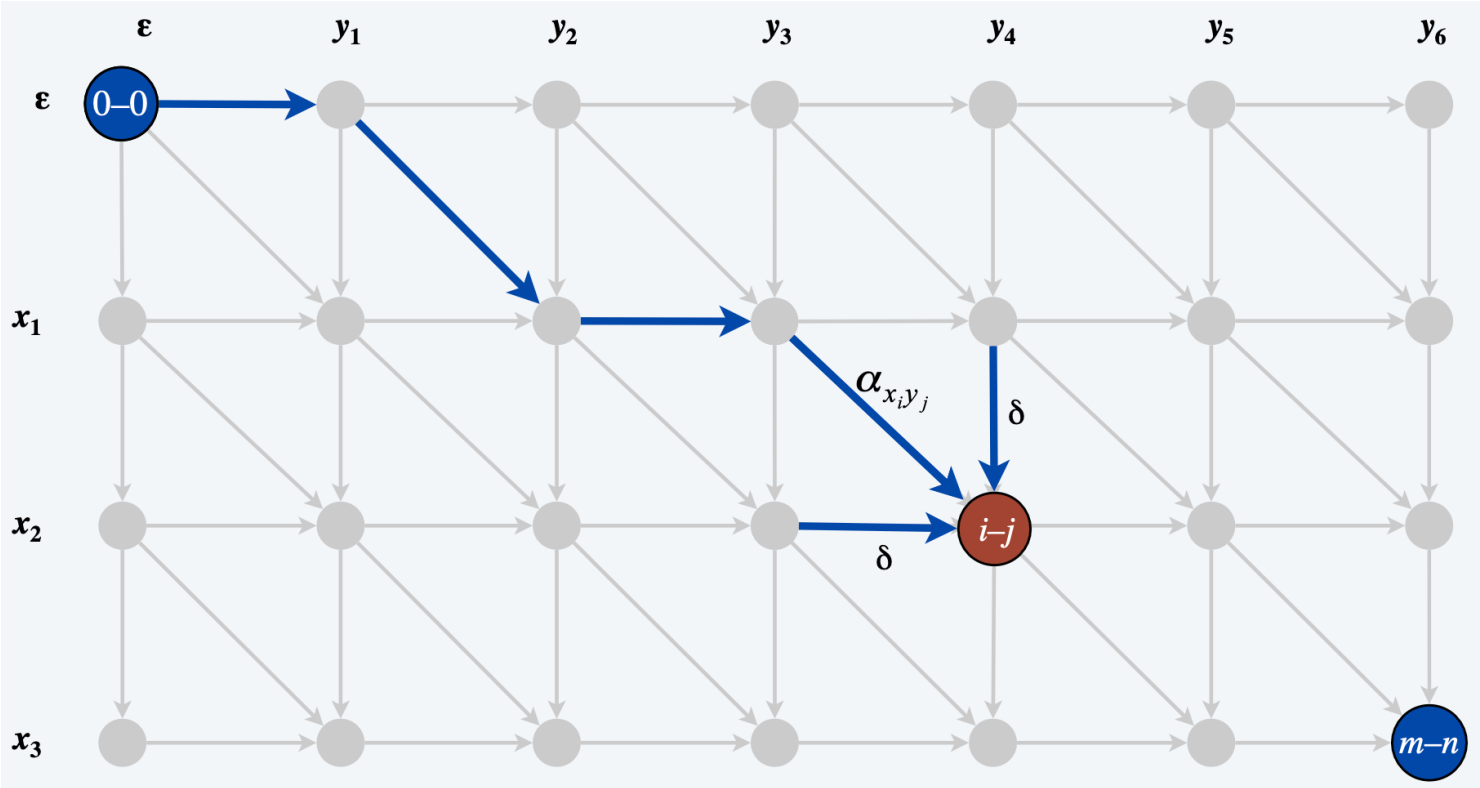
- **Edit distance graph:**
  - rows: x
  - columns: y
  - path: alignment
- **Example path:**
  - $- x_1 - x_2 \ldots x_m$
  - $y_1 y_2 y_3 y_4 \ldots y_n$



Shortest Path = Optimal Alignment

- **Lemma.** *f(i, j) = OPT(i, j)* for all *i* and *j*.

f(*i*, *j*) = length of shortest path from *(0, 0)* to *(i, j)*



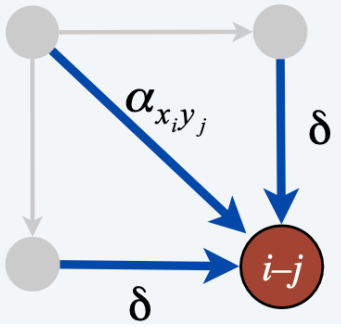
Shortest Path = Optimal Alignment

- **Lemma.** *f(i, j) = OPT(i, j)* for all *i* and *j*.
- **Pf.** (by strong induction on *i + j*)
  - Basis 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)* or *(i – 1, j)* or *(i, j – 1)*.

$$
\begin{aligned}
f(i,j) &= \min\{\alpha_{x_i y_j} + f(i-1,j-1),\ \delta + f(i-1,j),\ \delta + f(i,j-1)\} \\
&= \min\{\alpha_{x_i y_j} + OPT(i-1,j-1),\ \delta + OPT(i-1,j),\ \delta + OPT(i,j-1)\} \\
&= OPT(i,j) \quad \blacksquare
\end{aligned}
$$

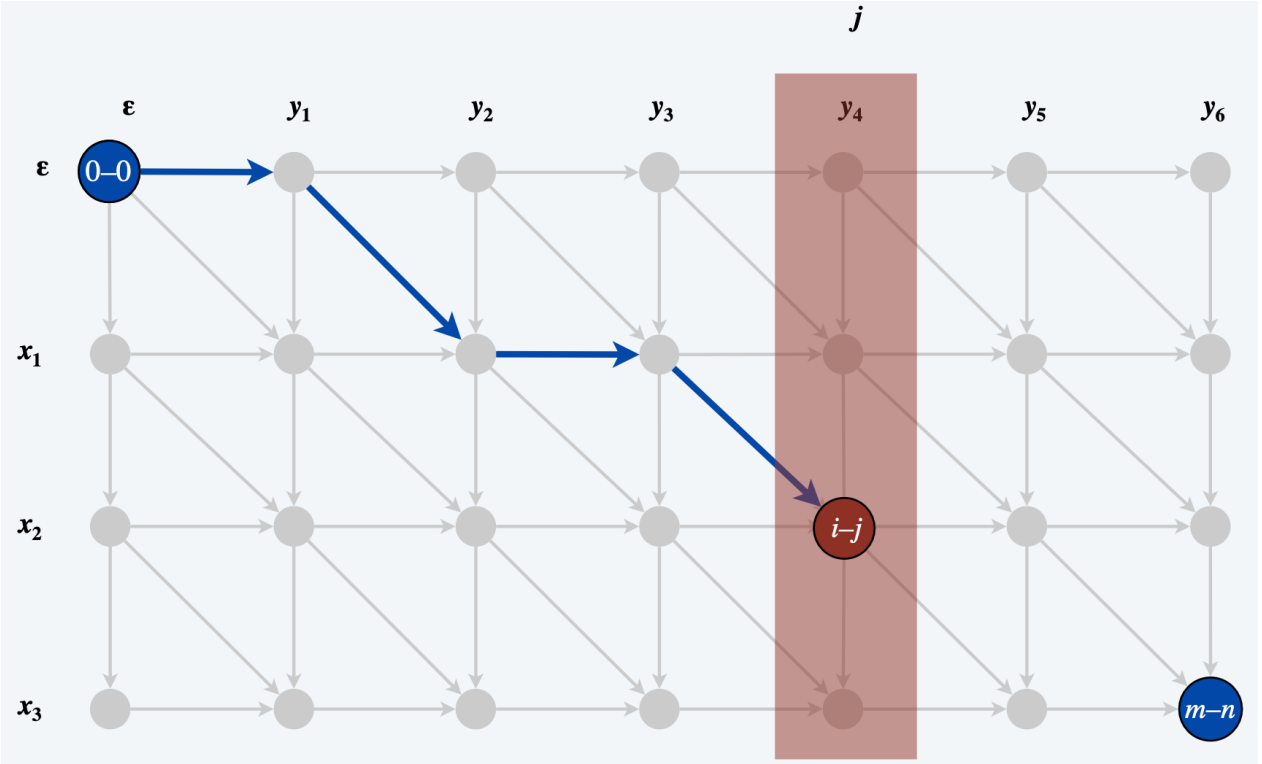
inductive hypothesis

Bellman equation



Hirschberg's Algorithm

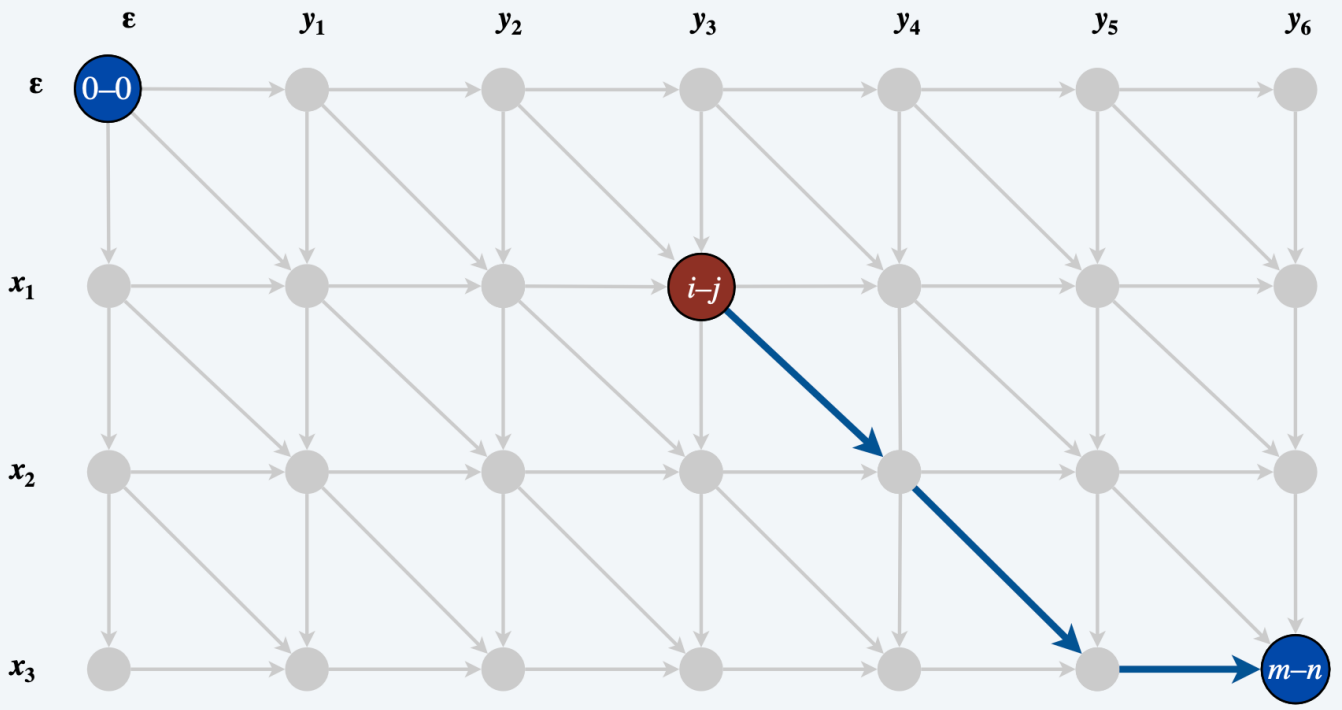
- **To compute *OPT(m, n)*:**
  - Let *f(i, j)* denote length of shortest path from *(0, 0)* to *(i, j)*.
  - **Lemma:** *f(i, j) = OPT(i, j)* for all *i* and *j*.
  - Can compute *f(·, j)* for any specific *j* in *O(mn)* time and *O(m)* space.



f(·, j) depends only on f(·, j – 1)

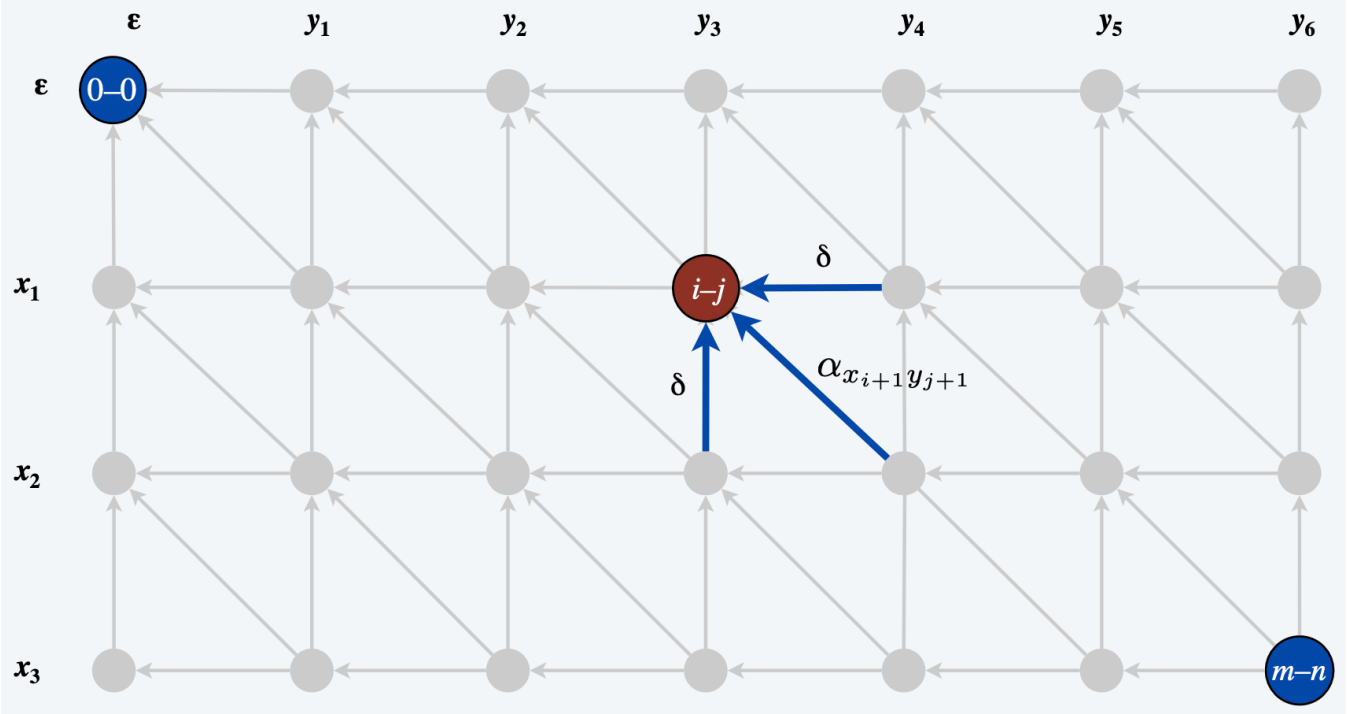
Hirschberg's Algorithm

- **To compute *OPT(m, n)*:**
  - Let *g(i, j)* denote length of shortest path from *(i, j)* to *(m, n)*.



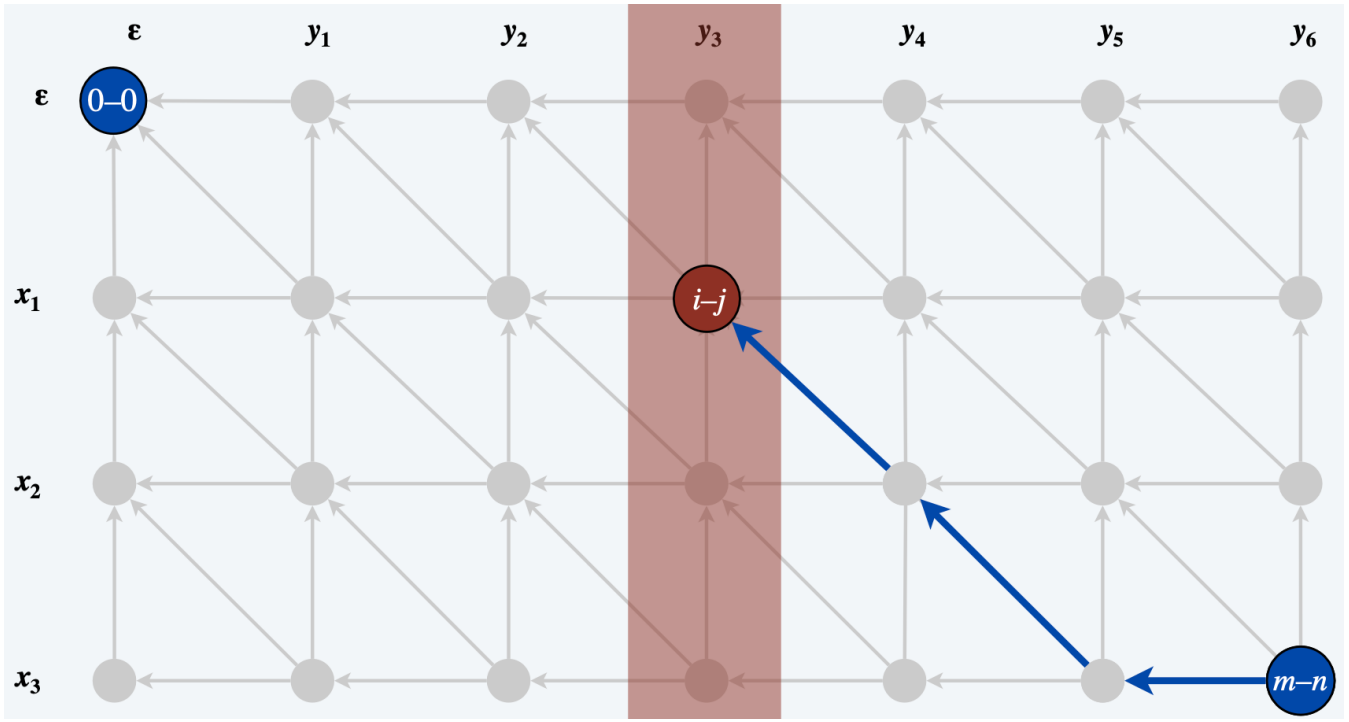
Hirschberg's Algorithm

- **To compute *OPT(m, n)*:**
  - Let *g(i, j)* denote length of shortest path from *(i, j)* to *(m, n)*.
  - Can compute *g(i, j)* by reversing edges and the roles of *(0, 0)* and *(m, n)*.



Hirschberg's Algorithm

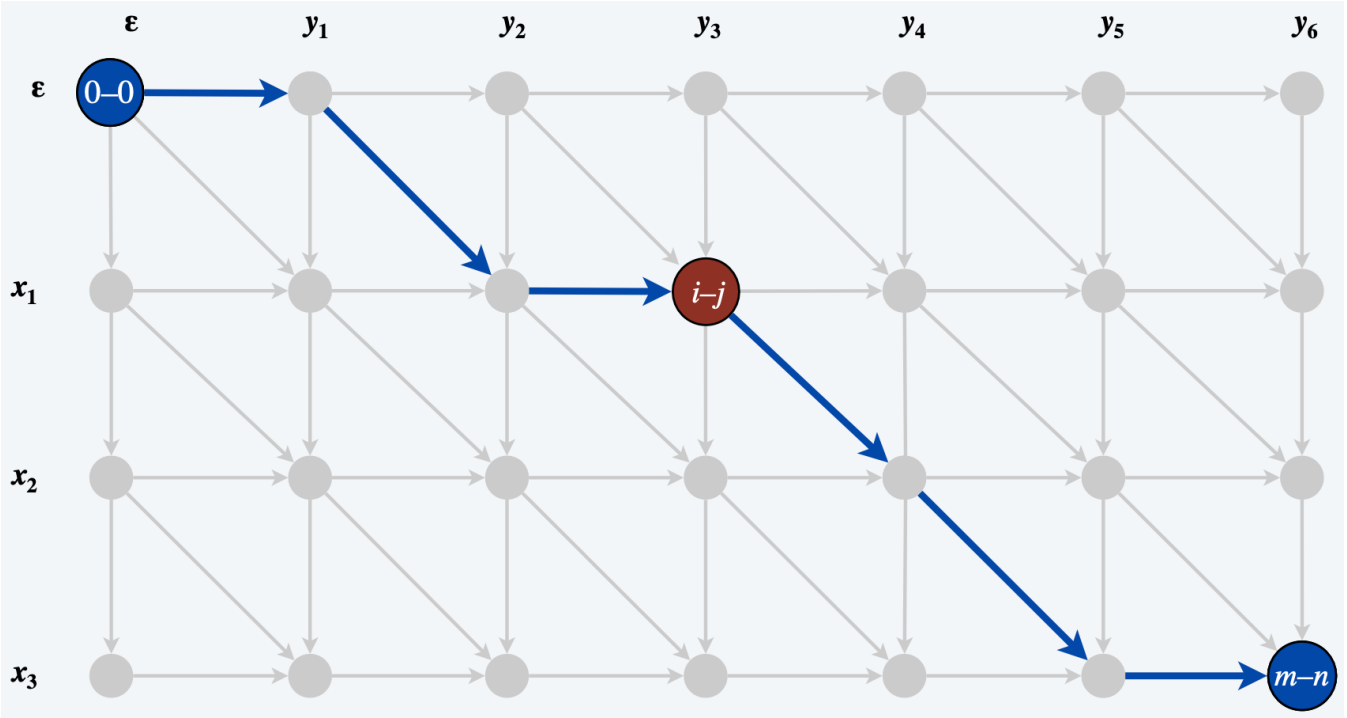
- **To compute *OPT(m, n)*:**
  - Let *g(i, j)* denote length of shortest path from *(i, j)* to *(m, n)*.
  - Can compute *g(i, j)* by reversing edges and the roles of *(0, 0)* and *(m, n)*.
  - Can compute *g(·, j)* for any specific *j* in *O(mn)* time and *O(m)* space.



g(·, j) depends only on g(·, j + 1)

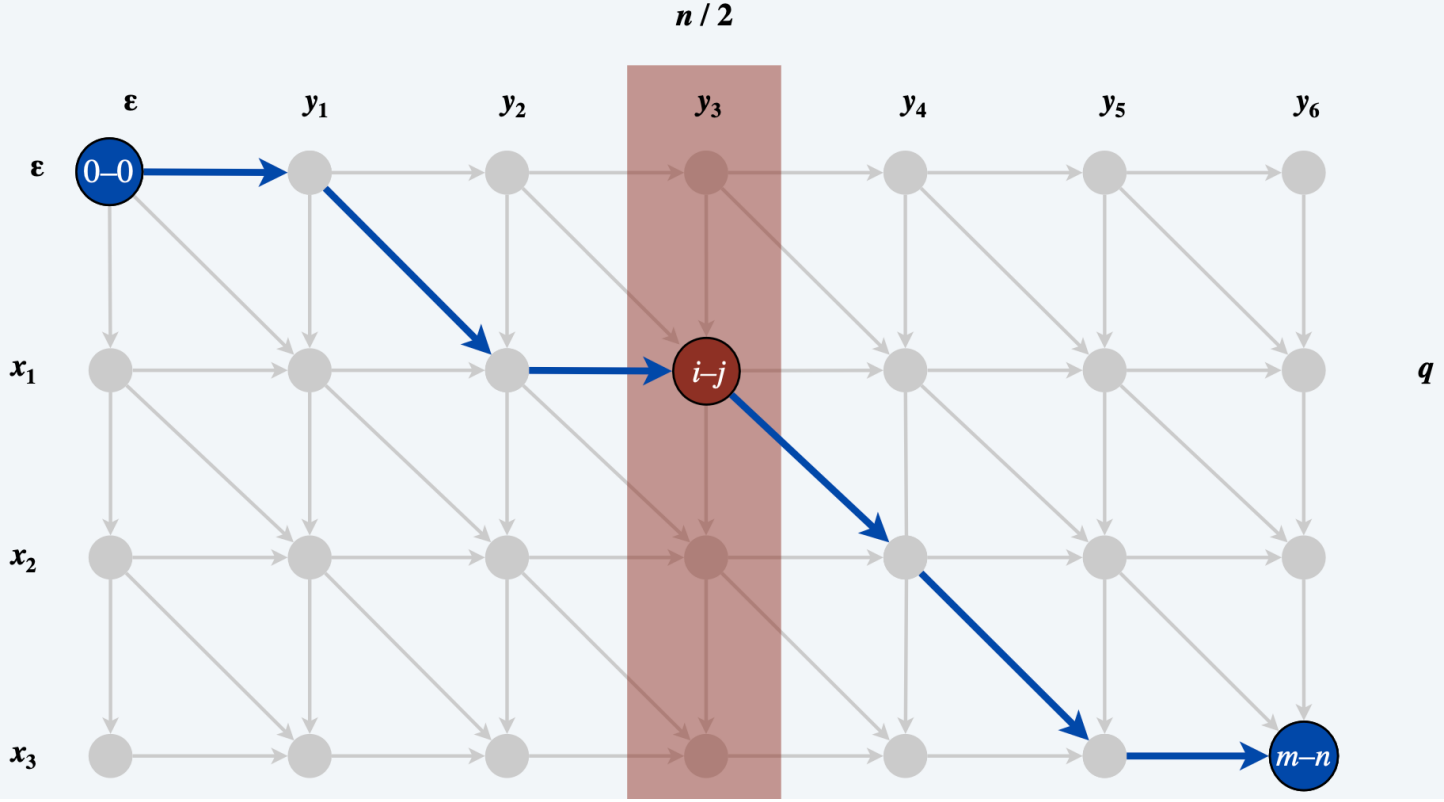
Hirschberg's Algorithm

- **Observation.** The length of a shortest path via (i, j) is $f(i, j) + g(i, j)$.



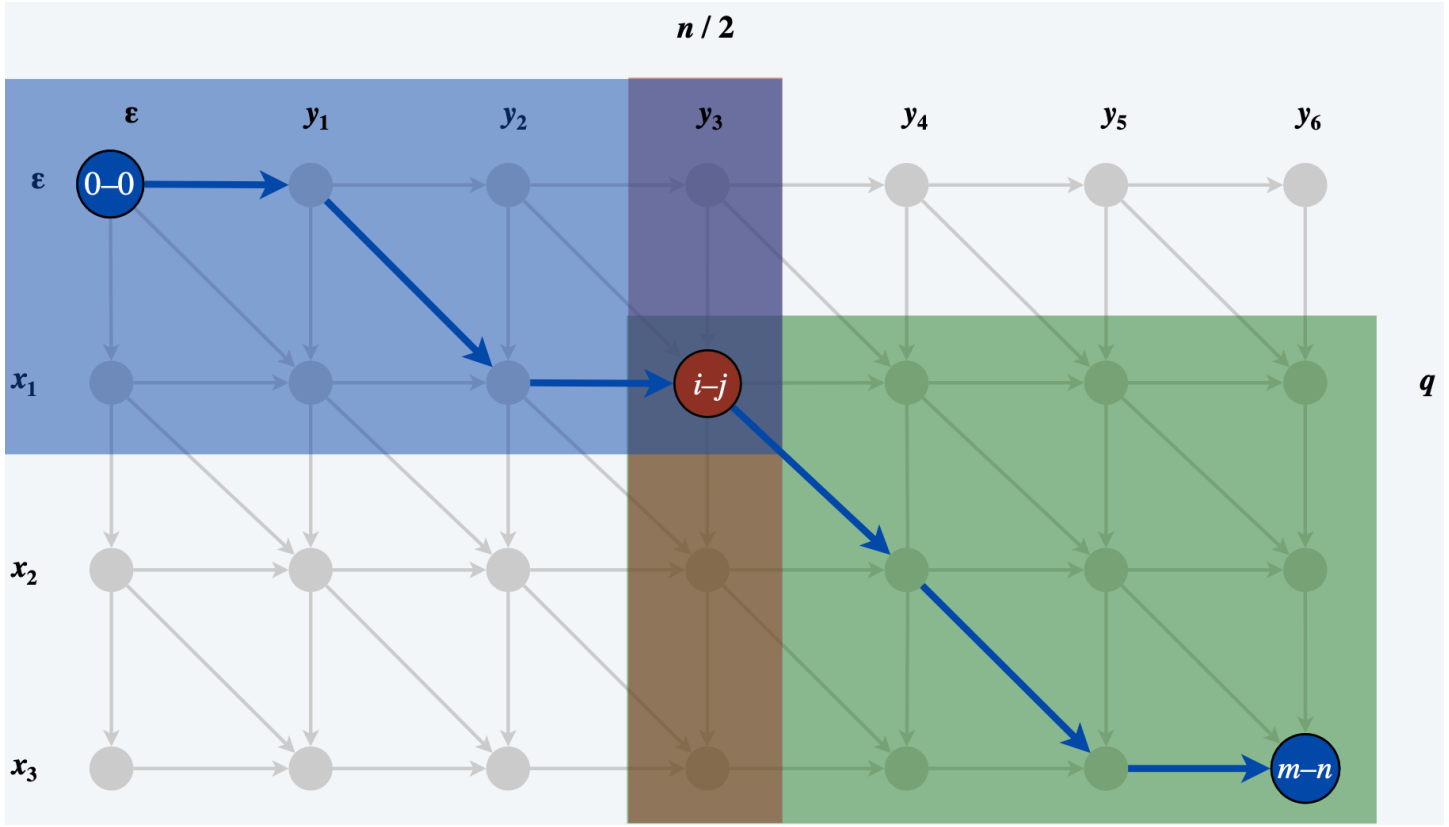
Hirschberg's Algorithm

- **Observation.** The length of a shortest path via (i, j) is $f(i, j) + g(i, j)$.
- **Observation.** 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 $(q, n/2)$.



Hirschberg's Algorithm: Divide and Conquer

- **Divide.** Find index q that minimizes $f(q, n/2) + g(q, n/2)$.
  - Save this dividing node $(q, n/2)$ as part of solution.
- **Conquer.** Recursively compute optimal alignment in each piece.



total problem size halved after each recursion

Hirschberg's Algorithm: Space

- **Theorem.** Hirschberg's algorithm uses $\Theta(m + n)$ space.
- **Pf.** (direct proof)
  - Each recursive call uses $\Theta(m)$ space to compute $f(\cdot, n/2)$ and $g(\cdot, n/2)$.
  - $\Theta(1)$ space needs to be maintained per recursive call to save the dividing node.
  - Recursion stops when input size becomes 1.
  - Number of recursive calls $\leq 1 + 2 + 4 + 8 + \ldots + n \leq 2n$.
  - So, $O(n)$ space in total. ▪

- **Q.** Does Hirschberg's algorithm also run in $O(mn)$ time?

Hirschberg's Algorithm: Running Time

- **Theorem.** Let *T(m, n)* = max running time of Hirschberg's algorithm on strings of lengths at most *m* and *n*. Then, *T(m, n) = O(mn log n)*.
- **Pf.** (direct proof)
  - *T(m, n)* is monotone nondecreasing in both *m* and *n*.
  - *T(m, n) ≤ 2T(m, n/2) + O(mn) ⇒ T(m, n) = O(mn log n)* ▪

- **Q.** Can the above analysis of *T(m, n)* be improved?
- **A.** Yes, because two subproblems are of size *(q, n/2)* and *(m – q, n/2)*.

Hirschberg's Algorithm: Running Time

- **Theorem.** Hirschberg's algorithm runs in $T(m, n) = O(mn)$ time.
- **Pf.** (by strong induction on $m + n$)
  - $O(mn)$ time to compute $f(\cdot, n/2)$ and $g(\cdot, n/2)$ and find dividing node $(q, n/2)$.
  - $T(q, n/2) + T(m - q, n/2)$ time for two recursive calls.
  - Choose constant $c > 0$ such that:

    ✓ $T(m, 1) \le cm$, $T(1, n) \le cn$, $T(m, n) \le cmn + T(q, n/2) + T(m - q, n/2)$
  - **Claim.** $T(m, n) \le 2cmn$

    ✓ Basis cases: $m = 1$ and $n = 1$.

    ✓ Inductive hypothesis: $T(m, n) \le 2cmn$ for all (m', n') with $m' + n' < m + n$.

    ✓ Inductive case:

$$T(m, n) \le T(q, n/2) + T(m - q, n/2) + cmn$$
$$\le 2cqn/2 + 2c(m - q)n/2 + cmn = cqn + cmn - cqn + cmn = 2cmn \blacksquare$$

inductive hypothesis

Exercise: Longest Common Subsequence

- **Problem.** Given two strings $X = x_1 x_2 \ldots x_m$ and $Y = y_1 y_2 \ldots y_n$, find a common subsequence that is as long as possible.
- **Alternative viewpoint.** Delete minimum number of characters from string X and string Y such that the resulting strings are the same.

- **Example.** LCS(GGCACCACG, ACGGCGGATACG) = GGCAACG
- **Applications.** Unix diff, git, bioinformatics, …

- **Q.** How to solve this problem via DP (in linear space)?

Longest Common Subsequence: Solution 1

- **Def.** *OPT(i, j) =* length of LCS of prefix strings $x_1x_2 \ldots x_i$ and $y_1y_2 \ldots y_j$
- **Goal.** *OPT(m, n)*
- **To compute *OPT(i, j)*:**
  - Case 1: $x_i = y_j$
    - ✓ *1* + length of LCS of prefix strings $x_1x_2 \ldots x_{i-1}$ and $y_1y_2 \ldots y_{j-1}$
  - Case 2: $x_i \neq y_j$
    - ✓ Delete x_i : length of LCS of prefix strings $x_1x_2 \ldots x_{i-1}$ and $y_1y_2 \ldots y_j$
    - ✓ Delete y_j : length of LCS of prefix strings $x_1x_2 \ldots x_i$ and $y_1y_2 \ldots y_{j-1}$
- **Bellman equation.**

$$OPT(i,j) = \begin{cases} 0 & \text{if } i = 0 \text{ or } j = 0 \\ 1 + OPT(i-1, j-1) & \text{if } x_i = y_j \\ \max\{OPT(i-1,j), OPT(i,j-1)\} & \text{if } x_i \neq y_j \end{cases}$$

Longest Common Subsequence: Solution 2

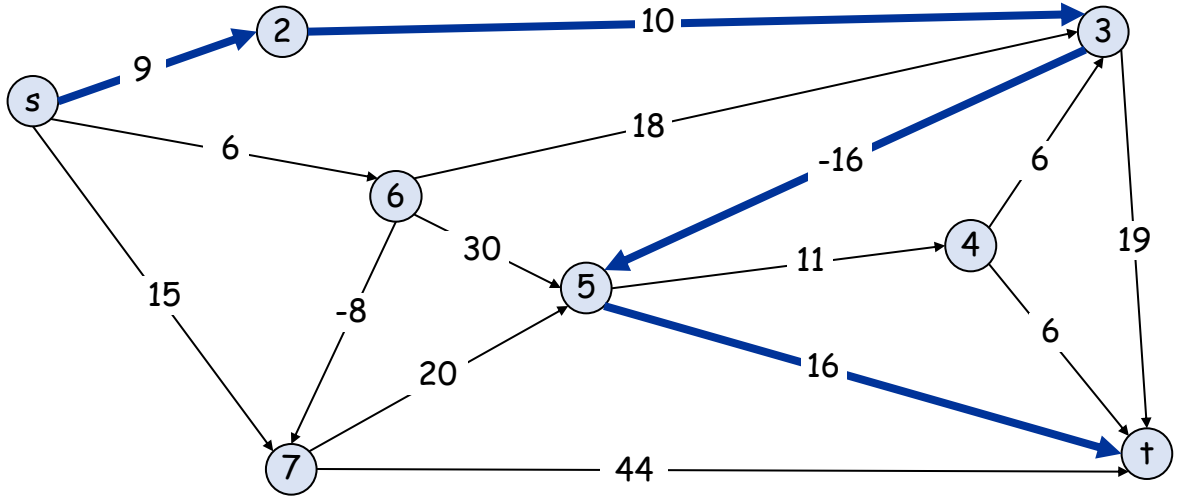
- **Alternatively.** Reduce this LCS problem to finding an optimal alignment of $X = x_1 x_2 \ldots x_m$ and $Y = y_1 y_2 \ldots y_n$.
  - Gap penalty $\delta = 1$; mismatch penalty $\alpha_{pp} = 0$ and $\alpha_{pq} = \infty$.
  - Edit distance = min number of gaps = min number of deletions from X and Y.
  - Length of LCS = $(m + n - \text{edit distance}) / 2$.
- **Running time.** $O(mn)$ **Space.** $O(m + n)$ (e.g., run Hirschberg)

- **Lower bound.** [Abboud-Backurs-Williams 2015] There exists no algorithm that runs in $O(n^{2-\varepsilon})$ to find LCS of two length-n strings unless SETH is false.

6. Shortest Paths with Negative Weights

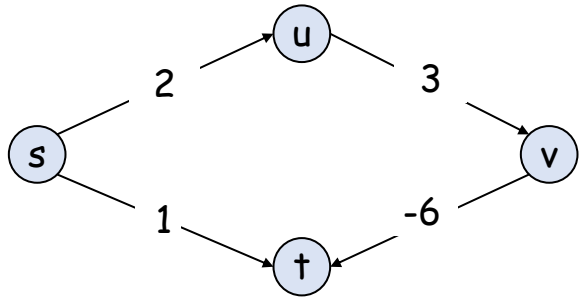
Shortest Paths with Negative Weights

- **Shortest-path problem.** Given a digraph $G = (V, E)$, with arbitrary edge weights ℓ_{vw}, find shortest path from source node s to destination node t.
- **Example.** Nodes represent agents in a financial setting and ℓ_{vw} is cost of transaction in which we buy from agent v and sell immediately to w.

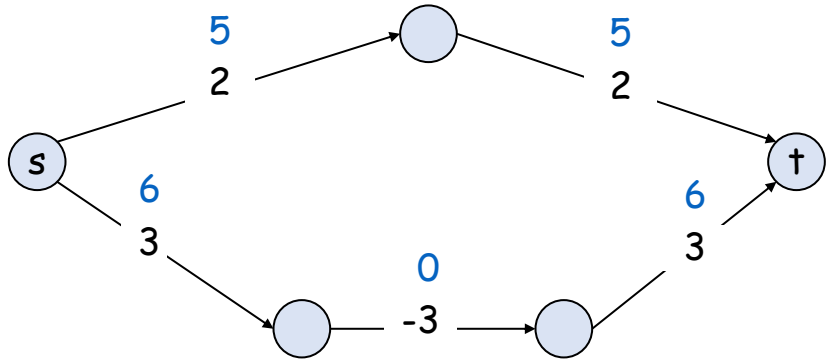


Shortest Paths: Failed Attempts

- **Dijkstra.** Can fail if there exist negative edge weights.

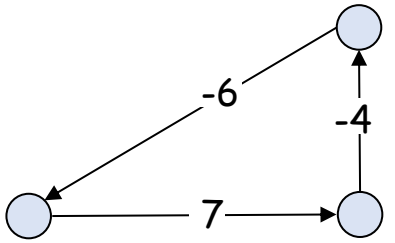


- **Reweighting.** Adding a constant to every edge weight can still fail.

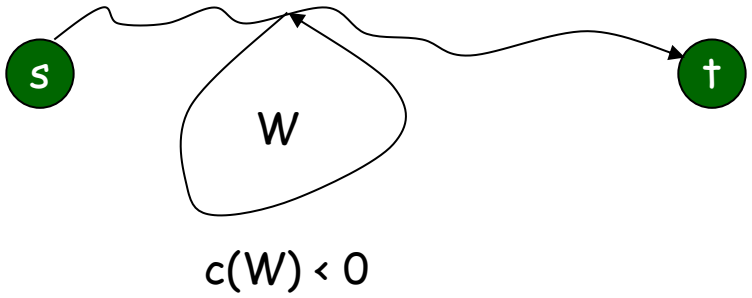


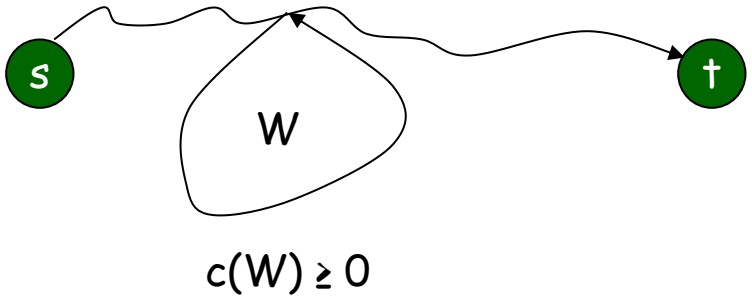
Negative Cycles

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



- **Observation 1.** If some *s-t* path contains a negative cycle, then there does not exist a shortest *s-t* path.
- **Observation 2.** If there exists no negative cycle, there exists a shortest *s-t* path that is simple (and has $\leq n - 1$ edges).





Shortest-Paths Problem with Negative Weights

- **Single-destination shortest-paths problem.** Given a digraph $G = (V, E)$, with arbitrary edge weights ℓ_{vw} (but no negative cycles) and a destination node t, find a shortest v-t path from every node v to t.

assume there exits a path from every node to t

- **Remark.** This single-destination shortest-paths problem is equivalent to single-source shortest-paths problem with edge directions reversed.

Shortest Paths: Dynamic Programming

- **Def.** *OPT(i, v)* = length of shortest *v-t* path *P* using ≤ *i* edges.
- **Goal.** *OPT(n – 1, v)*

  if no neg cycles, there exists a simple shortest path of length ≤ n -1

- **To compute *OPT(i, v)*:**
  - Case 1: *P* uses ≤ *i – 1* edges.
    - ✓ *OPT(i, v) = OPT(i – 1, v)*
  - Case 2: *P* uses exactly *i* edges.
    - ✓ Let *(v, w)* denote the first edge in *P*: pay the cost of ℓ_{vw} , then select the shortest *w-t* path using ≤ *i – 1* edges.

Shortest Paths: Dynamic Programming

- **Def.** *OPT(i, v)* = length of shortest *v-t* path *P* using ≤ *i* edges.
- **Goal.** *OPT(n – 1, v)*

if no neg cycles, there exists a simple shortest path of length ≤ n -1

- **Bellman equation:**

$$OPT(i,v) = \begin{cases} 0, & \text{if } i = 0 \text{ and } v = t \\ \infty, & \text{if } i = 0 \text{ and } v \neq t \\ \min\{OPT(i-1,v),\ \min_{w \in V}(OPT(i-1,w) + l_{vw})\} & \text{if } i > 0 \end{cases}$$

Shortest Paths: Algorithm

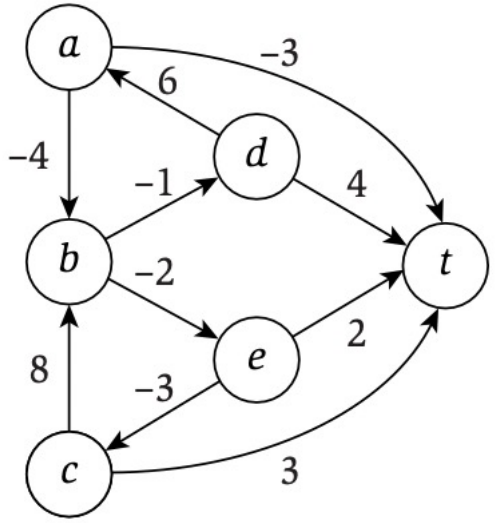
- **Bottom-up DP algorithm:**

```
Shortest-Path(G, t) {
   foreach node v ∈ V
      M[0, v] = ∞
   M[0, t] = 0

   for i = 1 to n - 1
      foreach node v ∈ V
         M[i, v] = M[i - 1, v]
         foreach edge (v, w) ∈ E
            M[i, v] = min{ M[i, v], M[i - 1, w] + ℓ_vw }
}
```

pull every neighbor w even if w not updated

- **Running time.** $O(mn)$ **Space.** $O(n^2)$

Shortest-Paths DP Algorithm: Demo



(a)

	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

(b)

$$OPT(i,v) = \begin{cases} 0, & \text{if } i = 0 \text{ and } v = t \\ \infty, & \text{if } i = 0 \text{ and } v \neq t \\ \min\{OPT(i-1,v),\ \min_{w \in V}(OPT(i-1,w) + l_{vw})\} & \text{if } i > 0 \end{cases}$$

Shortest Paths: Finding Shortest Paths

- **Finding the shortest paths:**
  - Approach 1: Maintain 2D array successor[*i, v*] that points to the next node on a shortest *v*-*t* path using $\leq i$ edges.
  - Approach 2: Compute optimal lengths M[*i, v*] and consider only edges with M[*i, v*] = M[*i* – *1, w*] + ℓ_{vw} . Any directed path in this subgraph is a shortest path.

- **Q.** Can we reduce the required space?

$$OPT(i,v) = \begin{cases} 0, & \text{if } i = 0 \text{ and } v = t \\ \infty, & \text{if } i = 0 \text{ and } v \neq t \\ \min\{OPT(i-1,v),\ \min_{w \in V}(OPT(i-1,w) + l_{vw})\} & \text{if } i > 0 \end{cases}$$

only OPT[i – 1, .] is used!

Shortest Paths: Practical Improvements

- **Space optimization.** Maintain two 1D arrays (instead of 2D arrays).
  - $d[v]$ = length of a shortest v-t path that we have found so far
  - successor[v] = next node on a v-t path (used to find shortest paths)
- **Remark.** This space-efficient algorithm is called Bellman-Ford-Moore.

- **Performance optimization.** If $d[w]$ was not updated in iteration $i - 1$, then no need to consider edges entering w in iteration i.
- **Remark.** This time-efficient implementation of Bellman-Ford-Moore is also known as the shortest path faster algorithm (SPFA).

Bellman-Ford-Moore: Efficient Implementation

- **Push-based DP algorithm with linear extra space:**

```
Bellman-Ford-Moore(G, s, t) {
    foreach node v ∈ V
        d[v] = ∞
        successor[v] = null
    d[t] = 0

    for i = 1 to n - 1
        foreach node w ∈ V
            if (d[w] has been updated in previous iteration)
                foreach node v such that (v, w) ∈ E
                    if (d[v] > d[w] + ℓ_vw)
                        d[v] = d[w] + ℓ_vw
                        successor[v] = w
        if (no d[w] value changed in iteration i)
            break
}
```

SPFA optimizes this for loop by keeping nodes updated in previous pass in a queue

push each v that has the updated w as a neighbor

terminate when no d[] update occurs

O(n) extra space

O(m) for each pass

Bellman-Ford-Moore: Analysis

- **Lemma 1.** After pass i, $d[v] \le$ length of a shortest v-t path using $\le i$ edges.
- **Pf.** (by induction on i)
  - Basis case: $i = 0$.
  - Inductive hypothesis: assume true after pass i.
  - Inductive case: Let P be any v-t path with $\le i + 1$ edges.
    - ✓ Let (v, w) be first edge in P and let P' be subpath from w to t.
    - ✓ By inductive hypothesis, because P' is a w-t path with $\le i$ edges, at the end of pass i we have $d[w] \le \ell(P')$.
    - ✓ After considering edge (v, w) in pass $i + 1$ (here w.l.o.g. consider pull-based): $d[v] \le \ell_{vw} + d[w]$. Then, since $d[w] \le \ell(P')$ after pass i and $d[w]$ never increases during the algorithm, we have $d[v] \le \ell_{vw} + \ell(P') = \ell(P)$. ▪

Bellman-Ford-Moore: Analysis

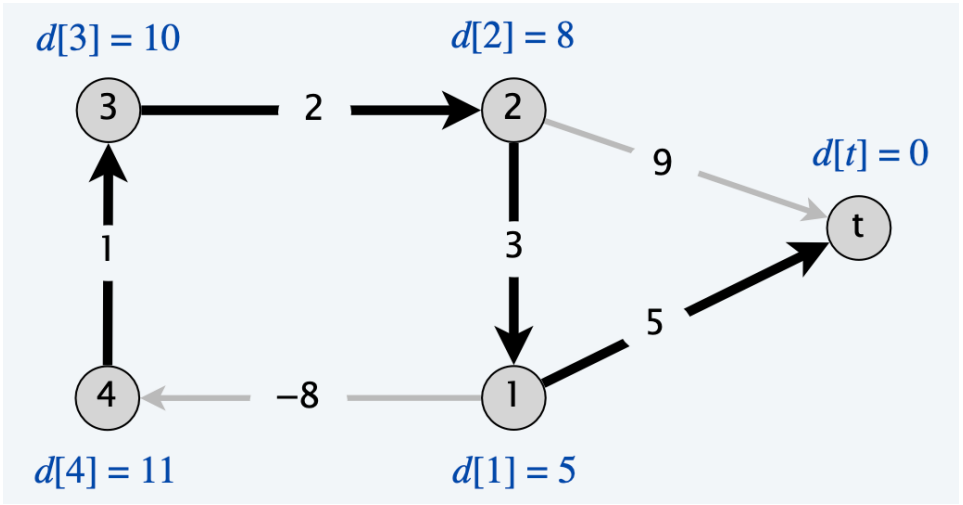
- **Theorem.** If no negative cycles, Bellman-Ford-Moore computes the lengths of the shortest *v-t* paths in $O(mn)$ time and $\Theta(n)$ extra space.
- **Pf.** (only left to show $d[v]$ = shortest *v-t* path length)
  - **Observation 2:** If no negative cycles, shortest path exists and has $\leq n - 1$ edges.
  - **Lemma 1:** After pass $n - 1$, $d[v] \leq$ length of shortest *v-t* path using $\leq n - 1$ edges.

- **Remark.** Bellman-Ford-Moore is typically faster in practice.
  - Edge (v, w) is considered in pass $i + 1$ only if $d[w]$ was updated in pass i.
  - If shortest path has k edges, then algorithm finds it after $\leq k$ passes.

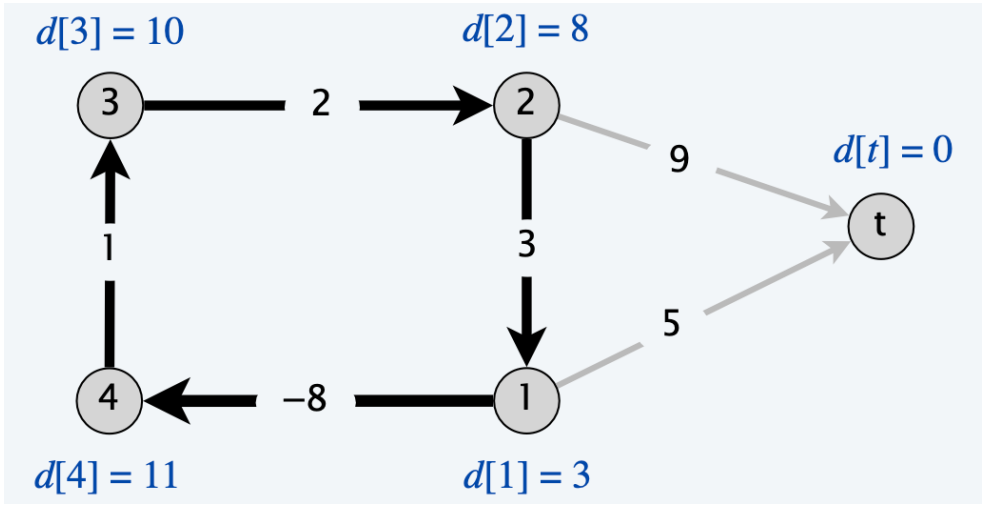
- **Q.** How to find a shortest *v-t* path of length $d[v]$ for every node v?

Bellman-Ford-Moore: Finding Shortest Paths

- **Def.** A successor graph consists of only edges {(*v*, successor[*v*])}.
- **Claim.** [This claim is false!] After pass *n – 1* of Bellman-Ford-Moore, the successor graph gives a directed path from *v* to *t* of length *d*[*v*].
- **Counterexample.** A successor graph may have directed cycles.
  - E.g., consider nodes updated in order: *t, 1, 2, 3, 4*



before updating 1



after updating 1

Bellman-Ford-Moore: Finding Shortest Paths

- **Lemma 2.** Any directed cycle W in successor graph is a negative cycle.
- **Pf.** (direct proof)
  - If successor[v] = w, we have $d[v] \geq d[w] + \ell_{vw}$. (They 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:

$$
\begin{array}{lcll}
d[v_1] & \geq & d[v_2] & + \ \ell(v_1, v_2) \\
d[v_2] & \geq & d[v_3] & + \ \ell(v_2, v_3) \\
\vdots & & \vdots & \vdots \\
d[v_{k-1}] & \geq & d[v_k] & + \ \ell(v_{k-1}, v_k) \\
d[v_k] & > & d[v_1] & + \ \ell(v_k, v_1) \quad \longleftarrow \text{ holds with strict inequality since we are updating } d[v_k]
\end{array}
$$

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

Bellman-Ford-Moore: Finding Shortest Paths

- **Theorem.** Assuming no negative cycles, Bellman-Ford-Moore finds a shortest *v*-*t* path for every node *v* in $O(mn)$ time and $\Theta(n)$ extra space.
- **Pf.** (direct proof)
  - **Lemma 2** + no neg cycles $\Rightarrow$ the successor graph cannot have a directed cycle.
  - 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*, then $d[v] = d[w] + \ell_{vw}$. (LHS and RHS are equal when successor[*v*] is set; $d[\cdot]$ did not change since algorithm terminated.)
  - Thus,

$$\begin{aligned} d[v_1] &= d[v_2] + \ell(v_1, v_2) \\ d[v_2] &= d[v_3] + \ell(v_2, v_3) \\ &\vdots \quad\quad \vdots \quad\quad \vdots \\ d[v_{k-1}] &= d[v_k] + \ell(v_{k-1}, v_k) \end{aligned}$$

P is a shortest path of length d[v]

d[t] = 0

  - Adding above equations yields $d[v] = d[t] + \ell(v_1, v_2) + \ell(v_2, v_3) + \ldots + \ell(v_{k-1}, v_k)$. ▪

Shortest Paths: Asymptotic Complexity

year	worst case	discovered by
1955	$O(n^4)$	Shimbel
1956	$O(m\, n^2\, W)$	Ford
1958	$O(m\, n)$	Bellman, Moore
1983	$O(n^{3/4}\, m \log W)$	Gabow
1989	$O(m\, n^{1/2} \log(nW))$	Gabow–Tarjan
1993	$O(m\, n^{1/2} \log W)$	Goldberg
2005	$O(n^{2.38}\, W)$	Sankowsi, Yuster–Zwick
2016	$\tilde{O}(n^{10/7} \log W)$	Cohen–Mądry–Sankowski–Vladu
20xx		

single-source shortest paths with weights between -W and W

7. Distance-Vector Protocols

Shortest-Paths Algorithms for Routing

- **Routing in a communication network.**
  - Node ≈ router
  - Edge ≈ direct communication link
  - Cost of edge ≈ latency of link ← the costs are non-negative, but Bellman-Ford-Moore is used anyway!

- **Dijkstra's algorithm.** Requires global information of network.
- **Bellman-Ford-Moore.** Uses only local knowledge of neighboring nodes.
- **Synchronization.** We don't expect routers to run in lockstep. The order in which each edges are processed in Bellman-Ford-Moore is not important. Moreover, algorithm converges even if updates are asynchronous.

Asynchronous Shortest-Paths Algorithm

- **Asynchronous DP algorithm:**

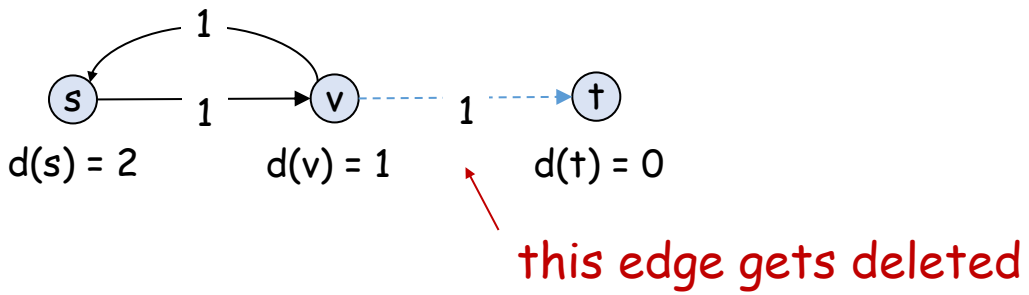
```
Asynchronous-Bellman-Ford-Moore(G, s, t) {
   foreach node v ∈ V
      d[v] = ∞
      successor[v] = null
   d[t] = 0
   Declare t to be active and all other nodes inactive

   while there exists an active node
      Choose an active node w
         foreach node v such that (v, w) ∈ E
            if (d[v] > d[w] + ℓ_vw)
               d[v] = d[w] + ℓ_vw
               successor[v] = w
               Declare v to be active
      Declare w to be inactive
}
```

no global in-order for loop for asynchronous version

Distance-Vector Routing Protocols

- **Distance-vector routing protocols.** "routing by rumor"
  - Each router maintains a vector of shortest path lengths (distances) to every other node and the first hops (directions) on each path.
  - Algorithm: each router performs *n* separate computations, one for each potential destination node, using information pushed by neighboring routers.
- **Example applications.** RIP, Xerox XNS RIP, Novell's IPX RIP, Cisco's IGRP, DEC's DNA Phase IV, AppleTalk's RTMP.
- **Caveat.** Edge costs may change during algorithm (or fail completely).

"counting to infinity"



Path-Vector and Link-State Routing Protocols

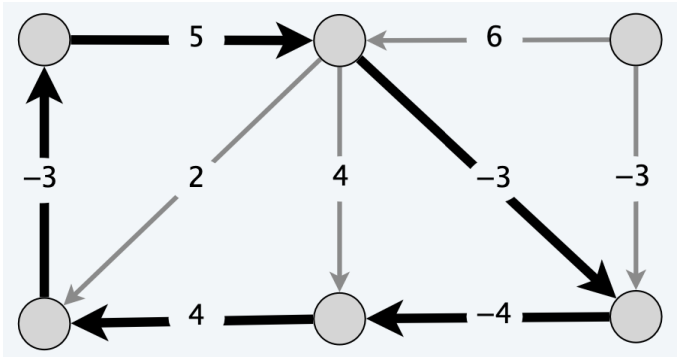
- **Path-vector routing protocols:**
  - Each router also stores the entire path.
  - Requires significantly more storage.
  - Avoids the "counting-to-infinity" problem and related difficulties.
  - Application: Border Gateway Protocol (BGP)
- **Link-state routing protocols:**
  - Each router stores the entire network topology.
  - Requires even more storage.
  - Independently calculates shortest paths based on Dijkstra's algorithm.
  - Applications: Open Shortest Path First (OSPF), Intermediate System to Intermediate System (IS-IS)

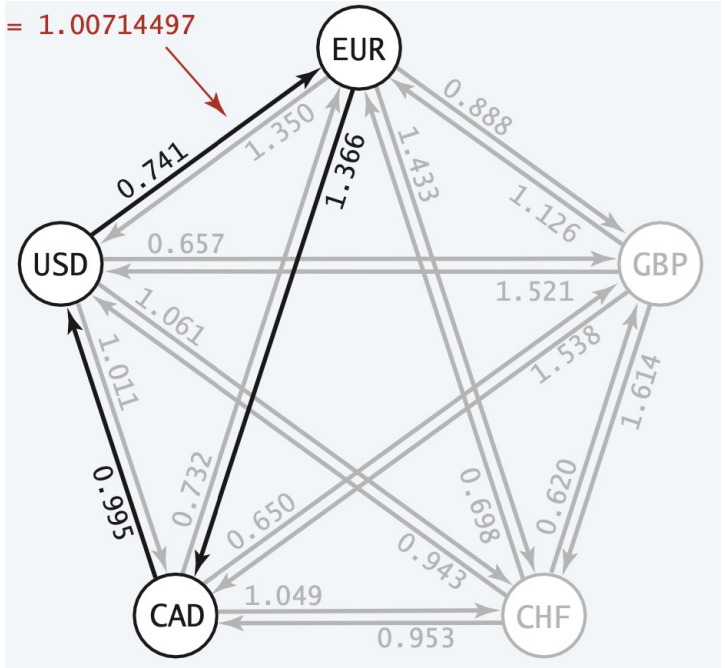
not just the distance and first hop

8. Negative Cycles

Detecting Negative Cycles

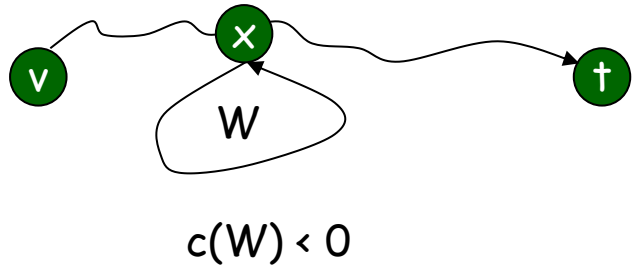
- **Negative cycle detection problem.** Given a directed graph $G = (V, E)$, with arbitrary edge weights ℓ_{vw}, find a negative cycle (if one exists).
- **Example.** [Currency conversion] Given n currencies and exchange rates between pairs of currencies, is there an arbitrage opportunity?
  - Fastest algorithm literally very valuable!
- **Q.** Can you convert this problem to a negative cycle detection problem?





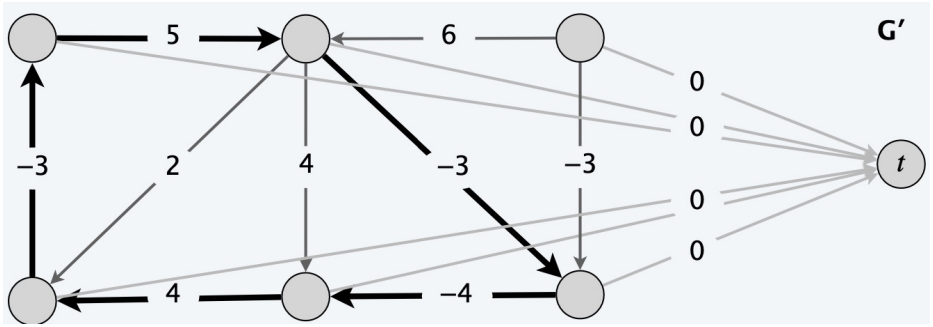
Detecting Negative Cycles

- **Lemma 3.** If $OPT(n, v) = OPT(n – 1, v)$ for every v, then no negative cycles.
  - Note: Lemma 3 assumes there exists a directed path from every node to t.
- **Pf.** The $OPT(n, v)$ values have converged ⇒ shortest v-t path exists. ▪
- **Lemma 4.** If $OPT(n, v) < OPT(n – 1, v)$ for some v, then (any) shortest v-t path of length n contains a cycle W. Moreover, W is a negative cycle.
- **Pf.** (by contradiction)
  - $OPT(n, v) < OPT(n – 1, v)$ ⇒ shortest v-t path P has exactly n edges.
  - By pigeonhole principle, the path P must contain a repeated node x.
  - Let W be any cycle in P.
  - Deleting W yields a v-t path with $< n$ edges.
  - Therefore, W is a negative cycle. ▪



Detecting Negative Cycles

- **Theorem 1.** Can find a negative cycle in $O(mn)$ time and $O(n^2)$ space.
- **Pf.** (constructive proof)
  - Construct graph G' by adding a new sink node t and connect all nodes to t with 0-length edges.
    - ✓ G' has $n' = n + 1$ nodes.
    - ✓ Every node has a directed path to t.
    - ✓ G has a negative cycle if and only if G' has a negative cycle.



  - Case 1: $OPT(n', v) = OPT(n' - 1, v)$ for every node v.
    - ✓ **Lemma 3** + every node can reach t ⇒ there exist no negative cycles.
  - Case 2: $OPT(n', v) < OPT(n' - 1, v)$ for some node v.
    - ✓ **Lemma 4** ⇒ can extract negative cycle from the v-t path of length exactly n' (cycle cannot contain t since no edge leaves t). ▪

Detecting Negative Cycles

- **Theorem 2.** Can find a negative cycle in $O(mn)$ time and $O(n)$ extra space.
- **Pf.** (constructive proof)
  - Construct graph G' as before.
  - Run Bellman-Ford-Moore on G' for $n' = n + 1$ passes (instead of n).
  - If no $d[v]$ values updated in pass n', then no negative cycles.
  - Otherwise, suppose $d[s]$ was updated in pass n'.
  - Let $pass(v)$ = last pass ($\leq n'$) in which $d[v]$ was updated.
  - Observe that $pass(s) = n'$, $pass(t) = 0$, and $pass(\text{successor}[v]) \geq pass(v) - 1$ for each $v \neq t$ (here w.l.o.g. consider push-based).
  - Following successor pointers ($\geq n'$ edges), we must eventually repeat a node.
  - **Lemma 2** $\Rightarrow$ the corresponding cycle is a negative cycle. ▪

More on Detecting Negative Cycles

- **Performance optimization:**
  - SPFA can be improved by using stack (DFS) instead of queue (BFS).
  - Tarjan's subtree disassembly trick: a practical speedup for shortest paths and negative cycle detection algorithms. [Page 304-307 of textbook]
- **Q.** Can we find negative cycles in (simple) undirected graphs?
  - A negative cycle in simple undirected graphs contains at least *3* edges.
- **A.** Yes, but more difficult (e.g., using *T*-joins). This same technique can be used to find simple shortest paths in undirected graphs that does not contain negative cycles.
- **Remark.** Some graph problems could be more challenging to solve in undirected graphs than in directed graphs.

Announcement

- **Assignment 4 has been released and the deadline is 2pm, May 11.**