6. Dynamic Programming

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Algorithmic Paradigms

Greed. Build up a solution incrementally, myopically optimizing some local criterion.

Divide-and-conquer. Break up a problem into two sub-problems, solve each sub-problem independently, and combine solution to sub-problems to form solution to original problem.

Dynamic programming. Break up a problem into a series of overlapping sub-problems, and build up solutions to larger and larger sub-problems.

Dynamic Programming History

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

Etymology.
- Dynamic programming = planning over time.
- Secretary of Defense 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"

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

Dynamic Programming Applications

Areas.
- Bioinformatics.
- Control theory.
- Information theory.
- Operations research.
- Computer science: theory, graphics, AI, systems, ….

Some famous dynamic programming algorithms.
- Unix diff for comparing two files.
- Viterbi for hidden Markov models.
- Smith-Waterman for sequence alignment.
- Bellman-Ford for shortest path routing in networks.
- Cocke-Kasami-Younger for parsing context free grammars.

6.1 Weighted Interval Scheduling

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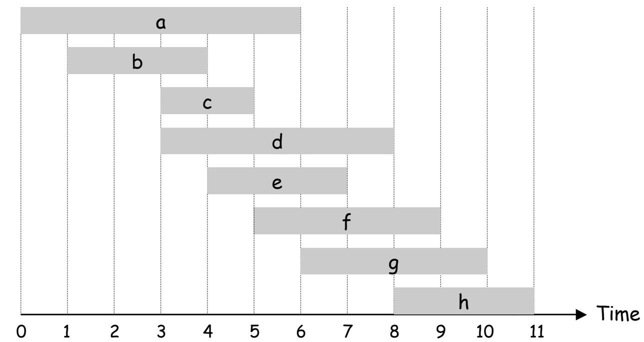
Weighted Interval Scheduling

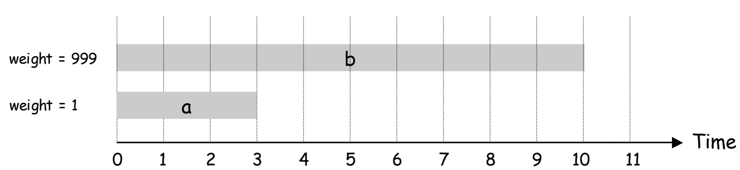
Weighted interval scheduling problem.
- Job j starts at s_j, finishes at f_j, and has weight or value v_j .
- Two jobs compatible if they don't overlap.
- Goal: find maximum weight subset of mutually compatible jobs.



Unweighted Interval Scheduling Review

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.

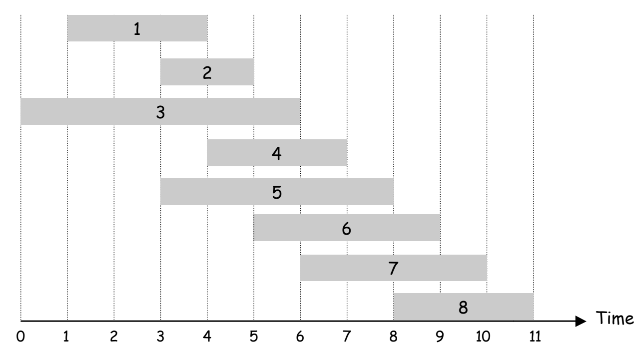
Observation. Greedy algorithm can fail spectacularly if arbitrary weights are allowed.



Weighted Interval Scheduling

Notation. Label jobs by finishing time: $f_1 \le f_2 \le \ldots \le f_n$.
Def. p(j) = largest index i < j such that job i is compatible with j.

Ex: p(8) = 5, p(7) = 3, p(2) = 0.



Dynamic Programming: Binary Choice

Notation. OPT(j) = value of optimal solution to the problem consisting of job requests 1, 2, ..., j.

- Case 1: OPT selects job j.
  - 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)

optimal substructure

- Case 2: OPT does not select job j.
  - must include optimal solution to problem consisting of remaining compatible jobs 1, 2, ..., j-1

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

Weighted Interval Scheduling: Brute Force

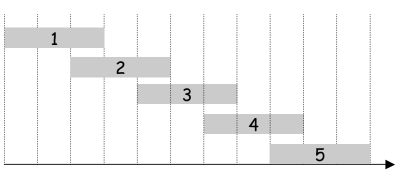
Brute force algorithm.

```
Input: n, s_1,…,s_n , f_1,…,f_n , v_1,…,v_n

Sort jobs by finish times so that f_1 ≤ f_2 ≤ ... ≤ f_n.

Compute p(1), p(2), …, p(n)

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

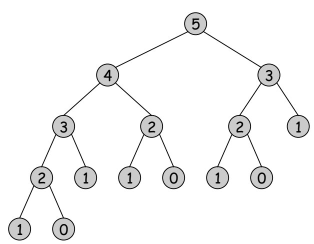

Weighted Interval Scheduling: Brute Force

Observation. Recursive algorithm fails spectacularly because of redundant sub-problems ⇒ exponential algorithms.

Ex. Number of recursive calls for family of "layered" instances grows like Fibonacci sequence.



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



Weighted Interval Scheduling: Memoization

Memoization. Store results of each sub-problem in a cache; lookup as needed.

```
Input: n, s_1,…,s_n , f_1,…,f_n , v_1,…,v_n

Sort jobs by finish times so that f_1 ≤ f_2 ≤ ... ≤ f_n.
Compute p(1), p(2), …, p(n)

for j = 1 to n
   M[j] = empty   ← global array
M[j] = 0

M-Compute-Opt(j) {
   if (M[j] is empty)
      M[j] = max(w_j + M-Compute-Opt(p(j)), M-Compute-Opt(j-1))
   return M[j]
}
```

Weighted Interval Scheduling: Running Time

Claim. Memoized version of algorithm takes O(n log n) time.

- Sort by finish time: O(n log n).
- Computing p(⋅) : O(n) after sorting by start time.

- `M-Compute-Opt(j)`: each invocation takes O(1) time and either
  - (i) returns an existing value `M[j]`
  - (ii) fills in one new entry `M[j]` and makes two recursive calls

- Progress measure Φ = # nonempty entries of `M[]`.
  - initially $\Phi = 0$, throughout $\Phi \leq n$.
  - (ii) increases Φ by 1 $\Rightarrow$ at most 2n recursive calls.

- Overall running time of `M-Compute-Opt(n)` is O(n). ▪

Remark. O(n) if jobs are pre-sorted by start and finish times.

Automated Memoization

Automated memoization. Many functional programming languages (e.g., Lisp) have built-in support for memoization.

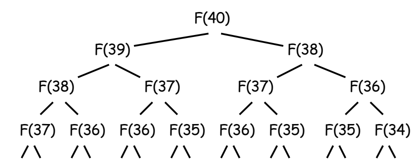
Q. Why not in imperative languages (e.g., Java)?

```
(defun F (n)
  (if
    (<= n 1)
    n
    (+ (F (- n 1)) (F (- n 2)))))
```

Lisp (efficient)

```
static int F(int n) {
   if (n <= 1) return n;
   else return F(n-1) + F(n-2);
}
```

Java (exponential)



Weighted Interval Scheduling: Finding a Solution

Q. Dynamic programming algorithms computes optimal value. What if we want the solution itself?
A. Do some post-processing.

```
Run M-Compute-Opt(n)
Run Find-Solution(n)

Find-Solution(j) {
   if (j = 0)
      output nothing
   else if (v_j + M[p(j)] > M[j-1])
      print j
      Find-Solution(p(j))
   else
      Find-Solution(j-1)
}
```

- # of recursive calls ≤ n $\Rightarrow$ O(n).

Weighted Interval Scheduling: Bottom-Up

Bottom-up dynamic programming. Unwind recursion.

```
Input: n, s_1,…,s_n , f_1,…,f_n , v_1,…,v_n

Sort jobs by finish times so that f_1 ≤ f_2 ≤ ... ≤ f_n.

Compute p(1), p(2), …, p(n)

Iterative-Compute-Opt {
   M[0] = 0
   for j = 1 to n
      M[j] = max(v_j + M[p(j)], M[j-1])
}
```

6.3 Segmented Least Squares

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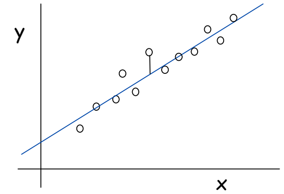
Segmented Least Squares

Least squares.

- Foundational problem in statistic and numerical analysis.
- 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 error:

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



Solution. Calculus ⇒ min error 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

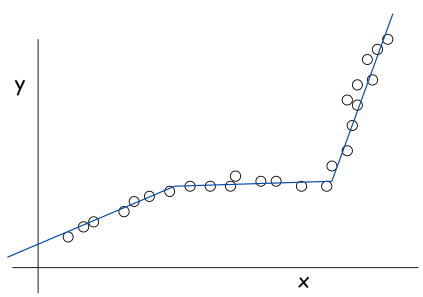
Segmented least squares.

- 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 f(x).

Q. What's a reasonable choice for f(x) to balance accuracy and parsimony?

goodness of fit

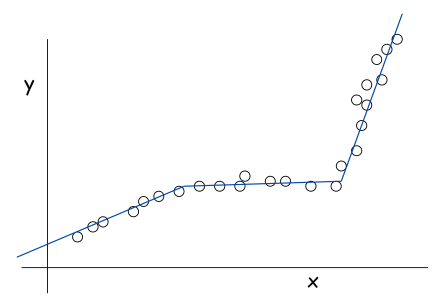
number of lines



Segmented Least Squares

Segmented least squares.

- 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:
  - the sum of the sums of the squared errors E in each segment
  - the number of lines L
- Tradeoff function: E + c L, for some constant c > 0.



Dynamic Programming: Multiway Choice

Notation.

- OPT(j) = minimum cost for points $p_1, p_{i+1}, \ldots, p_j$.
- e(i, j) = minimum sum of squares for points $p_i, p_{i+1}, \ldots, p_j$.

To compute OPT(j):

- Last segment uses points $p_i, p_{i+1}, \ldots, p_j$ for some i.
- Cost = e(i, j) + c + OPT(i-1).

$$OPT(j) = \begin{cases} 0 & \text{if } j = 0 \\ \min_{1 \le i \le j} \{ e(i,j) + c + OPT(i-1) \} & \text{otherwise} \end{cases}$$

Segmented Least Squares: Algorithm

```
INPUT: n, p1,…,pN , c

Segmented-Least-Squares() {
   M[0] = 0
   for j = 1 to n
      for i = 1 to j
         compute the least square error 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]
}
```

Running time. $O(n^3)$. can be improved to $O(n^2)$ by pre-computing various statistics

- Bottleneck = computing e(i, j) for $O(n^2)$ pairs, $O(n)$ per pair using previous formula.

6.4 Knapsack Problem

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Knapsack Problem

Knapsack problem.

- Given n objects and a "knapsack."
- Item i weighs $w_i > 0$ kilograms and has value $v_i > 0$.
- Knapsack has capacity of W kilograms.
- Goal: fill knapsack so as to maximize total value.

Ex: { 3, 4 } has value 40.

W = 11

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

Greedy: repeatedly add item with maximum ratio v_i / w_i.
Ex: { 5, 2, 1 } achieves only value = 35 $\Rightarrow$ greedy not optimal.

Dynamic Programming: False Start

Def. OPT(i) = max profit subset of items 1, …, i.

- Case 1: OPT does not select item i.
  - OPT selects best of { 1, 2, …, i-1 }
- Case 2: OPT selects item i.
  - accepting item i does not immediately imply that we will have to reject other items
  - without knowing what other items were selected before i, we don't even know if we have enough room for i

Conclusion. Need more sub-problems!

Dynamic Programming: Adding a New Variable

Def. OPT(i, w) = max profit subset of items 1, …, i with weight limit w.

- Case 1: OPT does not select item i.
  - OPT selects best of { 1, 2, …, i-1 } using weight limit w
- Case 2: OPT selects item i.
  - new weight limit = $w - w_i$
  - OPT selects best of { 1, 2, …, i-1 } using this new weight limit

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

Knapsack Problem: Bottom-Up

Knapsack. Fill up an n-by-W array.

```
Input: n, 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]
```


Knapsack Algorithm

W + 1 →

n + 1 ↓

	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, 2 }	0	1	6	7	7	7	7	7	7	7	7	7
{ 1, 2, 3 }	0	1	6	7	7	18	19	24	25	25	25	25
{ 1, 2, 3, 4 }	0	1	6	7	7	18	22	24	28	29	29	40
{ 1, 2, 3, 4, 5 }	0	1	6	7	7	18	22	28	29	34	34	40

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

W = 11

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

Knapsack Problem: Running Time

Running time. $\Theta(n\ W)$.
- Not polynomial in input size!
- "Pseudo-polynomial."
- Decision version of Knapsack is NP-complete. [Chapter 8]

Knapsack approximation algorithm. There exists a polynomial algorithm that produces a feasible solution that has value within 0.01% of optimum. [Section 11.8]

6.5 RNA Secondary Structure

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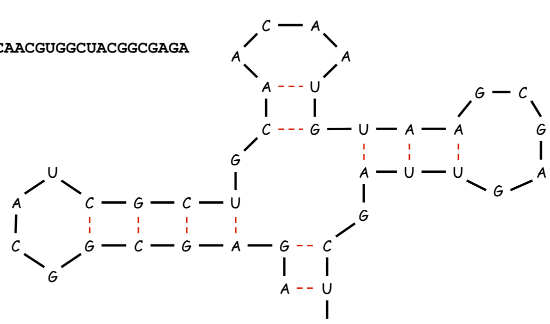
RNA Secondary Structure

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.

Ex: GUCGAUUGAGCGAAUGUAACAACGUGGCUACGGCGAGA



complementary base pairs: A-U, C-G

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 at least 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, then we cannot have $i < k < j < l$.

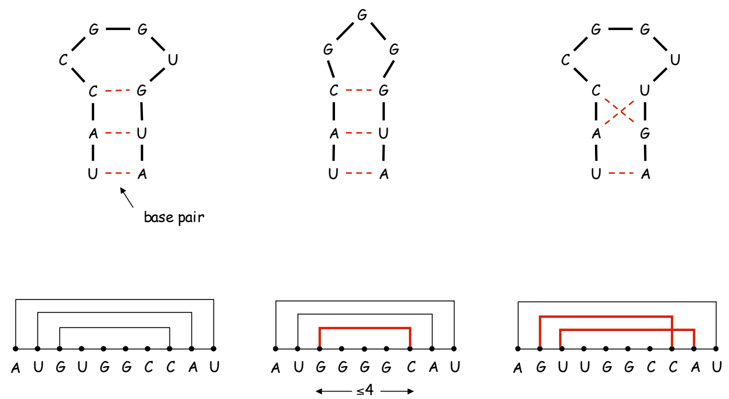
Free energy. Usual hypothesis is that an RNA molecule will form the secondary structure with the optimum total free energy.

approximate by number of base pairs

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.

RNA Secondary Structure: Examples

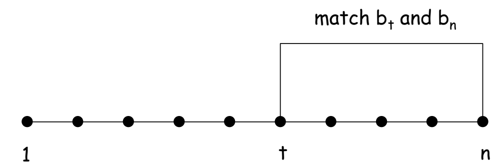
Examples.



ok   sharp turn   crossing

RNA Secondary Structure: Subproblems

First attempt. OPT(j) = maximum number of base pairs in a secondary structure of the substring $b_1 b_2 \ldots b_j$.



Difficulty. Results in two sub-problems.

- Finding secondary structure in: $b_1 b_2 \ldots b_{t-1}$. ← OPT(t-1)
- Finding secondary structure in: $b_{t+1} b_{t+2} \ldots b_{n-1}$. ← need more sub-problems

Dynamic Programming Over Intervals

Notation. OPT(i, j) = maximum number of base pairs in a secondary structure of the substring $b_i b_{i+1} \ldots b_j$.

- Case 1. If $i \geq j - 4$.
  - OPT(i, j) = 0 by no-sharp turns condition.

- Case 2. Base b_j is not involved in a pair.
  - OPT(i, j) = OPT(i, j-1)

- Case 3. Base b_j pairs with b_t for some $i \leq t < j - 4$.
  - non-crossing constraint decouples resulting sub-problems
  - $\text{OPT}(i, j) = 1 + \max_t \{ \text{OPT}(i, t-1) + \text{OPT}(t+1, j-1) \}$

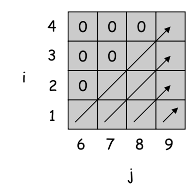
    take max over t such that $i \leq t < j-4$ and b_t and b_j are Watson-Crick complements

Remark. Same core idea in CKY algorithm to parse context-free grammars.

Bottom Up Dynamic Programming Over Intervals

Q. What order to solve the sub-problems?
A. Do shortest intervals first.

```
RNA(b1,…,bn) {
   for k = 5, 6, …, n-1
      for i = 1, 2, …, n-k
         j = i + k
         Compute M[i, j]
                         ↖ using recurrence
   return M[1, n]
}
```



Running time. $O(n^3)$.

Dynamic Programming Summary

Recipe.
- Characterize structure of problem.
- Recursively define value of optimal solution.
- Compute value of optimal solution.
- Construct optimal solution from computed information.

Dynamic programming techniques.
- Binary choice: weighted interval scheduling.
- Multi-way choice: segmented least squares.
- Adding a new variable: knapsack.
- Dynamic programming over intervals: RNA secondary structure.

Top-down vs. bottom-up: different people have different intuitions.

6.6 Sequence Alignment

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String Similarity

How similar are two strings?
- **ocurrance**
- **occurrence**

o	c	u	r	r	a	n	c	e	-
o	c	c	u	r	r	e	n	c	e

5 mismatches, 1 gap

o	c	-	u	r	r	a	n	c	e
o	c	c	u	r	r	e	n	c	e

1 mismatch, 1 gap

o	c	-	u	r	r	-	a	n	c	e
o	c	c	u	r	r	e	-	n	c	e

0 mismatches, 3 gaps

Edit Distance

Applications.
- Basis for Unix diff.
- Speech recognition.
- Computational biology.

Edit distance. [Levenshtein 1966, Needleman-Wunsch 1970, Smith-Waterman 1981]
- Gap penalty δ; mismatch penalty α_{pq}.
- Cost = sum of gap and mismatch penalties.

C	T	G	A	C	C	T	A	C	C	T
C	C	T	G	A	C	T	A	C	A	T

$\alpha_{TC} + \alpha_{GT} + \alpha_{AG} + 2\alpha_{CA}$

-	C	T	G	A	C	C	T	A	C	C	T
C	C	T	G	A	C	-	T	A	C	A	T

$2\delta + \alpha_{CA}$

Sequence Alignment

Goal: Given two strings $X = x_1\, x_2\, .\,.\,.\, x_m$ and $Y = y_1\, y_2\, .\,.\,.\, y_n$ find alignment of minimum cost.

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 no crossings.

Def. The pair x_i-y_j and $x_{i'}$-$y_{j'}$ cross if $i < i'$, but $j > j'$.

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

Ex: CTACCG vs. TACATG.
Sol: $M = x_2\text{-}y_1,\ x_3\text{-}y_2,\ x_4\text{-}y_3,\ x_5\text{-}y_4,\ x_6\text{-}y_6$.

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: Problem Structure

Def. $OPT(i, j)$ = min cost of aligning strings $x_1\, x_2\, .\,.\,.\, x_i$ and $y_1\, y_2\, .\,.\,.\, y_j$.

- Case 1: OPT matches x_i-y_j.
  - pay mismatch for x_i-y_j + min cost of aligning two strings $x_1\, x_2\, .\,.\,.\, x_{i-1}$ and $y_1\, y_2\, .\,.\,.\, y_{j-1}$
- Case 2a: OPT leaves x_i unmatched.
  - pay gap for x_i and min cost of aligning $x_1\, x_2\, .\,.\,.\, x_{i-1}$ and $y_1\, y_2\, .\,.\,.\, y_j$
- Case 2b: OPT leaves y_j unmatched.
  - pay gap for y_j and min cost of aligning $x_1\, x_2\, .\,.\,.\, x_i$ and $y_1\, y_2\, .\,.\,.\, y_{j-1}$

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

Sequence Alignment: Algorithm

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

Analysis. $\Theta(mn)$ time and space.
English words or sentences: $m, n \le 10$.
Computational biology: $m = n = 100{,}000$. 10 billions ops OK, but 10GB array?

6.7 Sequence Alignment in Linear Space

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Sequence Alignment: Linear Space

Q. Can we avoid using quadratic space?

Easy. Optimal value in O(m + n) space and O(mn) time.

- Compute OPT(i, •) from OPT(i-1, •).
- No longer a simple way to recover alignment itself.

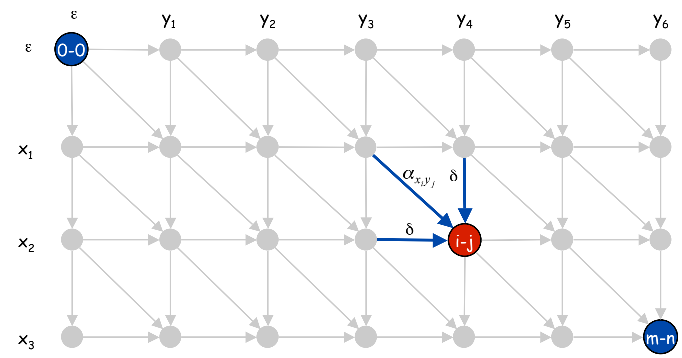
Theorem. [Hirschberg, 1975] Optimal alignment in O(m + n) space and O(mn) time.

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

Sequence Alignment: Linear Space

Edit distance graph.

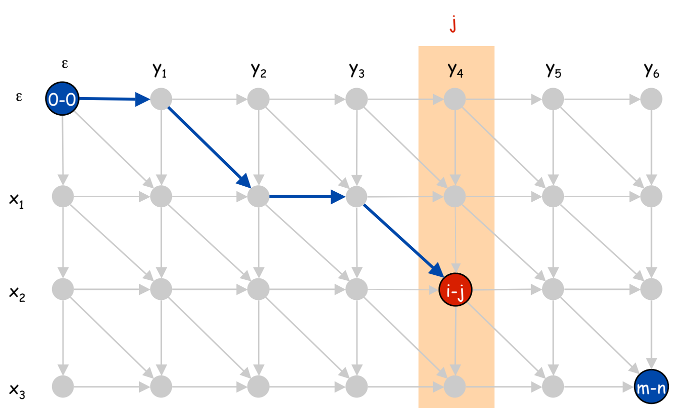
- Let f(i, j) be shortest path from (0,0) to (i, j).
- Observation: f(i, j) = OPT(i, j).



Sequence Alignment: Linear Space

Edit distance graph.

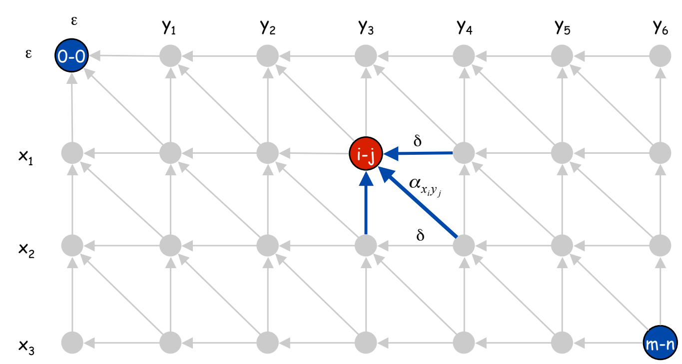
- Let f(i, j) be shortest path from (0,0) to (i, j).
- Can compute f (•, j) for any j in O(mn) time and O(m + n) space.



Sequence Alignment: Linear Space

Edit distance graph.

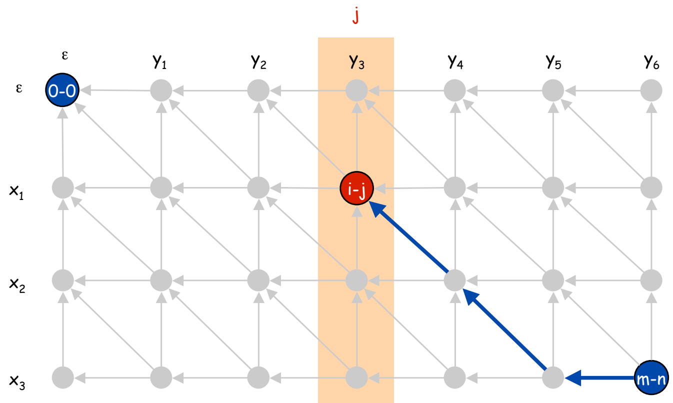
- Let g(i, j) be shortest path from (i, j) to (m, n).
- Can compute by reversing the edge orientations and inverting the roles of (0, 0) and (m, n)



Sequence Alignment: Linear Space

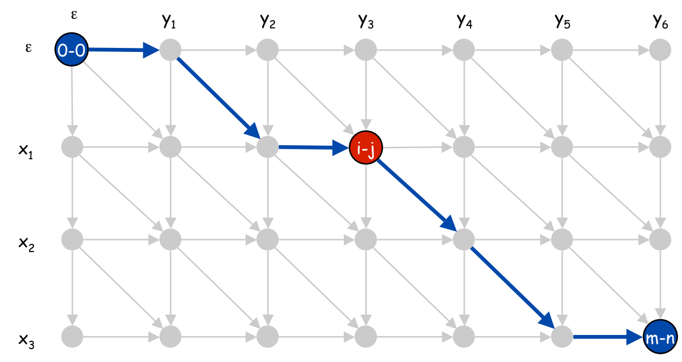
Edit distance graph.

- Let $g(i, j)$ be shortest path from (i, j) to (m, n).
- Can compute $g(\bullet, j)$ for any j in $O(mn)$ time and $O(m + n)$ space.



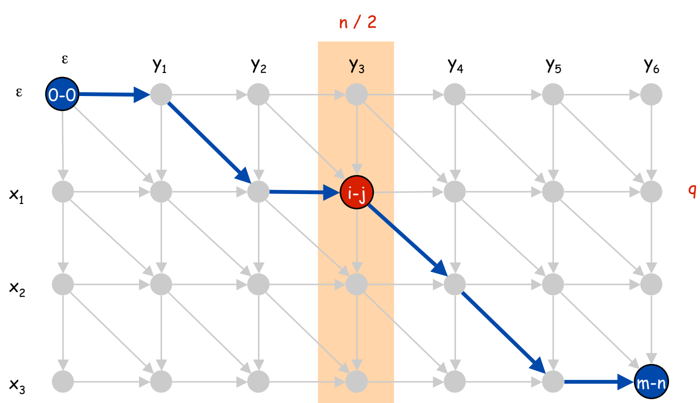
Sequence Alignment: Linear Space

Observation 1. The cost of the shortest path that uses (i, j) is $f(i, j) + g(i, j)$.



Sequence Alignment: Linear Space

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

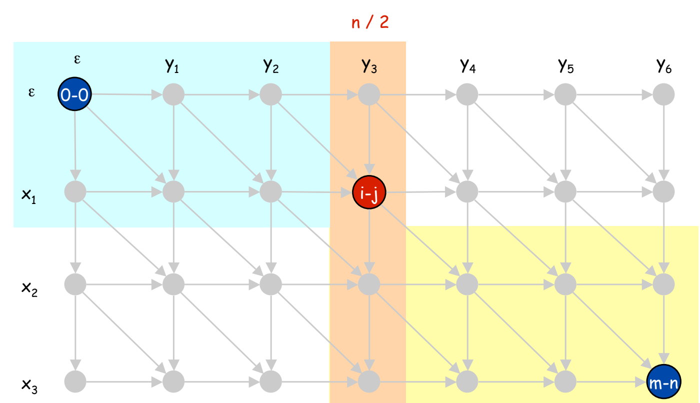


Sequence Alignment: Linear Space

Divide: find index q that minimizes $f(q, n/2) + g(q, n/2)$ using DP.

- Align x_q and $y_{n/2}$.

Conquer: recursively compute optimal alignment in each piece.



Sequence Alignment: Running Time Analysis Warmup

Theorem. Let T(m, n) = max running time of algorithm on strings of length at most m and n. T(m, n) = O(mn log 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 sub-problems are of size (q, n/2) and (m - q, n/2). In next slide, we save log n factor.

Sequence Alignment: Running Time Analysis

Theorem. Let T(m, n) = max running time of algorithm on strings of length m and n. T(m, n) = O(mn).

Pf. (by induction on n)

- O(mn) time to compute f(•, n/2) and g (•, 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:

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

- Base cases: m = 2 or n = 2.
- Inductive hypothesis: T(m, n) ≤ 2cmn.

$$\begin{aligned} T(m,n) &\le T(q,n/2) + T(m-q,n/2) + cmn \\ &\le 2cqn/2 + 2c(m-q)n/2 + cmn \\ &= cqn + cmn - cqn + cmn \\ &= 2cmn \end{aligned}$$