Dynamic Programming*

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Algorithm Course: Shanghai Jiao Tong University

Algorithm Course @ SJTU Xiaofeng Gao Dynamic Programming 1/56

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Outline

- Introduction
 - Introduction
- 2 Basic Methodology
 - Weighted Interval Scheduling
 - Segmented Least Squares
 - Knapsack Problem
- More Examples
 - RNA Secondary Structure
 - String Similarity
 - Sequence Alignment in Linear Space



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Algorithmic Paradigms

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

Divide-and-conquer: Break up a problem into 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 Applications

Areas

- Bioinformatics.
- Control theory.
- Information theory.
- Operations research.
- o Computer science: theory, graphics, AI, compilers, systems, ...

Some famous dynamic programming algorithms

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

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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.

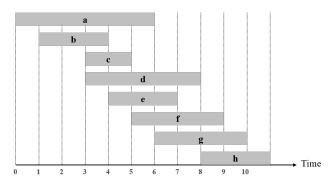
Goal: find maximum weight subset of mutually compatible jobs.

Weighted Interval Scheduling Problem

Job j starts at s_j , finishes at f_j , and has weight or value v_j .

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Unweighted Interval Scheduling Review

Recall: Greedy algorithm works if all weights are 1.

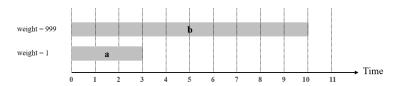
- o Consider jobs in ascending order of finish time.
- Add job to subset if it is compatible with previously chosen jobs.

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: $f_1 \le f_2 \le \cdots \le f_n$.

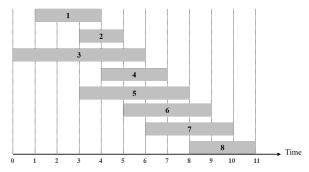
Definition: p(j) = largest index i < j such that job i is compatible with j.

Weighted Interval Scheduling

Notation: Label jobs by finishing time: $f_1 \le f_2 \le \cdots \le f_n$.

Definition: p(j) = largest index i < j such that job i is compatible with j.

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



Algorithm Course@SJTU

Binary Choice

Greedy template: OPT(j) = value of optimal solution to the problem consisting of job requests $1, 2, \dots, j$.

Optimal substructure:

Case 1: OPT selects job *j*.

- collect profit v_j
- o can't use incompatible jobs $\{p(j) + 1, p(j) + 2, \dots, j 1\}$
- must include optimal solution to problem consisting of remaining compatible jobs $1, 2, \dots, p(j)$

Case 2: OPT does not select job *j*.

• must include optimal solution to problem consisting of remaining compatible jobs $1, 2, \dots, j-1$

Binary Choice

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Case 2: OPT does not select job *j*.

• must include optimal solution to problem consisting of remaining compatible jobs $1, 2, \dots, j-1$

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



Brute Force Algorithm

Algorithm 1: Brute Force **Input:** n; s_1, \dots, s_n ; f_1, \dots, f_n ; v_1, \dots, v_n ; **Sort** jobs by finish times so that $f_1 < f_2 < \cdots < f_n$; Compute $p(1), p(2), \cdots, p(n)$; Function Compute-Opt (i): if i=0 then return 0; else return $\max\{v_i + \text{Compute-Opt}(p(j)), \text{Compute-Opt}(j-1)\};$

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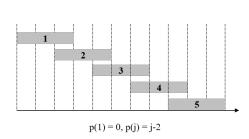
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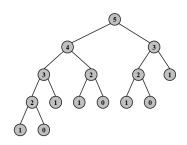
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Brute Force Algorithm

Observation: Recursive algorithm fails spectacularly because of redundant sub-problems \Rightarrow exponential algorithms.

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





Memoization

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

Algorithm 2: Memoization

```
Input: n; s_1, \dots, s_n; f_1, \dots, f_n; v_1, \dots, v_n
   Sort jobs by finish times so that f_1 < f_2 < \cdots < f_n;
2 Compute p(1), p(2), \dots, p(n);
3 for j = 1 \rightarrow n do
   M[j] = \text{empty};
M[0] = 0;
   Function M-Compute-Opt (i):
       if M[i] is empty then
           M[j] =
 8
              \max\{v_i + \text{M-Compute-Opt}(p(j)), \text{M-Compute-Opt}(j-1)\};
 9
       return M[i];
10
```

Running Time

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

- Sort by finish time: $O(n \log n)$.
- Computing $p(\cdot)$: $O(n \log n)$ via sorting by start time.
- M-Compute-Opt(j): each invocation takes O(1) time and either
 - \triangleright returns an existing value M[j]
 - \triangleright fills in one new entry M[j] and makes two recursive calls
- Progress measure $\Phi =$ number nonempty entries of $M[\cdot]$.
 - \triangleright initially $\Phi = 0$, throughout $\Phi \le n$.
 - \triangleright 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.



Finding a Solution from the OPT Value

```
Algorithm 3: Post-Processing

Run M-Compute-Opt(n);

Run Find-Solution(n);

Function Find-Solution (j):

if j = 0 then

output nothing;

else if v_j + M[p(j)] > M[j-1] then

print j;

Find-Solution (p(j));
```

Find-Solution(j-1);

```
• # of recursive calls 1 \le n \Rightarrow O(n);
```



10

Bottom-Up Dynamic Programming

Algorithm 4: Memoization

```
Input: n; s_1, \dots, s_n; f_1, \dots, f_n; v_1, \dots, v_n

1 Sort jobs by finish times so that f_1 \leq f_2 \leq \dots \leq f_n;

2 Compute p(1), p(2), \dots, p(n);

3 Function Iterative-Compute-Opt():

4 | M[0] = 0;

5 | for j = 1 \rightarrow n do

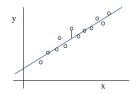
6 | M[j] = \max\{v_j + M[p(j)], M[j-1]\};
```

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- Foundational problem in statistic and numerical analysis.
- Given *n* points in the plane: $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$.
- \circ Find a line y = ax + b to minimize the sum of the squared error:



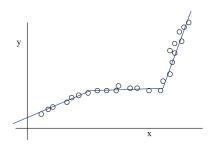
Solution: Calculus \Rightarrow min error is achieved when

$$a = \frac{n \sum_{i} x_{i} y_{i} - (\sum_{i} x_{i})(\sum_{i} y_{i})}{n \sum_{i} x_{i}^{2} - (\sum_{i} x_{i})^{2}}, b = \frac{\sum_{i} y_{i} - a \sum_{i} x_{i}}{n}$$

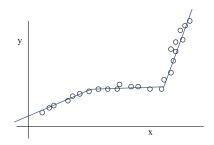


- Points lie roughly on a sequence of several line segments.
- Given *n* points in the plane: (x_1, y_1) , (x_2, y_2) , \cdots , (x_n, y_n) with $x_1 < x_2 < \cdots < x_n$, find a sequence of lines that minimizes f(x).

Question: What's a reasonable choice for f(x) to balance accuracy (goodness of fit) and parsimony (number of lines)?



- Points lie roughly on a sequence of several line segments.
- Given *n* points in the plane: $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ with $x_1 < x_2 < \dots < x_n$, find a sequence of lines that minimizes:
 - \triangleright the sum of the sums of the squared errors E in each segment
 - \triangleright the number of lines L
- Tradeoff function: E + cL, for some constant c > 0.



Multiway Choice

Notation:

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

Compute OPT(j):

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

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

Algorithm 5: Memoization

```
Input: n; p_1, \dots, p_N; c

1 Function Iterative-Compute-Opt():

2 M[0] = 0;

3 \text{for } j = 1 \rightarrow n \text{ do}

4 \text{for } i = 1 \rightarrow j \text{ do}

5 \text{compute the least square error } e_{ij} \text{ for the segment}

6 \text{for } j = 1 \rightarrow n \text{ do}

7 M[j] = \min_{1 \leq i \leq j} \{e_{ij} + c + M[i - 1]\};

8 \text{return } M[n];
```

Algorithm 6: Memoization

```
Input: n; p_1, \cdots, p_N; c

1 Function Iterative-Compute-Opt():

2 M[0] = 0;

3 \mathbf{for} \ j = 1 \rightarrow n \ \mathbf{do}

4 \mathbf{for} \ i = 1 \rightarrow j \ \mathbf{do}

5 \mathbf{compute} \ \text{the least square error} \ e_{ij} \ \text{for the segment}

6 \mathbf{for} \ j = 1 \rightarrow n \ \mathbf{do}

7 \mathbf{M}[j] = \min_{1 \leq i \leq j} \{e_{ij} + c + M[i-1]\};

8 \mathbf{return} \ M[n];
```

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

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

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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.

Knapsack Problem

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Example: $\{3,4\}$ has value 40.

_		
	W = 11	

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

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Example: $\{3,4\}$ has value 40.

W = 11

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1	1	1
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3	18	5
4	22	6
5	28	7

Greedy: repeatedly add item with maximum ratio v_i/w_i .

Example: $\{5, 2, 1\}$ achieves only value = $35 \Rightarrow$ greedy not optimal.

False Start

Definiton: $OPT(i) = \max \text{ profit subset of items } 1, \dots, i.$

Case 1: OPT does not select item i.

• OPT selects best of $\{1, 2, \dots, i-1\}$

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!

Adding a New Variable

Definiton: $OPT(i) = \max \text{ profit subset of items } 1, \dots, i \text{ with weight limit } w.$

Case 1: OPT does not select item i.

• OPT selects best of $\{1, 2, \dots, i-1\}$ using weight limit w

Case 2: OPT selects item i.

- new weight $limit = w w_i$
- OPT selects best of using $\{1, 2, \dots, i-1\}$ this new weight limit

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

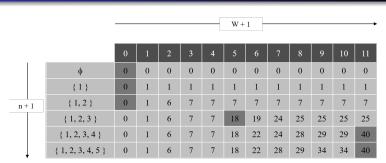
Bottom-Up Algorithm (Fill up an *n*-by-*W* array)

Algorithm 7: Knapsack Problem Algorithm using *n*-by-*W* Array

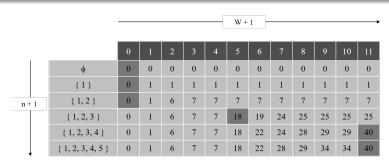
```
Input: n, W, w_1, \cdots, w_N, v_1, \cdots, v_N
1 for w = 0 \rightarrow W do
 M[0, w] = 0;
3 for i=1 \rightarrow n do
      for w = 1 \rightarrow W do
5
         if w_i > w then
          M[i, w] = M[i - 1, w];
6
          else
             M[i, w] = \max\{M[i-1, w], v_i + M[i-1, w-w_i]\} 
8
```

9 return M[n, W];

Knapsack Algorithm



Knapsack Algorithm



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

Running Time

Running time: $\Theta(nW)$.

- Not polynomial in input size!
- "Pseudo-polynomial".
- o Decision version of Knapsack is NP-complete.

Knapsack approximation algorithm: There exists a poly-time algorithm that produces a feasible solution that has value within 0.01% of optimum.

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RNA Secondary Structure

RNA:String $B = b_1 b_2 \cdots b_n$ 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.

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.

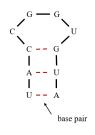
[No sharp turns.] The ends of each pair are separated by at least 4 intervening bases. If $(b_i, b_j) \in S$, then i < j - 4.

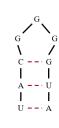
[Non-crossing.] If (b_i, b_j) and (b_k, b_l) are two pairs in S, then we cannot have i < k < j < l.

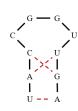
Free energy: Usual hypothesis is that an RNA molecule will form the secondary structure with the optimum total free energy.

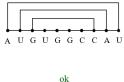
Goal: Given an RNA molecule $B = b_1 b_2 \cdots b_n$, find a secondary structure S that maximizes the number of base pairs

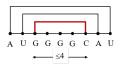
Examples

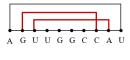










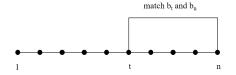


sharp turn

crossing

Subproblems

First attempt: $OPT(j) = \text{maximum number of base pairs in a secondary structure of the substring <math>b_1b_2 \cdots b_j$.



Difficulty: Results in two sub-problems.

- Finding secondary structure in: $b_1b_2 \cdots b_{t-1}$.
- Finding secondary structure in: $b_{t+1}b_{t+2}\cdots b_{n-1}$.

Dynamic Programming Over Intervals

Notation: $OPT(j) = \text{maximum number of base pairs in a secondary structure of the substring <math>b_i b_{i+1} \cdots b_j$.

- Case 1: If $i \ge j 4$.
 - OPT(i,j) = 0 by no-sharp turns condition.
- Case 2: Base b_i is not involved in a pair.
 - \circ OPT(i,j) = OPT(i,j-1)
- Case 3: Base b_j pairs with b_t for some $i \le t < j 4$.
 - o non-crossing constraint decouples resulting sub-problems
 - $\circ OPT(i,j) = 1 + \max_{t} \{ OPT(i,t-1) + OPT(t+1,j-1) \}$

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



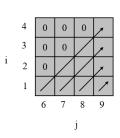
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Bottom Up Dynamic Programming Over Intervals

Question: What order to solve the sub-problems?

Answer: Do shortest intervals first.

```
RNA(b_{1},...,b_{n}) \{
for k = 5, 6, ..., n-1
for i = 1, 2, ..., n-k
j = i + k
Compute M[i, j]
return M[1, n]
using recurrence
\}
```



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

Dynamic Programming Summary

Recipe

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

Dynamic programming techniques

- o Binary choice: weighted interval scheduling.
- o Multi-way choice: segmented least squares.]
- Adding a new variable: knapsack.
- Dynamic programming over interval

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



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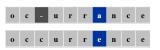
String Similarity: How similar are two strings?

							-
o c c	u	r	r	e	n	c	e

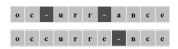
6 mismatches, 1 gap

How similar are two strings?

- ocurrance
- occurrence



1 mismatch, 1 gap



0 mismatches, 3 gaps



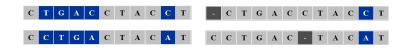
Edit Distance

Applications.

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

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

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



Sequence Alignment

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

Definiton: 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.

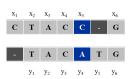
Definiton: The pair $x_i - y_j$ and $x_{i'} - y_{j'}$ cross if i < i', but j > j'.

$$M = \sum_{\substack{(x_i, y_j) \in M \\ \uparrow \\ \text{mismatch}}} \alpha_{x_i y_j} + \sum_{i: x_i \text{ unmatched}} \delta + \sum_{j: y_j \text{unmatched}} \delta$$

Example: CTACCG vs. TACATG.

Solution:
$$M = x_2 - y_1, x_3 - y_2, x_4 - y_3, x_5 - y_5$$

$$y_4, x_6 - y_6$$
.



Problem Structure

```
Definiton: OPT(i, j) = \min \text{ cost of aligning strings } x_1 x_2 \cdots x_i \text{ and } y_1 y_2 \cdots y_j.
```

Case 1: OPT matches $x_i - y_j$.

pay mismatch for $x_i - y_j$ + min cost of aligning two strings

$$x_1x_2\cdots x_{i-1}$$
 and $y_1y_2\cdots y_{j-1}$

Case 2a: OPT leaves x_i unmatched.

pay gap for x_i and min cost of aligning $x_1x_2 \cdots x_{i-1}$ and $y_1y_2 \cdots y_j$

Case 2b: OPT leaves y_j unmatched.

pay gap for y_j and min cost of aligning $x_1x_2 \cdots x_i$ and $y_1y_2 \cdots y_{j-1}$

Sequence Alignment

Algorithm 8: Sequence Alignment

1 Function

```
Sequence-Alignment (m, n, x_1x_2 \cdots x_m, y_1y_2 \cdots y_n, \beta, \alpha):
       for i = 0 \rightarrow m do
       M[i,0]=i\delta
3
       for i = 0 \rightarrow n do
4
       M[0,j]=j\delta
5
       for i = 1 \rightarrow m do
6
           for i = 1 \rightarrow n do
                M[i,j] = min(\alpha[x_i,y_j] + M[i-1,j-1],
8
                \delta + M[i-1,j], \delta + M[i,j-1]
       return M[m, n];
9
```

Sequence Alignment

Algorithm 9: Sequence Alignment

1 Function

```
Sequence-Alignment (m, n, x_1x_2 \cdots x_m, y_1y_2 \cdots y_n, \beta, \alpha):
       for i = 0 \rightarrow m do
       M[i,0] = i\delta
3
       for i = 0 \rightarrow n do
4
       M[0,j]=j\delta
5
       for i = 1 \rightarrow m do
6
           for i = 1 \rightarrow n do
               M[i,j] = min(\alpha[x_i,y_i] + M[i-1,j-1],
8
               \delta + M[i-1,j], \delta + M[i,j-1]
       return M[m, n];
9
```

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?

Outline

- Introduction
 - Introduction
- 2 Basic Methodology
 - Weighted Interval Scheduling
 - Segmented Least Squares
 - Knapsack Problem
- More Examples
 - RNA Secondary Structure
 - String Similarity
 - Sequence Alignment in Linear Space

Linear Space

Question: 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.

Linear Space

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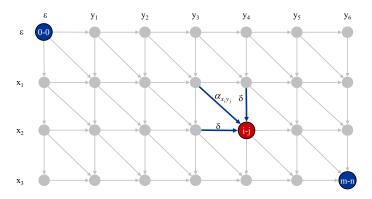
Theorem. [Hirschberg 1975] Optimal alignment in O(m+n) space and O(mn) time.

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

Programming Community Space Algorithm for Computing Maximal Common Subsequences D.S. Hinchberg Princeton University

The problem of finding a began common auto-quant of the origing has been subset in quadratic fine and space. An algorithm is premained which will subsequence from strings have been subset in quadratic fine and space. An algorithm is premained which will subsequence from strings have made to the subsequence from the problem of the subsequence from the subsequence of the strings of the subsequence of the strings of the subsequence of the subsequ

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



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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.

Induction: Last edge on shortest path to (i,j) is from (i-1,j-1), (i-1,j), or (i,j-1).

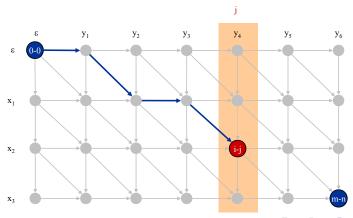
$$f(i,j) = \min\{a_{x_i y_i} + f(i-1,j-1), \delta + f(i-1,j), \delta + f(i,j-1)\}$$

$$= \min\{a_{x_i y_i} + OPT(i-1,j-1), \delta + OPT(i-1,j), \delta + OPT(i,j-1)\}$$

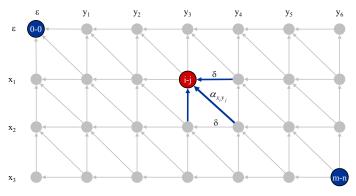
$$= OPT(i,j)$$



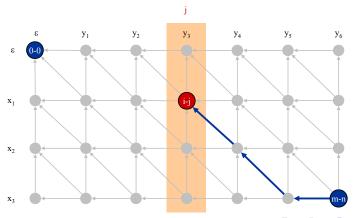
- \circ Let f(i,j) be shortest path from (0,0) to (i,j).
- Can compute f(*,j) for any j in O(mn) time and O(m+n) space.



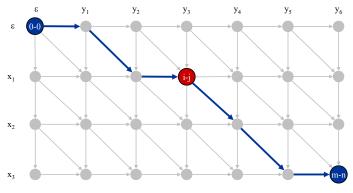
- Let g(i,j) be shortest path from (i,j) to (m,n).
- Can compute by reversing the edge orientations and inverting the roles of (0,0) and (m,n)



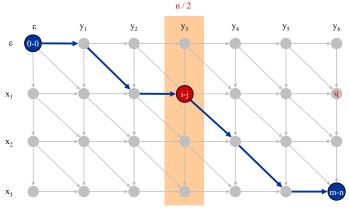
- Let g(i,j) be shortest path from (i,j) to (m,n).
- Can compute g(*,j) for any j in O(mn) time and O(m+n) space.



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

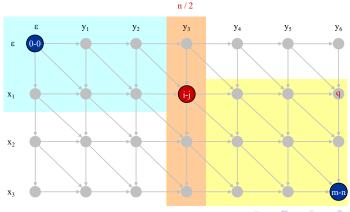


Observation 2: Let q be an index that minimizes f(q, n/2) + g(q, n/2). Then, the shortest path from (0, 0) to (m, n) uses (q, n/2).



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.



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.

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)

Proof: (by induction on n)

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

$$T(m,2) \le cm$$

 $T(2,n) \le cn$

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

Running Time Analysis (Continued)

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

Proof:

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

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

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

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

$$= 2cmn$$