Algorithm Design and Analysis (V)

Sequence Alignment

Guoqiang Li
School of Computer Science

Shanghai Jiao Tong University

Shortest Paths in DAGs, Revisited

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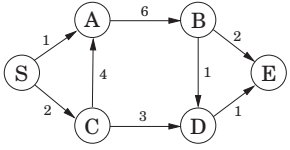

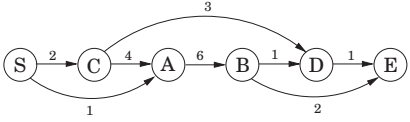

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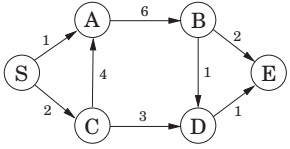

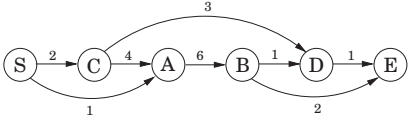

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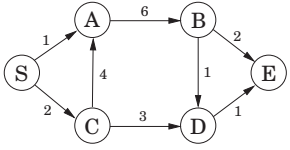

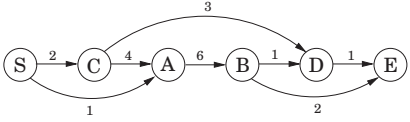

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If compute `dist` values in the left-to-right order, we can always be sure that by the time we get to a node v, all the information we need is prepared to compute `dist`(v).

Shortest Paths in DAGs, Revisited

Initialize all `dist`(.) value to ∞;
`dist`(s)=0;
for *each* $v \in V \backslash \{s\}$, *in linearized order* **do**
  `dist`(v) $= min_{(u,v) \in E}$\{`dist`(u) $+ l(u, v)$\};
end

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In dynamic programming we are given a DAG implicitly.

Longest Increasing Subsequences

Longest Increasing Subsequences

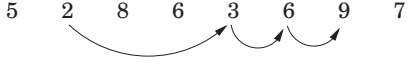
The input of longest increasing subsequence problem, is a sequence of numbers $a_1, \ldots, a_n$.

A subsequence is any subset of these numbers taken in order, of the form

$$a_{i_1}, a_{i_2}, \ldots, a_{i_k}$$

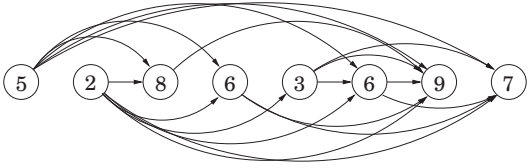
where $1 \leq i_1 < i_2 < \ldots < i_k \leq n$, and an increasing subsequence is one in which the numbers are getting strictly larger.

The task is to find the increasing subsequence of greatest length.



A graph of all permissible transitions:

- A node i for each element a_i,
- Directed edges (i, j) whenever it is possible for a_i and a_j to be consecutive elements:$i < j$ and $a_i < a_j$



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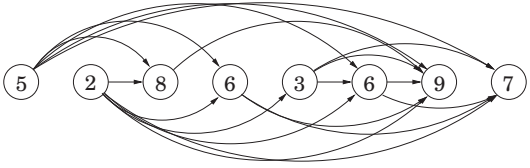

- This graph $G = (V, E)$ is a DAG, since all edges (i, j) have $i < j$
- There is a one-to-one correspondence between increasing subsequences and paths in this DAG.

The Algorithm

for $j = 1$ *to* n **do**
  $L(j) = 1 + \max\{L(i) \mid (i,j) \in E\}$;
end
`return(`$\max_j L(j)$`);`

Sequence Alignment

String Similarity

Q. How similar are two strings?

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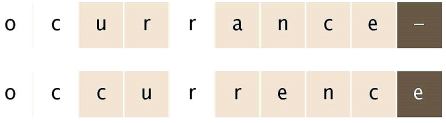
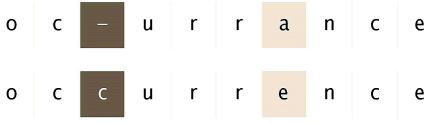
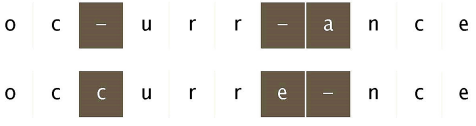


6 mismatches, 1 gap



1 mismatch, 1 gap



0 mismatches, 3 gaps

Edit Distance

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

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

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Example.

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

BLOSUM Matrix for Proteins

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	A	R	N	D	C	Q	E	G	H	I	L	K	M	F	P	S	T	W	Y	V
A	7	-3	-3	-3	-1	-2	-2	0	-3	-3	-3	-1	-2	-4	-1	2	0	-5	-4	-1
R	-3	9	-1	-3	-6	1	-1	-4	0	-5	-4	3	-3	-5	-3	-2	-2	-5	-4	-4
N	-3	-1	9	2	-5	0	-1	-1	1	-6	-6	0	-4	-6	-4	1	0	-7	-4	-5
D	-3	-3	2	10	-7	-1	2	-3	-2	-7	-7	-2	-6	-6	-3	-1	-2	-8	-6	-6
C	-1	-6	-5	-7	13	-5	-7	-6	-7	-2	-3	-6	-3	-4	-6	-2	-2	-5	-5	-2
Q	-2	1	0	-1	-5	9	3	-4	1	-5	-4	2	-1	-5	-3	-1	-1	-4	-3	-4
E	-2	-1	-1	2	-7	3	8	-4	0	-6	-6	1	-4	-6	-2	-1	-2	-6	-5	-4
G	0	-4	-1	-3	-6	-4	-4	9	-4	-7	-7	-3	-5	-6	-5	-1	-3	-6	-6	-6
H	-3	0	1	-2	-7	1	0	-4	12	-6	-5	-1	-4	-2	-4	-2	-3	-4	3	-5
I	-3	-5	-6	-7	-2	-5	-6	-7	-6	7	2	-5	2	-1	-5	-4	-2	-5	-3	4
L	-3	-4	-6	-7	-3	-4	-6	-7	-5	2	6	-4	3	0	-5	-4	-3	-4	-2	1
K	-1	3	0	-2	-6	2	1	-3	-1	-5	-4	8	-3	-5	-2	-1	-1	-6	-4	-4
M	-2	-3	-4	-6	-3	-1	-4	-5	-4	2	3	-3	9	0	-4	-3	-1	-3	-3	1
F	-4	-5	-6	-6	-4	-5	-6	-6	-2	-1	0	-5	0	10	-6	-4	-4	0	4	-2
P	-1	-3	-4	-3	-6	-3	-2	-5	-4	-5	-5	-2	-4	-6	12	-2	-3	-7	-6	-4
S	2	-2	1	-1	-2	-1	-1	-1	-2	-4	-4	-1	-3	-4	-2	7	2	-6	-3	-3
T	0	-2	0	-2	-2	-1	-2	-3	-3	-2	-3	-1	-1	-4	-3	2	8	-5	-3	0
W	-5	-5	-7	-8	-5	-4	-6	-6	-4	-5	-4	-6	-3	0	-7	-6	-5	16	3	-5
Y	-4	-4	-4	-6	-5	-3	-5	-6	3	-3	-2	-4	-3	4	-6	-3	-3	3	11	-3
V	-1	-4	-5	-6	-2	-4	-4	-6	-5	4	1	-4	1	-2	-4	-3	0	-5	-3	7

What is edit distance between these two strings?

P A L E T T E P A L A T E

Assume gap penalty $= 2$ and mismatch penalty $= 1$.

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

Merging

Goal. Given two strings $x_1 x_2 \dots x_m$ and $y_1 y_2 \dots y_n$, find a min-cost alignment.

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

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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

an alignment of CTACCG and TACATG

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

Sequence Alignment: Problem Structure

Definition $OPT(i, j)$: min cost of aligning prefix strings $x_1 x_2 \dots x_i$ and $y_1 y_2 \dots y_j$.

Goal. $OPT(m, n)$.

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Case 1. $OPT(i, j)$ matches $x_i - y_j$.
Pay mismatch for $x_i - y_j$ + min cost of aligning $x_1 x_2 \dots x_{i-1}$ and $y_1 y_2 ... y_{j-1}$.

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Case 2b. $OPT(i, j)$ leaves y_j unmatched.
Pay gap for y_j+ min cost of aligning $x_1 x_2 ... x_i$ and $y_1 y_2 \dots y_{j-1}$.

Bellman equation.

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

Sequence Alignment: Algorithm

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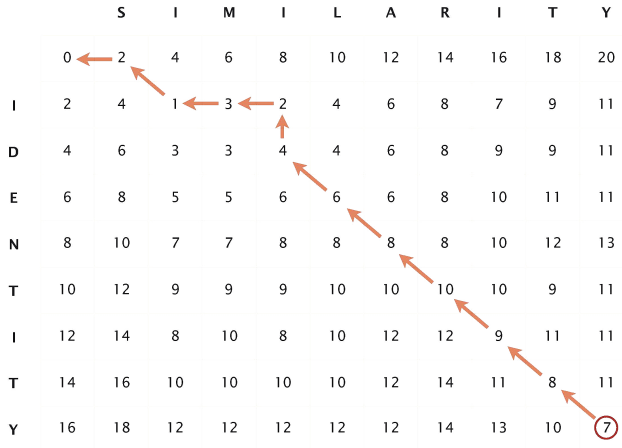
SequenceAlignment$(m, n, x_1, \ldots, x_m, y_1, \ldots, y_n, \delta, \alpha)$

for $i = 0$ *to* m **do**
  $M[i, 0] \leftarrow i\delta$;
end
for $j = 0$ *to* n **do**
  $M[0, j] \leftarrow j\delta$;
end
for $i = 1$ *to* m **do**
  for $j = 1$ *to* n **do**
    $M[i, j] \leftarrow \min\{\alpha_{x_i y_j} + M[i-1, j-1], \delta + M[i-1, j], \delta + M[i, j-1]\}$;
  end
end
Return $M[m, n]$;

Sequence Alignment: Traceback



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Proof.

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

Hirschberg's Algorithm

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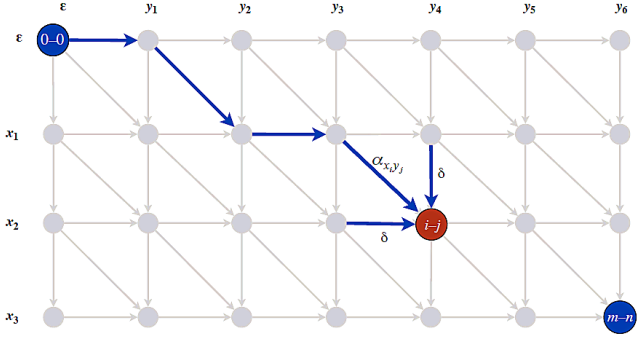
- Clever combination of divide-and-conquer and dynamic programming.
- Inspired by idea of Savitch from complexity theory.

Edit distance graph.

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



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- Thus,

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

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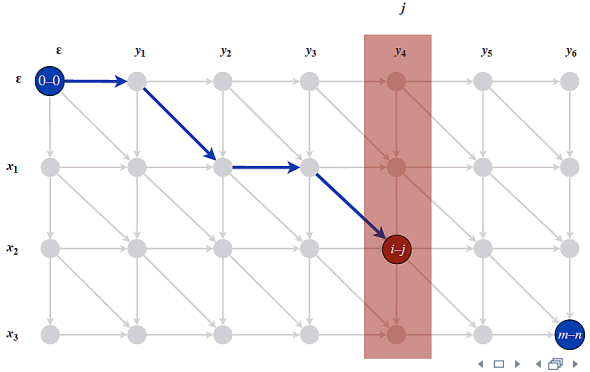
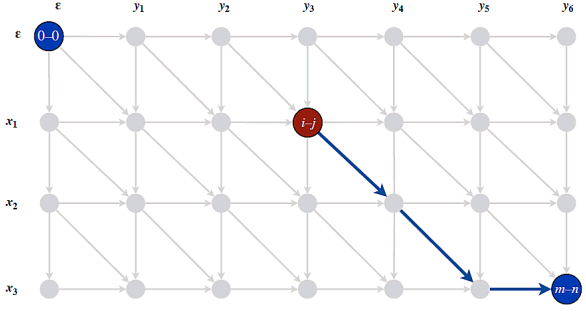
- Lemma: $f(i, j) = OPT(i, j)$ for all i and j.
- Can compute $f(\cdot, j)$ for any j in $O(mn)$ time and $O(m + n)$ space.



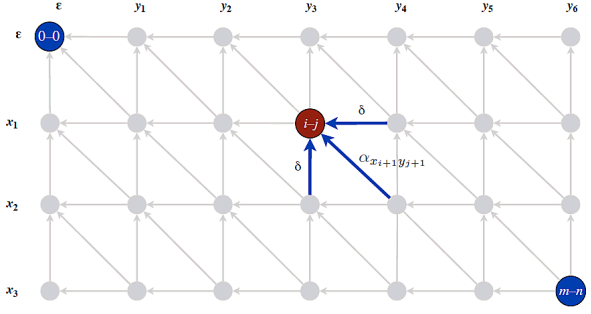
Edit distance graph.

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



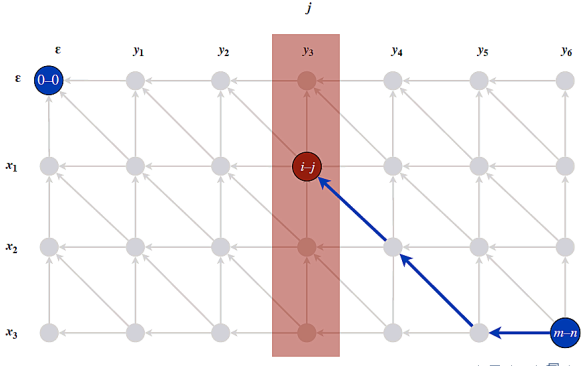
Edit distance graph.

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

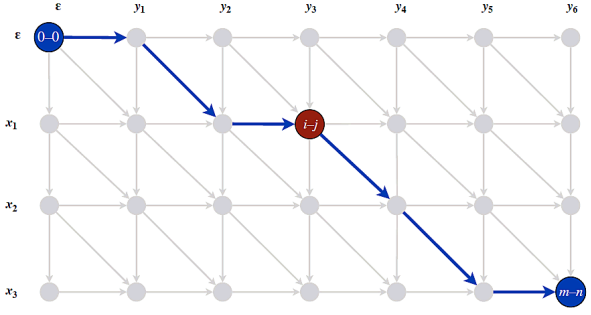


Edit distance graph.

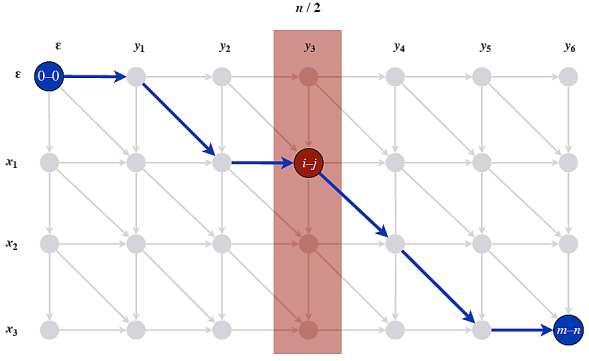
- Let $g(i, j)$ denote length of shortest path from (i, j) to (m, n).
- Can compute $g(\cdot, j)$ for any j in $O(mn)$ time and $O(m + n)$ space.



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



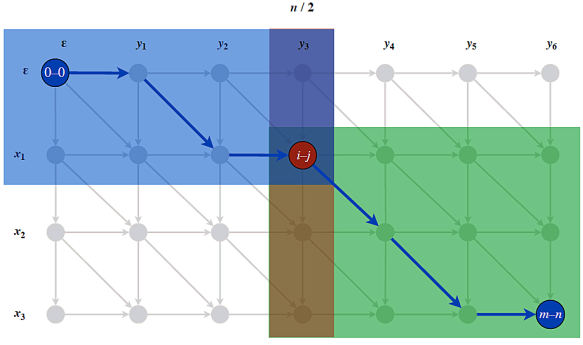
Observation 2. let q be an index that minimizes $f(q, n/2) + g(q, n/2)$. Then, there exists a shortest path from $(0, 0)$ to (m, n) that uses $(q, n/2)$.



Hirschberg's Algorithm

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

Conquer. Recursively compute optimal alignment in each piece.



Hirschberg's Algorithm: Space Analysis

Theorem

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

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Proof.

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Proof.

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

Exercise

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

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

Theorem

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

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Proof.

- $T(m, n)$ is monotone nondecreasing in both m and n.
- $$\begin{aligned} T(m, n) &\leq 2T(m, n/2) + O(mn) \\ &\Rightarrow T(m, n) = O(mn \log n) \end{aligned}$$

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

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Proof. [by strong induction on $m + n$]

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Proof. [by strong induction on $m + n$]

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

$$T(m, 2) \leq cm$$
$$T(2, n) \leq cn$$
$$T(m, n) \leq cmn + T(q, n/2) + T(m - q, n/2)$$

Claim

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

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

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

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

Longest common subsequence

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

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Example. **LCS(GGCACCACG, ACGGCGGATACG) = GGCAACG**.

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Example. **LCS(GGCACCACG, ACGGCGGATACG) = GGCAACG**.

Applications. Unix diff, git, bioinformatics.

Solution for LCS

$$LCS[i,j] = \begin{cases} 0, & \text{if } i = 0 \vee j = 0 \\ LCS[i-1, j-1] + 1, & \text{if } a[i] == b[j] \\ \max\{LCS[i-1, j], LCS[i, j-1]\}, & \text{otherwise.} \end{cases}$$

How about the longest common string?

Solution for LCS(substring)

$$LCS[i,j] = \begin{cases} 0, & \text{if } i = 0 \vee j = 0 \\ LCS[i-1, j-1] + 1, & \text{if } a[i] == b[j] \\ 0, & \text{otherwise.} \end{cases}$$

Referred Materials

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- Content of this lecture comes from Section 6.1 and 6.2 in [DPV07], Section 6.6 and 6.7 in [KT05].
- Suggest to read Section 6.2 in [KT05].