Design and Analysis of Algorithms V

Sequence Alignment

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Shortest Paths in DAGs, Revisited

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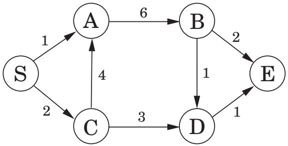
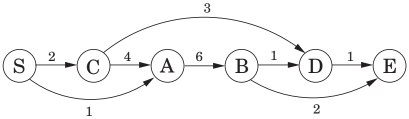
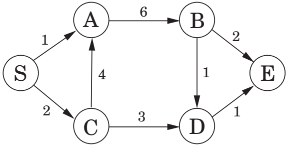
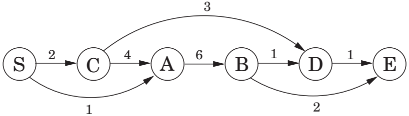




Shortest Paths in DAGs, Revisited





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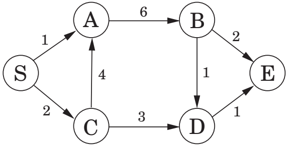
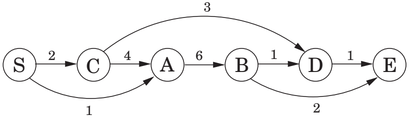
Shortest Paths in DAGs, Revisited





The special distinguishing feature of a DAG is that its nodes can be linearized, arranged on a line so that all edges go from left to right.

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 $\texttt{dist}(v)$.

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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This algorithm is solving a collection of subproblems, $\{\texttt{dist}(u) \mid u \in V\}$

Dynamic Programming

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In dynamic programming we are given a DAG implicitly.

Longest Increasing Subsequences

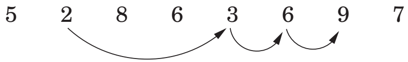
The input of longest increasing subsequence problem, is a sequence of numbers $a_1, \ldots, a_n$.

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.

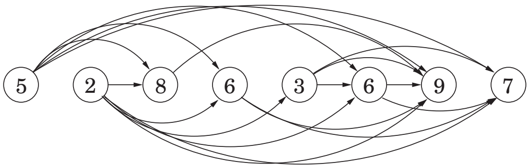
The task is to find the increasing subsequence of greatest length.



Graph Reformulation

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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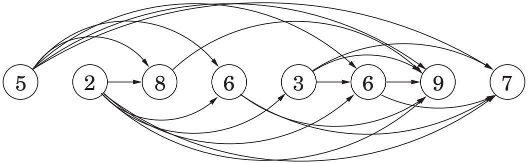

- This graph $G = (V, E)$ is a DAG, since all edges (i, j) have $i < j$
- There is a one-to-one correspondence between increasing subsequences and paths in this DAG.

The Algorithm

for $j = 1$ *to* n **do**

$\quad L(j) = 1 + \max\{L(i) \mid (i, j) \in E\}$;

end

`return(`$\max_j L(j)$`);`

Sequence Alignment

String Similarity

Q. How similar are two strings?

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Example. **ocurrance** and **occurrence**.

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o	c	u	r	r	a	n	c	e	–
o	c	c	u	r	r	e	n	c	e

6 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

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

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Example.

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

BLOSUM Matrix for Proteins

	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

Exercise

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 $x_1x_2\ldots x_m$ and $y_1y_2\ldots y_n$, find a min-cost alignment.

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Definition The cost of an alignment M is:

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

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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 $x_1 x_2 \ldots x_i$ and $y_1 y_2 \ldots y_j$.

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

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

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 $y_1 y_2 \dots y_{j-1}$.

Sequence Alignment: Problem Structure

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, ..., x_m, y_1, ..., y_n, δ, α)
for i = 0 to m do
    M[i, 0] ← iδ;
end
for j = 0 to n do
    M[0, j] ← jδ;
end
for i = 1 to m do
    for j = 1 to n do
        M[i, j] ← min{α_{x_i y_j} + M[i − 1, j − 1], δ + M[i − 1, j], δ + M[i, j − 1]};
    end
end
RETURN M[m, n];
```

Sequence Alignment: Traceback

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		S	I	M	I	L	A	R	I	T	Y
	0	2	4	6	8	10	12	14	16	18	20
I	2	4	1	3	2	4	6	8	7	9	11
D	4	6	3	3	4	4	6	8	9	9	11
E	6	8	5	5	6	6	6	8	10	11	11
N	8	10	7	7	8	8	8	8	10	12	13
T	10	12	9	9	9	10	10	10	10	9	11
I	12	14	8	10	8	10	12	12	9	11	11
T	14	16	10	10	10	10	12	14	11	8	11
Y	16	18	12	12	12	12	12	14	13	10	7

Sequence Alignment: Analysis

Theorem

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

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Proof.

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

Hirschberg's Algorithm

Sequence Alignment in Linear Space

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

Sequence Alignment in Linear Space

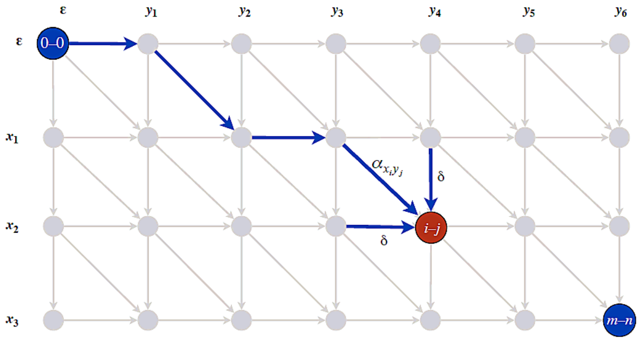
[Hirschberg] There exists an algorithm to find an optimal alignment in $O(mn)$ time and $O(m+n)$ space.

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

Hirschberg's Algorithm

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

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- Last edge on shortest path to (i,j) is from $(i-1,j-1)$, $(i-1,j)$, or $(i,j-1)$.
- 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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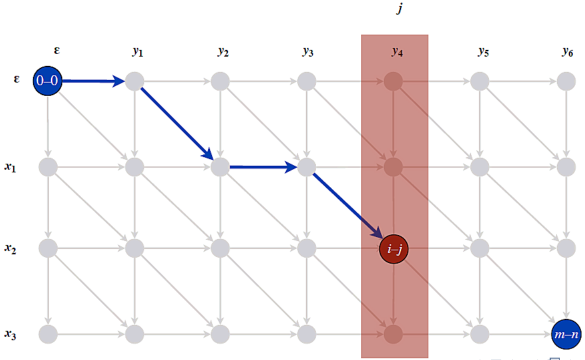
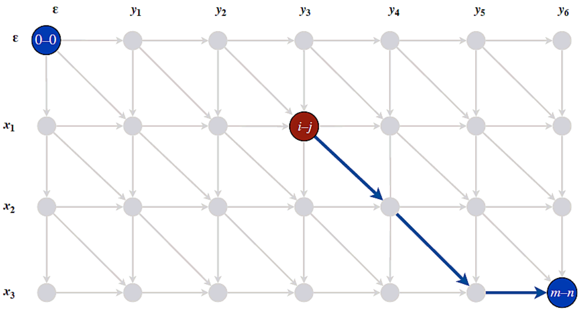
- Can compute $f(\cdot, j)$ for any j in $O(mn)$ time and $O(m)$ space.



Hirschberg's Algorithm

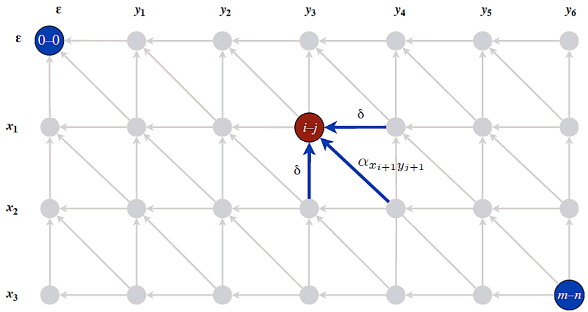
Edit distance graph.

- 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).



Hirschberg's Algorithm

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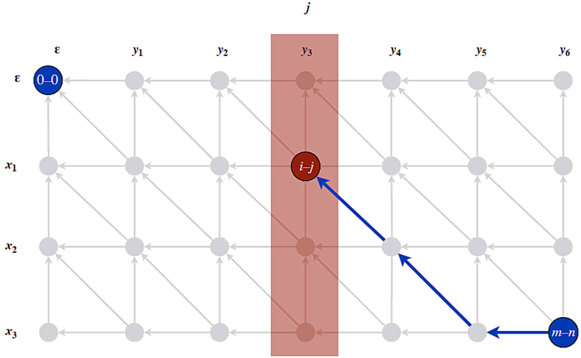
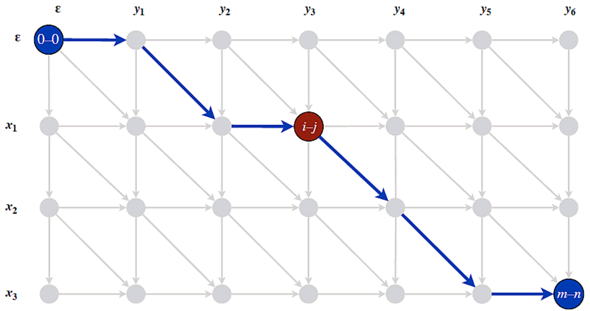
Edit distance graph.

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



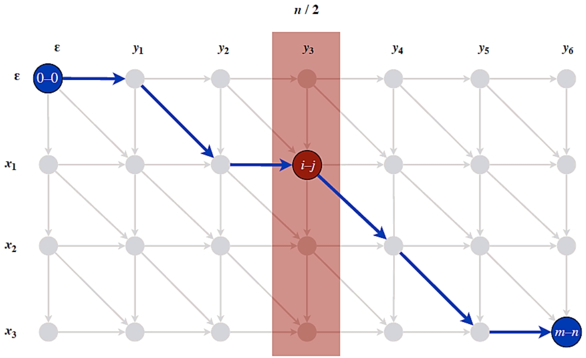
Hirschberg's Algorithm

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



Hirschberg's Algorithm

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

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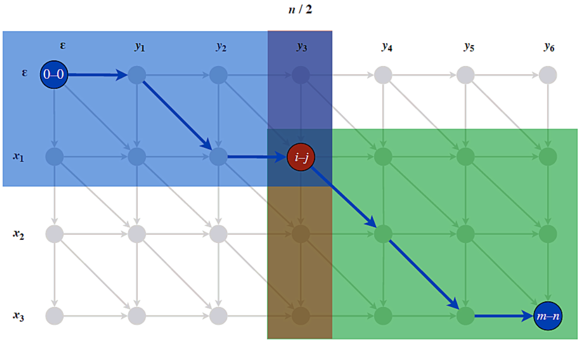
Divide. Find index q that minimizes $f(q, n/2) + g(q, n/2)$; save node i-j as part of solution.

Conquer. Recursively compute optimal alignment in each piece.



Hirschberg's Algorithm: Space Analysis

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Theorem

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

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Proof.

Hirschberg's Algorithm: Space Analysis

Theorem

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

Proof.

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

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. $O(mn \log m \log n)$

Running Time Analysis Warmup

Theorem

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

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Proof.

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

$$\begin{aligned} T(m,n) &\le 2T(m,n/2) + O(mn) \\ &\Rightarrow T(m,n) = O(mn \log n) \end{aligned}$$

Running Time Analysis Warmup

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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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Running Time Analysis

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

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

Running Time Analysis

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Theorem

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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:

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

Running Time Analysis

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Claim

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

Running Time Analysis

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Claim

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

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

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

Longest common subsequence

Problem. Given two strings $x_1 x_2 \ldots x_m$ and $y_1 y_2 \ldots y_n$, find a common subsequence that is as long as possible.

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Applications. Unix diff, git, bioinformatics.

Quiz

How about the longest common string?

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].