



Algorithms: Design  
and Analysis, Part II

# Dynamic Programming

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Sequence Alignment:  
Optimal Substructure

# Problem Definition

Recall: sequence alignment. [Needleman-Wunsch score = Similarity measure between strings]

Example:  
A G G C T  
A G G - C A  
total penalty =  $\alpha_{\text{gap}} + \alpha_{AT}$

Input: strings  $X = x_1 \dots x_m, Y = y_1 \dots y_n$  over some alphabet  $\Sigma$  (like  $\{A, C, G, T\}$ )  
- Penalty  $\alpha_{\text{gap}} > 0$  for inserting a gap,  
 $\alpha_{ab}$  for matching  $a \neq b$  [presumably  $\alpha_{aa} = 0$  if  $a = b$ ]

Feasible Solutions: alignments - i.e., insert gaps to equalize lengths of the strings

Goal: alignment with minimum-possible total penalty.

# A Dynamic Programming Approach

Key step: identify subproblems. As usual, will look at structure of an optimal solution for clues.

[i.e., develop a recurrence + then reverse engineer the subproblems]

Structure of optimal solution: Consider an optimal alignment of  $X, Y$  and its final position:

——  $X + \text{gaps}$  ——  
——  $Y + \text{gaps}$  ——

Final position

Question: How many relevant possibilities are there for the contents of the final position?

(A) 2  
(B) 3

(C) 4  
(D)  $m \cdot n$

Case 1:  $x_m, y_n$  matched

Case 2:  $x_m$  matched with a gap

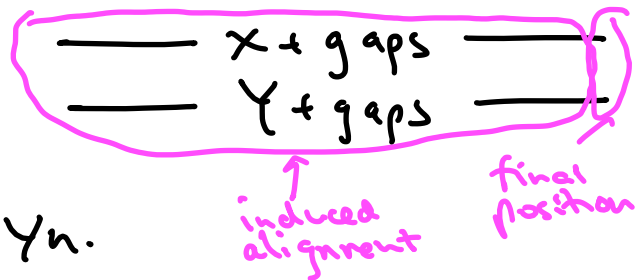
Case 3:  $y_n$  matched with a gap

[pointless to have 2 gaps]

# Optimal Substructure

- ①  $x_m \in Y_n$
- ②  $x_m \in \text{gap}$
- ③  $y_n \in \text{gap}$

Point: narrow optimal solution down to 3 candidates.



Optimal substructure: let  $X' = X - x_m$ ,  $Y' = Y - y_n$ .

If case ① holds, then induced alignment of  $X'$  &  $Y'$  is optimal.

If case ② holds, then induced alignment of  $X'$  &  $Y$  is optimal.

If case ③ holds, then induced alignment of  $X$  &  $Y'$  is optimal.

# Optimal Substructure (Proof)

Proof: [of Case 1, other cases are similar]

By contradiction. Suppose induced alignment of  $X', Y'$  has penalty  $P$  while some other one has penalty  $P^* < P$ .

$\Rightarrow$  appending  $\begin{pmatrix} x_n \\ 1 \\ y_n \end{pmatrix}$  to the latter, get an alignment of  $X$  and  $Y$  with penalty  $P^* + \alpha_{x_n y_n} < \underbrace{P + \alpha_{x_n y_n}}_{\substack{\text{penalty of} \\ \text{original alignment}}}$

*Contents of first position*  $\rightarrow$

$\Rightarrow$  contradicts optimality of original alignment of  $X$  &  $Y$

QED!