

In bioinformatics, there is a sequence comparison problem, defined as follows. Assume to score 2 for a match, -3 for a mismatch, and -1 for an insertion or deletion; then derive the matching with the highest score. What if score -1.5 for a mismatch? Briefly describe the algorithm and illustrate your algorithm by the following two sequences, ACGCTGA and AACTGT.

Ans.

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假設 $X = \langle ACGCTGA \rangle$, $Y = \langle AACTGT \rangle$ 花 39:27

令一個矩陣 M , 其中 $M[i, j]$ 存放, X 和 Y comparison 的最高分數。

推測其遞迴的表示法為

$$M[i, j] = \max \begin{cases} M[i-1, j-1] + 2, & \text{if } x_i == y_j \\ M[i-1, j-1] - 3, & \text{if } x_i \neq y_j \\ M[i-1, j] - 1, & \text{if delete } x_i \\ M[i, j-1] - 1, & \text{if insert } y_j \end{cases}$$

如果最高分是 $\begin{cases} \text{match, 標記 } \nwarrow^m \\ \text{ismatch, 標記 } \nwarrow^x \\ \text{delete, 標記 } \uparrow \\ \text{insert, 標記 } \leftarrow \end{cases}$

由 Dynamic Programming 得最高分

$\begin{matrix} & \emptyset & A & A & C & T & G & T \\ \emptyset & 0 & \nwarrow^{-1} & \nwarrow^{-2} & \nwarrow^{-3} & \nwarrow^{-4} & \nwarrow^{-5} & \nwarrow^{-6} \\ A & \uparrow^{-1} & \nwarrow^2 & \nwarrow^1 & \nwarrow^0 & \nwarrow^{-1} & \nwarrow^{-2} & \nwarrow^{-3} \\ C & \uparrow^{-2} & \uparrow^1 & \nwarrow^0 & \nwarrow^3 & \nwarrow^2 & \nwarrow^1 & \nwarrow^0 \\ G & \uparrow^{-3} & \uparrow^0 & \nwarrow^{-1} & \uparrow^2 & \nwarrow^1 & \nwarrow^4 & \nwarrow^3 \\ C & \uparrow^{-4} & \uparrow^{-1} & \nwarrow^{-2} & \nwarrow^1 & \nwarrow^0 & \uparrow^3 & \nwarrow^2 \\ T & \uparrow^{-5} & \uparrow^{-2} & \nwarrow^{-3} & \uparrow^0 & \nwarrow^3 & \nwarrow^2 & \nwarrow^5 \\ G & \uparrow^{-6} & \uparrow^{-3} & \nwarrow^{-4} & \uparrow^{-1} & \uparrow^2 & \nwarrow^5 & \nwarrow^4 \\ A & \uparrow^{-7} & \uparrow^{-4} & \nwarrow^{-5} & \nwarrow^{-2} & \uparrow^1 & \uparrow^4 & \nwarrow^3 \end{matrix}$

得最高分 = 3

$\begin{matrix} \text{old} = & A & & \cancel{A} & - & C & & T & G & A & - \\ & | & & & & | & & | & | & & \\ \text{new} = & A & - & - & A & C & T & G & - & T \end{matrix}$

如果 mismatch 權重改成 -1.5

$$M[i, j] = \begin{cases} M[i-1, j-1] + 2 & , \text{ if } x_i == y_j \\ M[i-1, j-1] - 1.5 & , \text{ if } x_i \neq y_j \\ \max \begin{cases} M[i-1, j] - 1 & , \text{ delete } x_i \\ M[i, j-1] - 1 & , \text{ insert } y_j \end{cases} \end{cases}$$

	∅	A	A	C	-	T	G	T
∅	0	-1	-2	-3	-4	-5	-6	
A	↑-1	↖^m₂	↖^m₂	←1	←0	←-1	←-2	
C	↑-2	↑1	↑1	↖^m₄	←3	←2	←1	
G	↑-3	↑0	↑0	↑3	↖^x_{2.5}	↖^m₅	←4	
C	↑-4	↑1	↑1	↖^m₂	↖^x_{1.5}	↑4	↖^x_{3.5}	
T	↑-5	↑-2	↑-2	↑1	↖^m₄	↑3	↖^m₆	
G	↑-6	↑-3	↑-3	↑0	↑3	↖^m₆	↑5	
A	↑-7	↖^m₄	↖^m₋₁	↑-1	↑2	↑5	↑4	

最高分數為 4

old: - A C - G ~~∅~~ T ~~G~~ A
 new: A A C T G - T - -