
1 Recursions

1.1 Definitions

S^1, S^2 target and query sequences

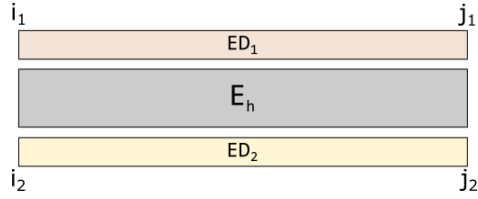
i_1, j_1, i_2, j_2 interaction boundaries

si_1, sj_1, si_2, sj_2 seed boundaries

N the maximum interaction length (~ 150)

M the enclosed unpaired positions in one loop (~ 15)

General energy computation:



$$E_{i_2, j_2}^{i_1, j_1} = E_h(i_2, j_2) + ED_1(i_1) + ED_2(j_2)$$

Optimization task:

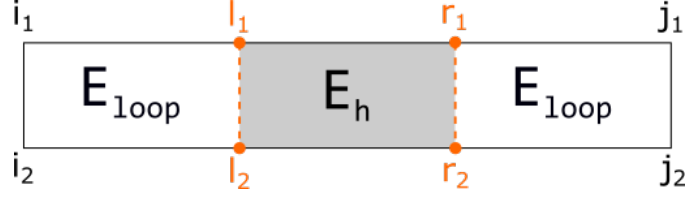
$$\min_{\substack{j_1 - i_1 \leq N \\ j_2 - i_2 \leq N}} \left(E_h(i_2, j_2) \right)$$

1.2 Initialization

$$\forall_{\substack{si_1 \leq i_1 \leq j_1 \leq sj_1 \\ si_2 \leq i_2 \leq j_2 \leq sj_2}} E_h(i_2, j_2) = \infty$$

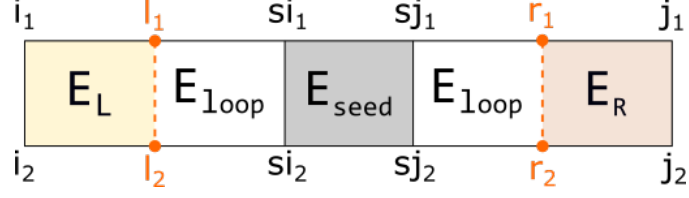
$$E_h(si_2, sj_2) = E_{seed}$$

1.3 Recursion 1 ($O(N^4)$ space + time)



$$\begin{array}{l}
 \forall \\
 si_1 - N \leq i_1 \leq si_1 \\
 si_2 - N \leq i_2 \leq si_2 \\
 \forall \\
 sj_1 \leq j_1 \leq sj_1 + N \\
 sj_2 \leq j_2 \leq sj_2 + N
 \end{array}
 E_h(i_1, j_1) = \begin{cases}
 \infty & : \text{if no matching base pair} \\
 \infty & : \text{if } j_1 - i_1 > N \text{ oder } j_2 - i_2 > N \\
 \min_{\substack{i_1 < l_1 \leq r_1 < j_1 \\ i_2 < l_2 \leq r_2 < j_2 \\ l_1 - i_1 - 1 \leq M \\ j_1 - r_1 - 1 \leq M \\ l_2 - i_2 - 1 \leq M \\ j_2 - r_2 - 1 \leq M}} & \left(E_{loop}(i_1, l_1) + E_h(l_1, r_1) + E_{loop}(r_1, j_1) \right) \\
 & : \text{otherwise.}
 \end{cases}$$

1.4 Recursion 2 ($O(N^2)$ space + $O(N^4)$ time)



$$E_h(i_1, j_1) = \begin{cases} \infty & : \text{if } j_1 - i_1 > N \text{ oder } j_2 - i_2 > N \\ \left(E_L(i_1) + E_{seed} + E_R(j_1) \right) & \\ : \text{otherwise.} \end{cases}$$

$$\forall_{\substack{si_1 - N \leq i_1 \leq si_1 \\ si_2 - N \leq i_2 \leq si_2}} E_L(i_1) = \begin{cases} \infty & : \text{if no matching base pair} \\ \min_{\substack{l_1 - i_1 - 1 \leq M \\ l_2 - i_2 - 1 \leq M}} \left(E_L(l_1) + E_{loop}(i_1, l_1) \right) & \\ : \text{otherwise.} \end{cases}$$

$$\forall_{\substack{sj_1 \leq j_1 \leq sj_1 + N \\ sj_2 \leq j_2 \leq sj_2 + N}} E_R(j_1) = \begin{cases} \infty & : \text{if no matching base pair} \\ \min_{\substack{j_1 - r_1 - 1 \leq M \\ j_2 - r_2 - 1 \leq M}} \left(E_{loop}(r_1, j_1) + E_R(r_1) \right) & \\ : \text{otherwise.} \end{cases}$$