
1 Recursions

1.1 Definitions

S^1, S^2 target and query sequences

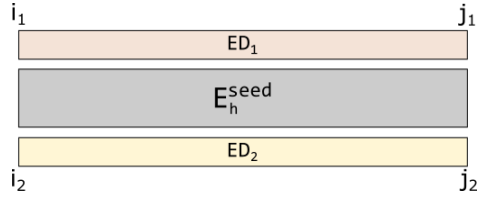
i_1, j_1, i_2, j_2 interaction boundaries

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:



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

Optimization task:

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

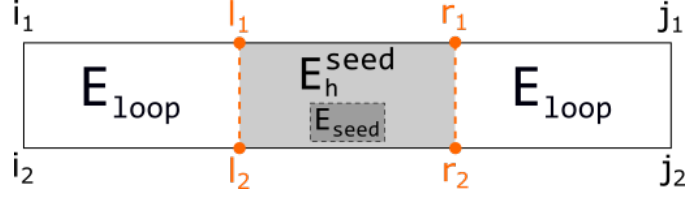
1.2 Initialization

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

$$E_h^{seed}(si_1, sj_1) = E_{seed}$$

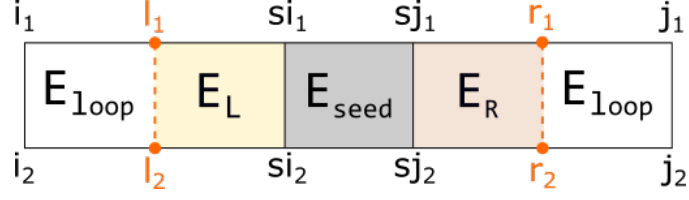
with E_{seed} including E_{init} .

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



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

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



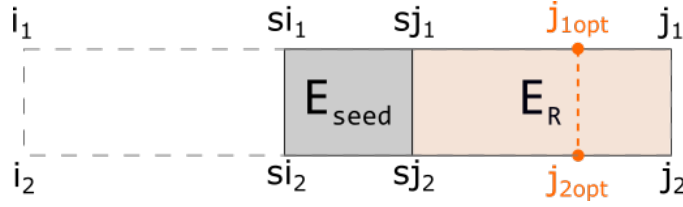
$$E_h^{seed}(i_1, j_1) = \begin{cases} \infty & : \text{if } j_1 - i_1 > N \text{ oder } j_2 - i_2 > N \\ \left(E_L(i_1) + E_{seed} + E_R(j_1) \right) & \\ \infty & : \text{otherwise.} \end{cases}$$

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

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

1.5 Recursion 3 ($O(N^2)$ space + $O(N^2)$ time)

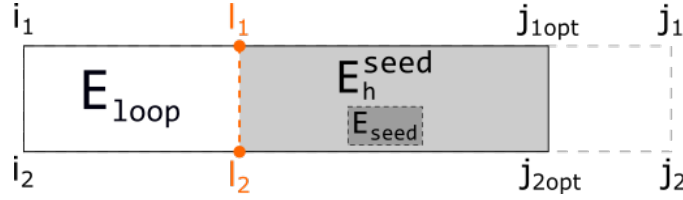
First find j_1 and j_2 that minimize right side. Call them j_{1opt} and j_{2opt} .



$$\arg \min_{j_1, j_2} \left(E_{seed} + E_R^{(sj_1, j_1)} \right)$$

with E_R defined as in Recursion 2.

Then minimize over entire interaction up to j_{1opt} and j_{2opt} .



$$\forall_{\substack{si_1 - N \leq i_1 \leq j_{1opt} \\ si_2 - N \leq i_2 \leq j_{2opt}}} E_h^{seed}(i_1, j_{1opt}) = \begin{cases} \infty & : \text{if no matching base pair} \\ \min_{\substack{l_1 - i_1 - 1 \leq M \\ l_2 - i_2 - 1 \leq M}} \left(E_{loop}(i_1, l_1) + E_h^{seed}(l_1, j_{1opt}) \right) & \\ \text{otherwise.} & \end{cases}$$