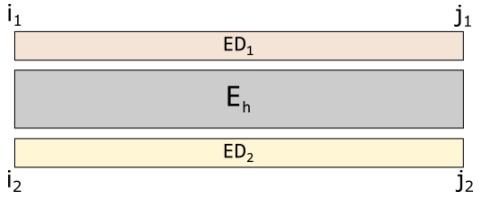
1 Recursions

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:



$$E\binom{i_1,j_1}{i_2,j_2} = E_h\binom{i_1,j_1}{i_2,j_2} + ED_1\binom{i_1}{j_1} + ED_2\binom{i_2}{j_2}$$

Optimization task:

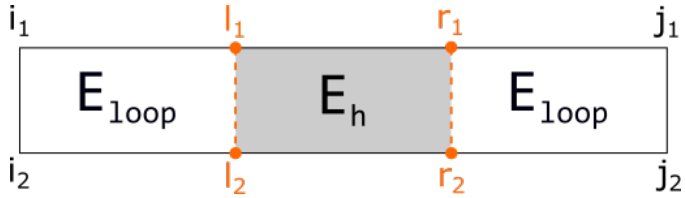
$$\min_{\substack{j_1-i_1<=N \\ j_2-i_2<=N}} \left(E_h\binom{i_1,j_1}{i_2,j_2} \right)$$

1.2 Initialization

$$\forall_{\substack{si_1<=i_1<=j_1<=sj_1 \\ si_2<=i_2<=j_2<=sj_2}} E_h\binom{i_1,j_1}{i_2,j_2} = \infty$$

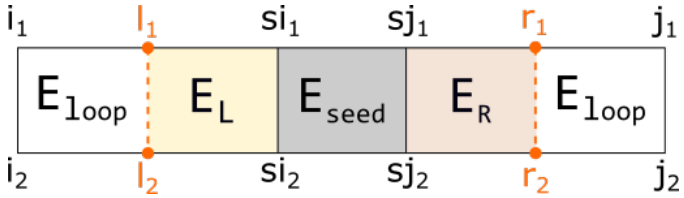
$$E_h\binom{si_1,sj_1}{si_2,sj_2} = E_{seed}$$

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



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

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



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

$$\underset{\substack{si_1-N<=i_1<=si_1 \\ si_2-N<=i_2<=si_2}}{\forall} E_L\binom{i_1}{i_2} = \begin{cases} \infty \\ \quad : \text{if no matching base pair} \\ \min\limits_{\substack{l_1-i_1-1<=M \\ l_2-i_2-1<=M}} \left(E_{loop}\binom{i_1,l_1}{i_2,l_2} + E_L\binom{l_1}{l_2}\right) \\ \quad : \text{otherwise.} \end{cases}$$

$$\underset{\substack{sj_1<=j_1<=sj_1+N \\ sj_2<=j_2<=sj_2+N}}{\forall} E_R\binom{j_1}{j_2} = \begin{cases} \infty \\ \quad : \text{if no matching base pair} \\ \min\limits_{\substack{j_1-r_1-1<=M \\ j_2-r_2-1<=M}} \left(E_R\binom{r_1}{r_2} + E_{loop}\binom{r_1,j_1}{r_2,j_2}\right) \\ \quad : \text{otherwise.} \end{cases}$$