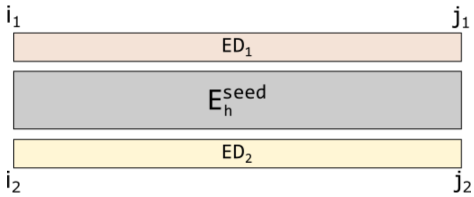
1 Recursions

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:



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

Optimization task:

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

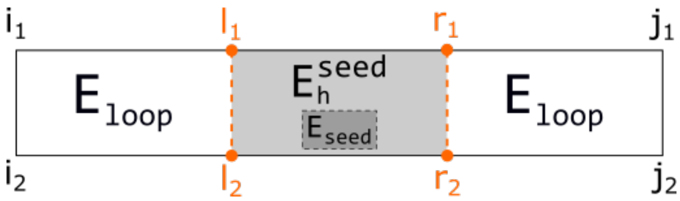
1.2 Initialization

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

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

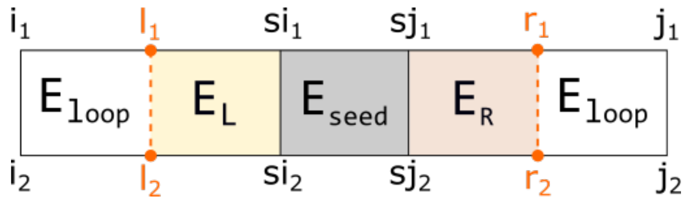
with E_{seed} including E_{init}.

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



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

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



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

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

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

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

First find j1 and j2 that minimize right side. Call them j_{1opt} and j_{2opt}.

$$\arg\min_{j1,j2}\left(E_{seed} + E_R\binom{sj_1,j_1}{sj_2,j_2}\right)$$

with E_R defined as in Recursion 2.
Then minimize over entire interaction up to j_{1opt} and j_{2opt}.

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