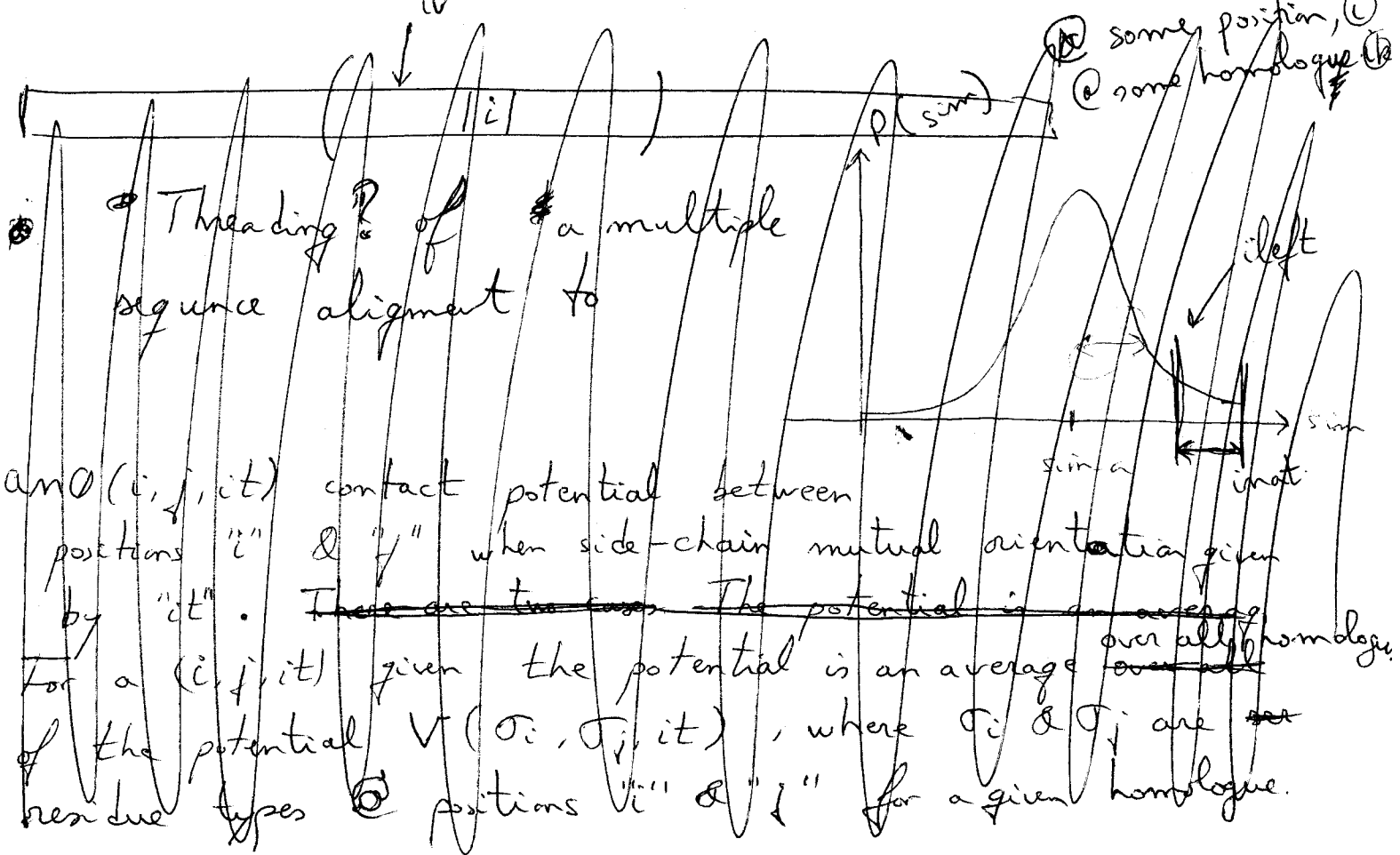
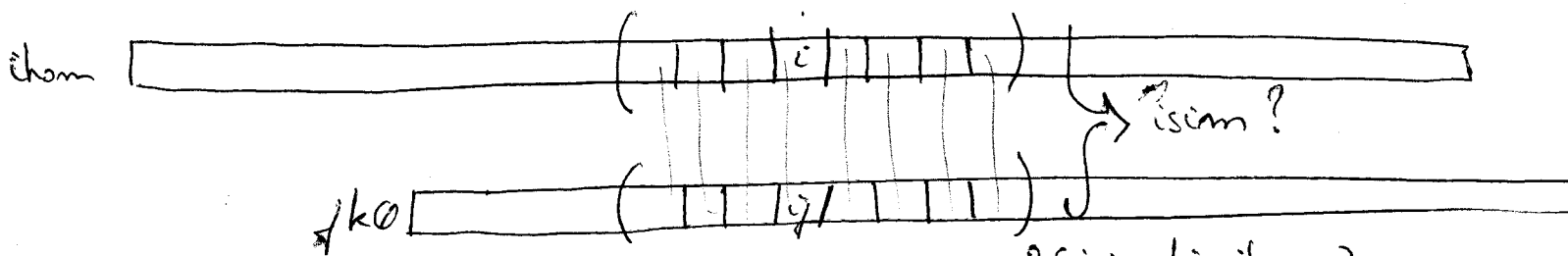


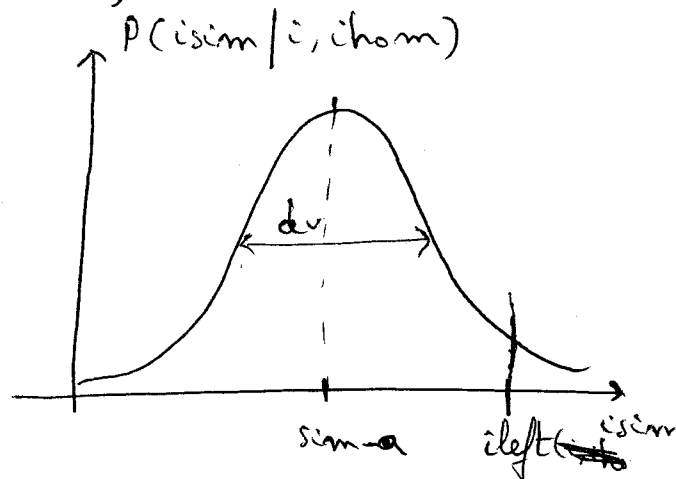
Threading of a multiple sequence alignment to

and $\phi(i, j, it)$ contact potential between positions "i" & "j" when side-chain mutual orientation given by "it". ~~There are two cases. The potential is an average~~ For a (i, j, it) given the potential is an average ~~over all~~ ^{over all homologues} of the potential $V(\sigma_i, \sigma_j, it)$, where σ_i & σ_j are ~~are~~ residue types @ positions "i" & "j" for a given homologue.

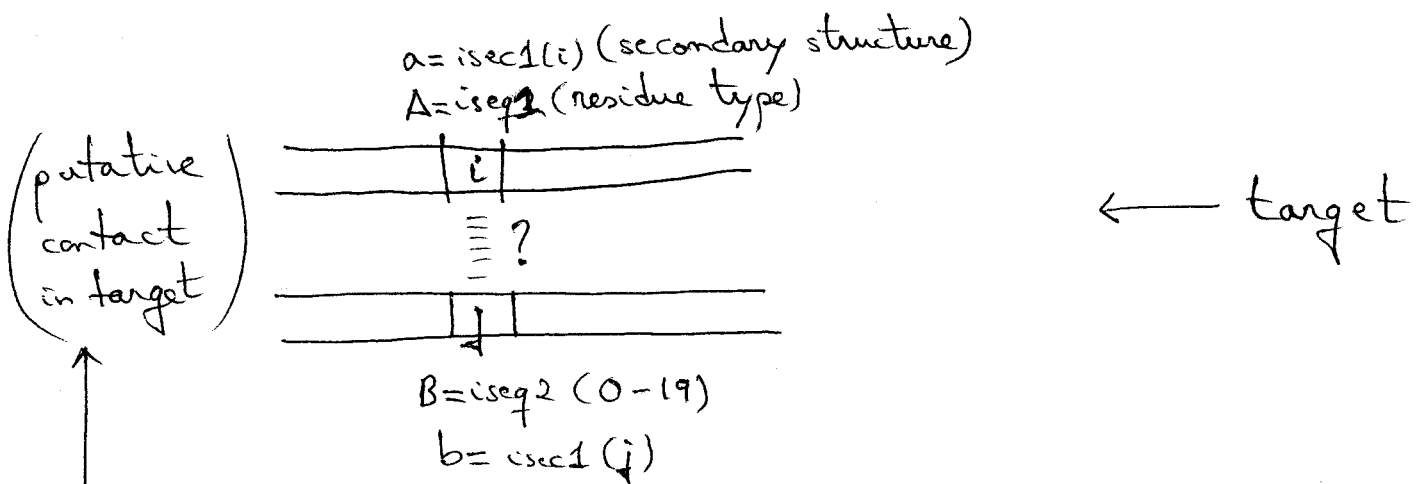
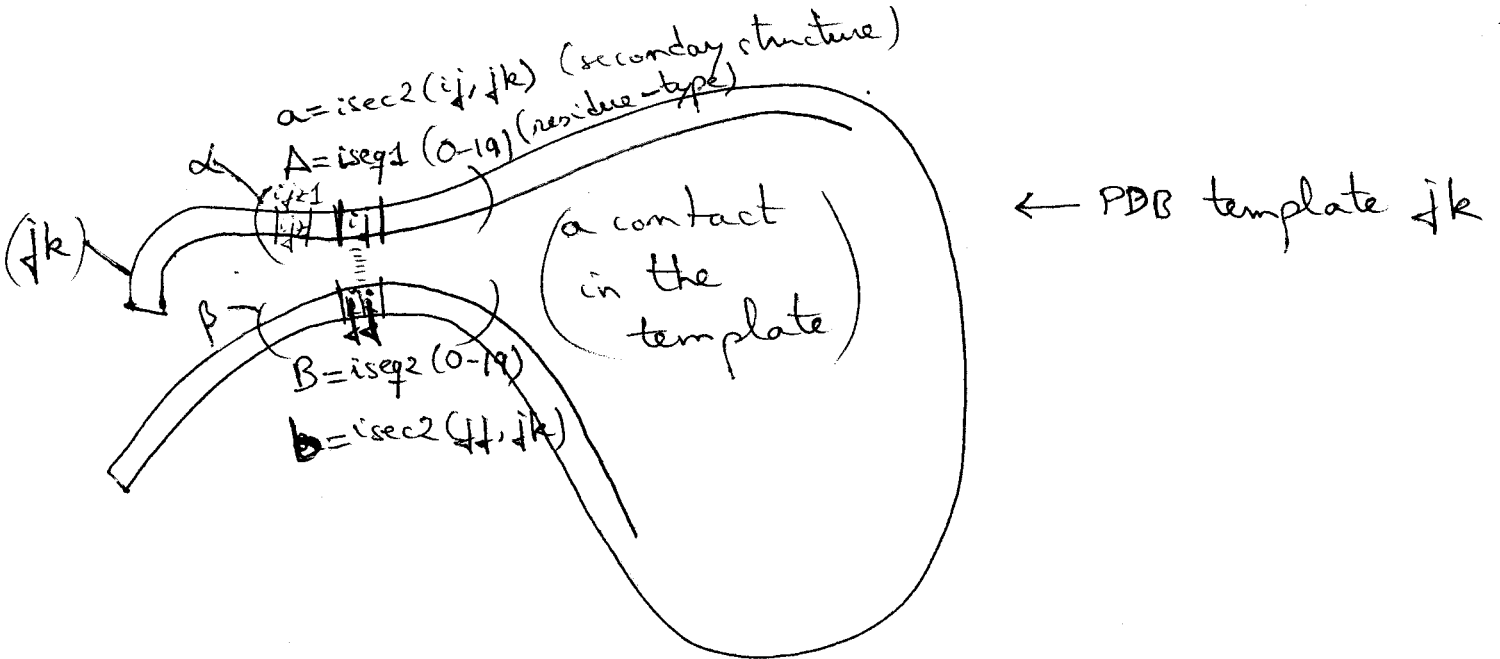



~~ilft(i, ichom) denotes values of isim -> ilft(i, ichom) denote homologous segments~~

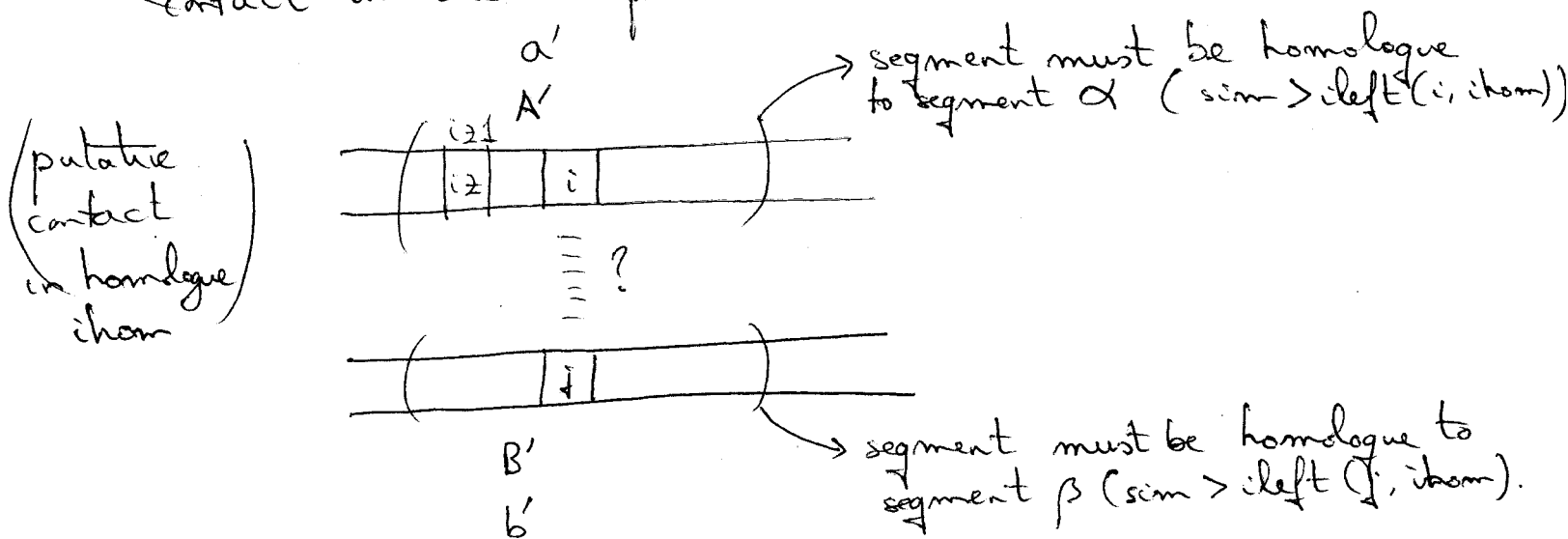
a chunk of ~~2~~ ^{cwin2} amino acids that we may find with

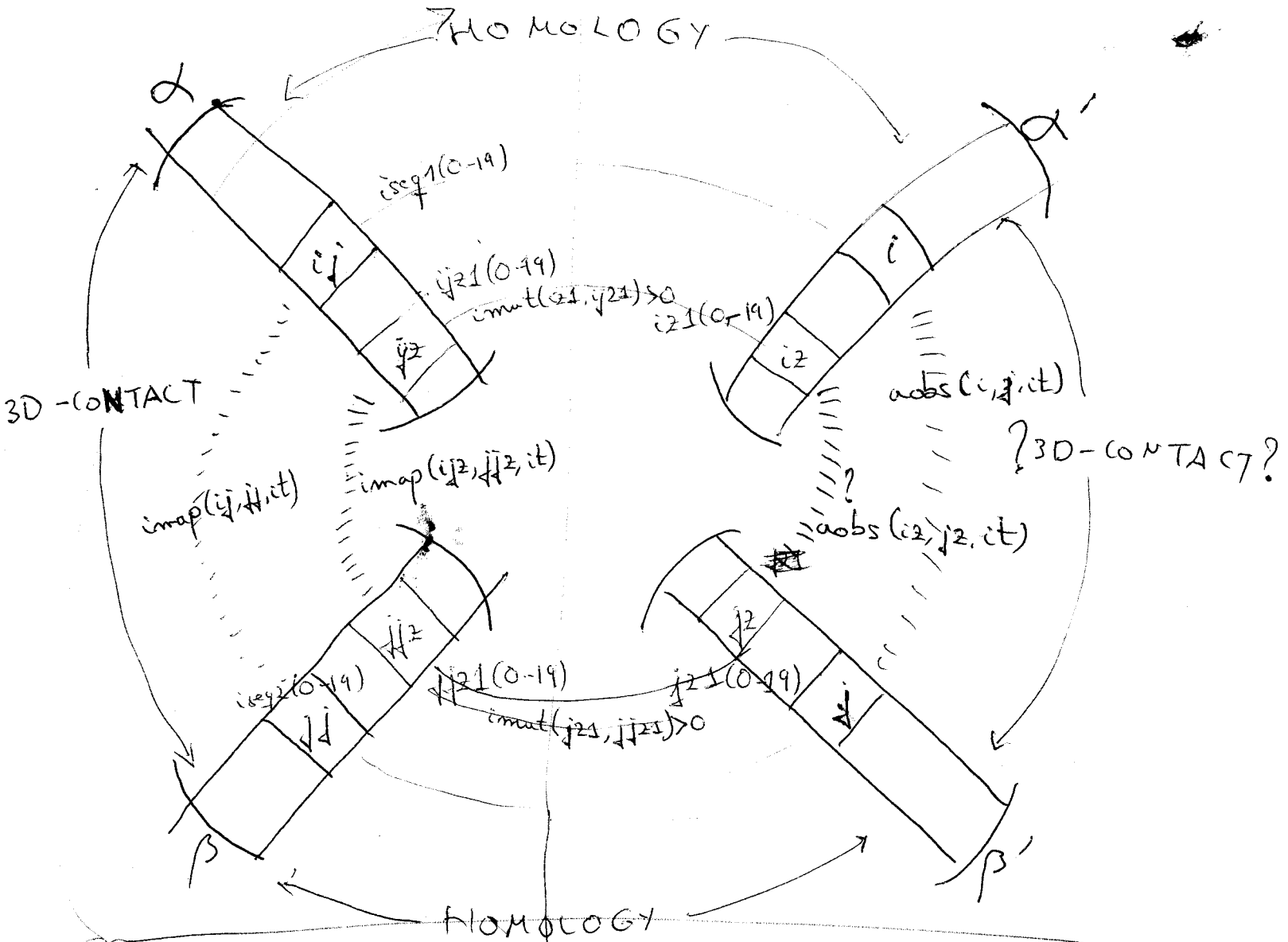


For each PDB structure, find the contact map $\text{imap}(i, j, it)$



types and secondary structure of the putative contact must coincide to types and secondary structure of the contact in the template





template PDB struct \longleftrightarrow homologue to target sequence

$$\text{aobs}(i, j, it) += sf * \text{imap}(ij, it)$$

\uparrow combined homology of (α, α') , (β, β')

\uparrow conditions for this statement to happen.

- (1) secondary structure of ij must be same as ^{predicted} second. struct of "i" in target.
- (2) secondary structure of ij must be same as predicted secondary struct. of "j" in target.
- (3) residue type @ ij same as residue type @ i
- (4) residue type @ ij same as residue type @ j
- (5) residue type @ i_2 evolutionarily related to residue type @ i_2
- (6) residue type @ j_2 evolutionarily related to residue type @ j_2
- (7) (α, α') & (β, β') must be homologues