
Algorithm SMC method for protein segment construction

- 1: $x_0^{(j)} = \emptyset, j = 1, 2, \dots, N$
 - 2: **for** i from 1 to $l - 3$ **do**
 - 3: **for** j from 1 to N **do**
 - 4: Construct list $L_i^{(j)}$ of possible pairs (ϕ', ψ') for amino acid i
 - 5: **for** n from 1 to 100 **do**
 - 6: Propagate $x_{i-1}^{(j)} \rightarrow x_i^{(j,n)}$ as follows:
 - 7: Draw one (ϕ_i, ψ_i) pair from $L_i^{(j)}$ and $\omega_i \sim p(\omega_i)$, and sample up to n_s side chain positions for χ_i .
 - 8: **if** $i = 1$ **then**
 - 9: Let $\{s_{i,j,n}^{(k)}\}_{k=1}^{N_s}$ contain the n_s positions for χ_1
 - 10: **else**
 - 11: Propagate $\{s_{i-1,j,n}^{(k)}\}_{k=1}^{N_s} \rightarrow \{s_{i,j,n}^{(k)}\}_{k=1}^{N_s}$ using embedded side chain filter: set $\{s_{i,j,n}^{(k)}\}_{k=1}^{N_s}$ to be the N_s vectors of $\chi_{1:i}$ with the lowest energies among the $N_s \times n_s$ combinations of $\chi_{1:i-1}$ with χ_i .
 - 12: **end if**
 - 13: **end for**
 - 14: **end for**
 - 15: Sample N particles from $\{x_i^{(j,1)}, \dots, x_i^{(j,100)}\}_{j=1}^N$ to be $x_i^{(1)}, \dots, x_i^{(N)}$
 - 16: **end for**
 - 17: Do final processing (including analytical closure for last three amino acid positions) and output conformations.
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