Three-Dimensional Reconstruction Using the Encounter Probabilities

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Given an encounter probability profile of the first bead in a Rouse chain of N bead, we use the expected encounter model in the Rouse chain to give estimate on the 3D organization of the chain. Given the encounter profile e, we minimize the goal function of the form

$$min\{f(d)\} \tag{1}$$
$$Ad \leq b \tag{2}$$
$$A_{eq}d = b_{eq} \tag{3}$$
$$l_b \leq d \leq u_b \tag{4}$$
$$c(d) \leq 0 \tag{5}$$
$$c_{eq}(d) = 0 \tag{6}$$

where d is a vector of the distances of bead from bead 1, $f = \sum d_j$, $A \in M_{[N \times N]}$ is a matrix such that

$$A_{ii} = \begin{cases} -1 & \text{if } \exists j \quad ; \|e_j - e_i\| \leq \epsilon \\ 0 & \text{else} \end{cases} \tag{7}$$

$$A_{ij} = \begin{cases} 1/|J| & \text{if } \|e_j - e_i\| \leq \epsilon \\ 0 & \text{else} \end{cases} \tag{8}$$

for small ϵ of choice, and J is the group of all indices j such that $\|e_j - e_i\| \leq \epsilon$ for each i. The vector b is the zero vector, $b = 0$, l_b is the lower bound, set to be a vector of all ones, u_b is the upper bound set to be a vector of all N. The non linear constraint

$$c(d) = \sum_{i=1}^{N} \left(\frac{d_i^{-1.5}}{\sum_{i=1}^{n} d_i^{-1.5}} - e_i \right)^2 \tag{9}$$