Protein Folding Prediction in 3D Cubic Lattice in HP Model

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In this article we develop the idea of the heuristic algorithm for 2D HP models described by Traykov et al. [3] and thus allows to solve the 3D HP lattice model for protein folding problem. The algorithm divided the protein sequence S of k non intersected segments $S_1 \cdots S_k$ which are supposed to be small and $S = S_1 \cup S_2 \cup \cdots \cup S_k$. On the first step the algorithm finds optimal folding for segment S_1 and saved. On the second step, the algorithm finds optimal folding for $S_1 \cup S_2$ taking into account the saved folding, and so on. The algorithm shows the optimal result in cubic lattice, after the processing of all segments. We compare the obtained results with the results of well-known in the literature algorithms for solving the 3D HP lattice model such as the genetic algorithm [2], a metaheuristic algorithm for ant colony optimization[4], and evolutionary algorithm with backtracking[1].

References

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