

EFFECTIVE OPTIMIZATION ALGORITHMS FOR FRAGMENT-ASSEMBLY BASED PROTEIN STRUCTURE PREDICTION

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Despite recent developments in protein structure prediction, an accurate new fold prediction algorithm remains elusive. One of the challenges facing current techniques is the size and complexity of the space containing possible structures for a query sequence. Traditionally, to explore this space fragment assembly approaches to new fold prediction have used stochastic optimization techniques. Here we examine deterministic algorithms for optimizing scoring functions in protein structure prediction. Two previously unused techniques are applied to the problem, called the Greedy algorithm and the Hill-climbing algorithm. The main difference between the two is that the latter implements a technique to overcome local minima. Experiments on a diverse set of 276 proteins show that the Hill-climbing algorithms consistently outperform existing approaches based on Simulated Annealing optimization (a traditional stochastic technique) in optimizing the root mean squared deviation (RMSD) between native and working structures.