Point Matching Under Non-Uniform Distortions and Protein Side Chain Packing Based on an Efficient Maximum Clique Algorithm

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Abstract

We developed maximum clique-based algorithms for spot matching for two-dimensional gel electrophoresis images, protein structure alignment and protein side-chain packing, where these problems are known to be NP-hard. Algorithms based on direct reductions to the maximum clique can find optimal solutions for instances of size (the number of points or residues) up to 50~150 using a standard PC. We also developed pre-processing techniques to reduce the sizes of graphs. Combined with some heuristics, many realistic instances can be solved approximately.

Keywords: maximum clique, electrophoresis, point matching, side-chain packing, structure alignment