

AN APPLICATION OF COMMUNITY STRUCTURE IN COMPLEX NETWORKS TO RESEARCH ON PROTEIN FOLDING

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Abstract. Complex networks have become an important field in complexity studies. The community structure in complex networks is a particular issue with practical applications. This paper constructs a protein folding conformation network, and explores the community structure of this protein folding network using the clustering method. In the community structure, we look for the vertex of the centrality, which is a hub of the community structure. Consequently, the space of protein folding conformation is divided by community structures. We can then search for optimal conformation in each community structure parallelly, so that one can get the protein structure that is close to nature both easily and effectively. The study explores a new way for researching and predicting protein structures.

Keywords. complex network, community structure, clustering analysis, protein folding, search space

1 Introduction

Complex networks have become an important field in complexity studies. In the past few years, many systems in diverse fields were modeled as complex networks, including technological systems, biological networks, ecological webs and social systems^[1]. The community structure in complex networks is important with many practical applications. Communities in a social network might represent real social groupings, perhaps by interest or background; communities in a citation