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Topological properties of four networks in protein structures

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In this paper, we investigate the complex networks of interacting amino acids in protein structures. The cellular networks and their random controls are treated for the four threshold distances between atoms. The numerical simulation and analysis are relevant to the topological properties of the complex networks in the structural classification of proteins, and we mainly estimate the network's metrics from the resultant network. The cellular network is shown to exhibit a small-world feature regardless of their structural class. The protein structure presents the positive assortative coefficients, when the topological property is described as a tendency for connectivity of high-degree nodes. We particularly show that both the modularity and the small-wordness are significantly followed the increasing function against nodes.

Keywords: Biological network, Global efficiency, Assortative coefficient, Modularity, Small-worldness

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I. Introduction

In the past two decades, the complex networks have been ubiquitous in many biological, ecological, technological, informational, and infrastructural systems [1] and many research efforts have provoked considerable interest in complex systems. The network has emerged as a crucial framework in biological networks when researchers study and analyze an open and novel problem in complex systems [2]. The most important properties of biological networks are the structural and the topological ones involving interacting amino acids. Biological systems have been simulated and analyzed in networks such as the protein-protein interaction network [3], metabolic pathways network [4], gene regulatory network [5], and proteins as networks of amino acids [6]. From the protein–protein interactions form biomolecular networks, it has been recently argued that one perturbing protein is able to trigger a cascade of effects that change or modify the synthesis and folding of several other proteins not necessarily directly interacting with the targeted one [7]. As a similar result, another problem, it has been also documented that the extinction of one species in an ecological system produces a cascade problems that propagate well beyond the nearest neighbors of the extinguished species [8]. The proteins in the biological systems have performed diverse biochemical functions and also provided structural basis in living cells. It is important to understand how proteins consistently fold into their native-state structures, the relevance of structure to their function, and their network analysis. Characteristically, the network analysis of protein structures is able to be supported to understand possible relevance of various network metrics.

Many researches of proteins are ubiquitous in scientific fields of the network. There have been of much interest for metabolic networks, gene regulatory networks, protein–protein interaction networks as long evolutionary history. The protein contact network is exclusive among other intra-cellular networks. The unique method of synthesis has designated a linear chain of amino acids and folded into a stable three dimensional structure through contact lengths among the residues. The degree distribution in cellular networks follows a Poisson distribution or a power-law distribution. The degree distribution in random network follows a Poisson distribution, which indicates that most nodes have roughly the same number of links, approximately equal to the network's average degree [9]. In contrast, a scale-free network has a power-law degree distribution, $p(k) \sim k^{-\gamma}$,