ABSTRACT

Network representation of protein structures is an information-rich mode of examining protein structure, dynamics and its interactions with biomolecules. Graph spectral methods are extremely useful and powerful in analysing complex networks. This thesis is concerned with development of graph spectral methods for analysing networks and applying them to protein structure analysis. Some of the key problems of network science that are addressed here are network similarity assessment and identification of key components in networks. A new network similarity score (NSS) has been developed and has shown to be useful in comparing different networks considering both local and global changes. The applicability of this scoring scheme as a protein structure model validation tool has been demonstrated using models from various sources such as CASP experiments, mutant structures and molecular simulation trajectories. Also, a method to identify nodes and edges crucial in the network has been developed using NSS and perturbation analysis.

Although the methods developed in the thesis are inspired by the topology and functions related to protein structures, they are general and are applicable to problems in many other disciplines.