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Discovering Functional Interdependence Relationship in PPI Networks for Protein Complex Identification

Winnie W. M. Lam* and Keith C. C. Chan, *Member, IEEE*

***Abstract*—Protein molecules interact with each other in protein complexes to perform many vital functions, and different computational techniques have been developed to identify protein complexes in protein–protein interaction (PPI) networks. These techniques are developed to search for subgraphs of high connectivity in PPI networks under the assumption that the proteins in a protein complex are highly interconnected. While these techniques have been shown to be quite effective, it is also possible that the matching rate between the protein complexes they discover and those that are previously determined experimentally be relatively low and the "false-alarm" rate can be relatively high. This is especially the case when the assumption of proteins in protein complexes being more highly interconnected be relatively invalid. To increase the matching rate and reduce the false-alarm rate, we have developed a technique that can work effectively without having to make this assumption. The name of the technique called protein complex identification by discovering functional interdependence (PCIFI) searches for protein complexes in PPI networks by taking into consideration both the functional interdependence relationship between protein molecules and the network topology of the network. The PCIFI works in several steps. The first step is to construct a multiple-function protein network graph by labeling each vertex with one or more of the molecular functions it performs. The second step is to filter out protein interactions between protein pairs that are not functionally interdependent of each other in the statistical sense. The third step is to make use of an information-theoretic measure to determine the strength of the functional interdependence between all remaining interacting protein pairs. Finally, the last step is to try to form protein complexes based on the measure of the strength of functional interdependence and the connectivity between proteins. For performance evaluation, PCIFI was used to identify protein complexes in real PPI network data and the protein complexes it found were matched against those that were previously known in MIPS. The results show that PCIFI can be an effective technique for the identification of protein complexes.**

I. Introduction

PROTEIN molecules in protein–protein interaction (PPI) networks interact with each other in subnetworks, called protein complexes [18], [21]. Since protein complexes can play important roles in the understanding of cellular organizations and functions, such as replication, transcription, and control of gene expression, etc. [16], much recent effort has been made to discover protein complexes experimentally. Unfortunately, as laboratory experiments are time consuming and expensive, the number of experimentally identified protein complexes is still far from complete [27]. To reduce costs and time, some attempts have been made to use computational techniques to search for protein complexes in PPI networks automatically so that biological experiments can be better directed [19]. These techniques are mostly graph clustering algorithms. Given a PPI network represented in a graph, these graph clustering algorithms can be used to discover densely connected regions. Under the assumption that the proteins in protein complexes are more highly interconnected, these regions are expected to have higher chance to correspond to known protein complexes.

Among the graph clustering algorithms that have been used to discover protein complexes, MCODE [5] is one of the most popular. It discovers protein complexes based on the connectivity between protein molecules in a PPI network. Under the assumption that the proteins in a protein complex are more densely connected with each other [31], MCODE makes use of a local search algorithm that operates in three stages: vertex weighting, complex prediction, and postprocessing. Given a PPI network graph, MCODE first weights all its vertices based

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