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Predicting Protein Interactions by using Various Algorithms on Biological Networks

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Abstract- *To identify the protein complexes is very important to understand the function and organization of cellular principles. Protein complexes are usually identified by various algorithms among Protein to Protein interactions networks. Various algorithms based on the concept graph clustering, dense region and spectrometry. A comparison is given for comparing various algorithms to identify the algorithm which is best for identifying the prediction of protein interactions. We propose that comparison made easy to identify which algorithm is used on biological networks.*

I. INTRODUCTION

With the gap between the sequence data and their functional annotations becomes increasing wider, many computational methods have been proposed to annotate functions for unknown proteins. However designing effective methods to make good use of various biological resources is still a big challenge for researchers due to function diversity of proteins. Designing an effective method to make good use of various biological resources is still a big challenge, due to heterogeneity, complexity and diversity of these biological data. According to differences between the ways to integrate data resources, the computational methods can be classified into four categories: multiple feature vector based method, multi-classifier based method, kernel based method and network based method. Recently, more and more researchers have put their focuses on developing effective methods to annotate protein functions based on network, since functions of cell are performed not by single protein but by a group of proteins that work together, and network is a good way to describe the relationship between proteins. Moreover, a large number of network-based algorithms provide us effective tools to mine information from networks, which also helps us to understand the complicated mechanism of cell life actives.

II. Methodology

Protein-protein interactions and protein complexes represent important relationships in biological pathways. For that reason, we have included these interactions in the learning process as relational information that may influence the final predictions. The classical data mining approach represents data in a propositional manner, i.e., one table featuring one row per protein and a list of columns (or features) for each specific protein. Propositional representation of the data used in the present study would require thousands of Boolean attributes per protein (one for each of the potential interacting partners in the entire proteome), and where most of the columns would have no values. By contrast, using a relational representation [25] it is sufficient to define one binary predicate and to include as many instances as true interaction partners exist. Relational representation also allows us to consider sequence features of the interaction partner in the learning process through a link with its identifier. For example, we can annotate a protein A with the membrane trafficking pathway because protein A is involved in a complex interaction with protein B, which contains a transmembrane region.

Protein domain is the unit of protein function and structure. The functions of an unknown protein can be inferred by identifying

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whether it consists of the protein domain with the function annotations. There are also some network-based methods that combine protein domain information with PPI to predict protein functions. the global information of the networks is ignored. Some methods such as Markov Clustering algorithm (MCL), PageRank-Nibble are proposed to find protein complexes based on random walk technique which can exploit the global structure of networks. The global clustering methods mine complexes from PPI networks by partitioning the networks into separated subgraphs. G-N algorithm which partitions the PPI networks by iteratively removing the edges with the highest edge betweens. Another famous global clustering method is Markov Clustering algorithm (MCL) [7], [8] which detects protein complexes by simulating random walkers in PPI networks. The random walker starts on an initial node and moves to a neighboring node based on the probabilities of the connecting edges. If the walker goes into a dense region, it would be hard to get out of the region. Based on this concept, MCL partitions the PPI networks into non-overlapping subgraphs by using two operators called expansion and inflation. Since the random walk technique implicitly exploits the global structure of networks, MCL obtains robust and performance for protein complex detection. However, MCL can only generate non-overlapping subgraphs, whereas protein complexes are highly overlapped and there are many multi-functional proteins which involve in different function modules [9]. To overcome this limitation, some methods have been proposed to identifying overlapping protein complexes based on MCL algorithm [10]. Local clustering algorithms detect protein complexes by considering local neighbors instead of global networks. Based on maximal clique algorithm (CMC), Liu et al. [11] detect protein complexes by finding all the maximal cliques. Adamcsek et al. [14] develop a software package, named CFinder, based on clique percolation method (CPM) [13] which detects the k-cliques and join two adjacent k-cliques if they share (k _ 1) common nodes. However, it is too strict to require that a protein complex always contains a maximal clique.

Consequently, some methods have been proposed to find local dense subgraphs. Most of these algorithms initiate a cluster from a single node and iteratively add a neighbor node according to different heuristic criteria. Then they take post-processing step to filter out low density clusters and heavily overlapping clusters. MCODE [10] algorithm first weights every node based on its local neighborhood densities, and then selects nodes with high weights as seeds. It detects protein complexes by extending the seeds. DPClus [11] algorithm is different from MCODE. It weights each edge based on the common neighbors between its two proteins and assigns weights to nodes by their weighted degrees. DPClus selects the node with the highest weight as the seed node and iteratively adds close nodes to construct protein complexes. Li et al. [12] improve DPClus algorithm by modifying the strategy of seed selecting and cluster expanding based on subgraph diameter and subgraph density. Recently, many new clustering methods based on local density have been proposed, including HC-PIN [13], SPICi [14], Cluster ONE [15] and so on. However these methods ignore the inherent architecture of protein complexes. Previous studies [16] reveal that a protein complex is generally composed of a core and attachments. The proteins in core as the heart of protein complex are highly connected and co-expressed, and have the greatest degree of functional similarity. The proteins in attachments often connect to the proteins in core and assist the core to perform subordinate functions. With respect to the core-attachment structure of protein complex, Leung et al. [17] design CORE algorithm, a statistic framework to identify the core of protein complex. The proteins in core are determined by two factors: whether two proteins interact or not and the number of the common neighbors between them. Then CORE algorithm calculates the pvalue for all pairs of proteins to detect core. Wu et al. [18] introduce a core-attachment based method (COACH) to detect protein complexes in two stages. They firstly detect the cores from the neighborhood graphs of vertices based on local density. Then the protein complexes are generated by including attachments into the cores. In [9], it is pointed out that COACH achieves better prediction performance than other methods which fail to consider intrinsic structure of protein complexes. Recently, some core-attachment based approaches have been proposed [10], [19]. However, there are no uniform or standard definition for the core and attachments of protein complexes, which arouses our substantial interests in developing method with respect to the core-attachment structure. The merit of local clustering algorithms is that they can detect overlapping protein complexes and can be implemented easily. However, they generate protein complexes by using some heuristic rules and fail to take consideration of the information of entire PPI networks.

PageRank-Nibble method [24] is a non-heuristic local clustering algorithm, which starts from a single vertex and looks for a cluster of good conductance in its neighborhoods. This method absorbs the neighborhoods to generate cluster with respect to their PageRank values which reflect the degree of closeness to the starting nodes from the entire PPI networks perspective. Moreover, the method measures the quality of cluster by using conductance. Leskovec et al. [25] have pointed out that a good community is supposed to have low conductance. Consequently, Voevodski et al. [26] and Hodgkinson and Karp [27] use PageRank-Nibble algorithm to detect protein complexes. Their experimental results show that the algorithm find better clusters than other popular graph partition methods. However, PageRank-Nibble algorithm detects protein complexes without considering the core-attachment structure of protein complexes. Moreover, in [26], PageRank-Nibble algorithm assigns values to the neighbors of a node by dividing the value of the node evenly among its neighbors. Whereas in order to find better clusters, the neighbors that tend to construct clusters with the node should get higher values. Based on the facts mentioned above, we develop a weighted PageRank-Nibble algorithm which adds weight on edges according to their topological features and assigns the neighbors with different probability. Then we propose a new method named WPNCA to detect protein complexes from PPI networks using weighted PageRank-Nibble algorithm and core-attachment structure. We have conducted experiment on yeast data. The experimental results show that WPNCA outperforms the existing methods in terms of both accuracy and p-value.

Coupling graph is a new and very useful graphical model for representing intrinsic associations between pairs of subgraphs in a complex. In bioinformatics, coupling graphs can be used to reveal the structural interactions of protein-protein interacting complexes,

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genephenotype association networks, microRNA-gene expression regulatory networks, and so on. The frequent coupling subgraphs of these coupling graph databases play an important role in discovering the essential patterns hidden in the coupling graph databases. However, mining the frequent coupling subgraphs from a coupling graph database is very challenging, as existing subgraph mining algorithms perform poorly on coupling subgraph mining. The huge number of irrelevant subgraphs generated by the existing algorithm is the big hurdle to the efficiency. To overcome this obstacle, we have introduced a new algorithm by using a novel graph transformation and restoration technique.

A. Comparisons

Closed Coupling graph is a new and very useful graphical model for representing intrinsic associations between pairs of subgraphs in a complex. In bioinformatics, coupling graphs can be used to reveal the structural interactions of protein-protein interacting complexes, genephenotype association networks, microRNA-gene expression regulatory networks, and so on. The frequent coupling subgraphs of these coupling graph databases play an important role in discovering the essential patterns hidden in the coupling graph databases. However, mining the frequent coupling subgraphs from a coupling graph database is very challenging, as existing subgraph mining algorithms perform poorly on coupling subgraph mining. The huge number of irrelevant subgraphs generated by the existing algorithm is the big hurdle to the efficiency. To overcome this obstacle, we have introduced a new algorithm by using a novel graph transformation and restoration technique. The prediction method described can generate many different annotation systems depending on the configuration parameters used. For the current problem of predicting pathway associations, we have configured a RLE with a minimum frequency of 0.2 and a maximum depth of 4 as the WARMR parameters. These parameters were selected to build decision trees with different attributes depending on the specific pathway, since we are interested in predicting a range of proteins related to each pathway in parallel to the molecular variability of the proteins in the corresponding pathway. Of the various configurations produced, we applied a tradeoff between performance (measured as AUPRC in test data set) and diversity of rules for each pathway when making our selection. This means that a system with better performance could have been selected at the expense of decreasing (or even removing) the diversity among the proteins predicted, which would be similar to the features of just one pathway protein rather than several techniques. CFinder algorithm which detects k-cliques and then merges the adjacent k-cliques as modules.

Local Clique Merging Algorithm (LCMA) generates overlapping clusters based on local clique merging. It first locates local cliques in an interaction graph and then merges the detected local cliques according to their affinity to form maximum density subgraphs. The Markov cluster (MCL) algorithm is a popular method to predict protein complexes by simulating random walks within graphs. DPCLus detects protein complexes by keeping track of the periphery of a detected cluster. Liu et al gave an algorithm called CMC (Clustering-based on Maximal Cliques) which uses maximun cliques to discover complexes from weighted PPI networks. COACH is a core-attachment-based method which detects protein complexes in two stages. First, it detects protein-complex cores as the "hearts" of protein complexes and then includes the attachment proteins into these cores to form biologically meaningful structures.

II. Comparison of Various Methods used for Protein Complexes

B. Table 1. Comparison of various methods used for identifying protein complexes

percent	Methods	MF			CC			BP		
		Precision	Recall	Fmeasure	Precision	Recall	Fmeasure	Precision	Recall	Fmeasure
10%	ThrRW	0.63	0.44	0.52	0.54	0.36	0.44	0.49	0.36	0.41
	DCS	0.78	0.4	0.53	0.64	0.31	0.42	0.55	0.3	0.39
	ZhangDC	0.7	0.25	0.37	0.61	0.24	0.34	0.5	0.23	0.32
	MRF	0.47	0.19	0.27	0.23	0.2	0.21	0.25	0.2	0.22
	UBiRW	0.62	0.24	0.35	0.69	0.26	0.38	0.64	0.23	0.32
	WAC	0.56	0.08	0.14	0.50	0.03	0.07	0.56	0.08	0.14
	RLC	0.60	0.25	0.35	0.68	0.24	0.36	0.63	0.23	0.34
20%	ThrRW	0.62	0.43	0.51	0.53	0.35	0.43	0.49	0.34	0.40
	DCS	0.75	0.41	0.53	0.64	0.3	0.41	0.55	0.3	0.39
	ZhangDC	0.71	0.25	0.37	0.62	0.25	0.36	0.52	0.24	0.32
	MRF	0.37	0.21	0.27	0.24	0.19	0.21	0.26	0.21	0.23
	UBiRW	0.62	0.23	0.34	0.68	0.26	0.38	0.64	0.22	0.33
	WAC	0.56	0.09	0.15	0.51	0.04	0.07	0.56	0.09	0.15
	RLC	0.60	0.24	0.34	0.64	0.22	0.33	0.63	0.22	0.33
50%	ThrRW	0.59	0.39	0.47	0.51	0.33	0.40	0.48	0.30	0.37
	DCS	0.77	0.33	0.46	0.66	0.25	0.36	0.56	0.26	0.36
	ZhangDC	0.74	0.2	0.31	0.65	0.22	0.33	0.54	0.21	0.3
	MRF	0.35	0.18	0.24	0.22	0.16	0.19	0.22	0.17	0.19
	UBiRW	0.60	0.21	0.31	0.66	0.25	0.36	0.62	0.20	0.30
	WAC	0.56	0.09	0.16	0.51	0.03	0.06	0.56	0.09	0.16
	RLC	0.63	0.21	0.31	0.70	0.21	0.32	0.64	0.2	0.31
80%	ThrRW	0.50	0.32	0.39	0.47	0.27	0.34	0.44	0.23	0.30
	DCS	0.83	0.22	0.35	0.72	0.18	0.29	0.63	0.18	0.28
	ZhangDC	0.83	0.12	0.21	0.72	0.16	0.26	0.63	0.15	0.24
	MRF	0.32	0.09	0.14	0.18	0.08	0.11	0.16	0.09	0.11
	UBiRW	0.54	0.16	0.25	0.62	0.20	0.30	0.58	0.16	0.25
	WAC	0.56	0.09	0.16	0.51	0.03	0.07	0.56	0.09	0.16
	RLC	0.74	0.14	0.24	0.77	0.15	0.26	0.53	0.14	0.22

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The results in Table 2 compare the MSCF algorithm with a snp threshold of 30% to other classical algorithms. From Table 2, the F-score of the MSCF algorithm is the highest, while the Sp and Sn of the MSCF are higher than the most algorithms. Thus, the MSCF algorithm has better performance. The MSCF algorithm gives less perfect matches and larger average sizes because all the proteins on the boundary are added into the complex. Future work will determine whether the proteins on the boundary belong to the complex. Given the already extensive literature on biclustering algorithms, it is important to structure the analysis to be presented. To achieve this, we classified the surveyed biclustering algorithms along four dimensions: . The type of biclusters they can find. The bicluster type is determined by the merit functions that define the type of homogeneity that they seek in each bicluster. The way multiple biclusters are treated and the bicluster structure produced. Some algorithms find only one bicluster, others find nonoverlapping biclusters, others, more general, extract multiple, overlapping biclusters. The specific algorithm used to identify each bicluster. Section 5 shows that some proposals use greedy methods, while others use more expensive global approaches or even exhaustive enumeration. The domain of application of each algorithm. Biclustering applications range from a number of microarray data analysis tasks to more exotic applications like recommendation systems, direct marketing and elections analysis. Biclustering algorithms may have two different objectives: to identify one or to identify a given number of biclusters. Some approaches attempt to identify one bicluster at a time.

Cheng and Church and Sheng et al. identify a bicluster, mask it with random numbers, and repeat the procedure in order to eventually find other biclusters. Lazzeroni and Owen attempt to discover one bicluster at a time in an iterative process where a plaid model is obtained. Ben-Dor et al. also follow this strategy. Other biclustering approaches discover one set of biclusters at a time. Hartigan identifies two biclusters at the time by splicing each existing bicluster into two pieces at each iteration. CTWC performs two-way clustering on the row and column dimensions of the data matrix separately. It uses a hierarchical clustering algorithm that generates stable clusters of rows and columns, at each iteration and, consequently, discovers a set of biclusters.

Table 2

Table 2 Comparisons with other algorithms

Algorithms	PC	Ave	PM	Sp	Sn	F-score
MCODE[7]	59	7.11	7	0.10	0.68	0.19
Cfinder[9]	156	7.88	14	0.20	0.52	0.28
MCL[11]	446	5.60	7	0.32	0.29	0.31
DPClus[13]	149	3.10	12	0.23	0.63	0.34
CMC[14]	319	3.78	17	0.32	0.43	0.37
COACH[15]	334	4.58	14	0.33	0.39	0.36
CP-DR[16]				0.87	0.39	0.54
HC-PIN(λ=0.5)[17]	133	6.24	6	0.26	0.36	0.30
HC-PIN(λ=1.0)[17]	148	7.53	5	0.22	0.35	0.27
IPCA[25]	535	5.36	16	0.52	0.55	0.53
EPOF[20]	1835	12.57	5	0.75	0.39	0.51
MSCF	590	9.59	10	0.69	0.59	0.64

Notes: PC: Number of predicted complexes; Ave: Average size; PM: Number of perfect matching.

Protein interaction networks contain helpful information for understanding the role of proteins in cells and predicting function for un-annotated proteins. a new approach that uses topology of protein–protein interaction network for assigning function to un-annotated proteins. This method combines three topological feature of interaction network to predict function relativity of each protein pairs. The proposed approach provides a general concept of relativity in the networks which can be used in defining relativity of two nodes in various graph-based problems. Ultimately, more high-resolution maps of RNA–protein interactions can be revealed to understand their biological roles in greater depth and detail. Coupling graph is a new and very useful graphical model for representing intrinsic associations between pairs of subgraphs in a complex. In bioinformatics, coupling graphs can be used to reveal the structural interactions of protein-protein interacting complexes, genephenotype association networks, microRNA-gene expression regulatory networks, and so on. The frequent coupling subgraphs of these coupling graph databases play an important role in discovering the essential patterns hidden in the coupling graph databases. However, mining the frequent coupling subgraphs from a coupling graph database is very challenging, as existing subgraph mining algorithms perform poorly on coupling subgraph mining. The huge number of irrelevant subgraphs generated by the existing algorithm is the big hurdle to the efficiency. To overcome this obstacle, we have introduced a new algorithm by using a novel graph transformation and restoration technique.

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III Conclusion

A coupling graph is transformed into a generic graph, and then subgraph mining is conducted on the transformed coupling graphs. We have proved that the transformation and restoration are equivalent. Experimental results carried out on a data set containing 10,511 coupling graphs have demonstrated that the proposed algorithm not only shortens the mining time, but also reduces the memory usage. The usefulness of frequent coupling subgraphs has also been demonstrated on identifying antibody- specific B-cell epitopes. the functional information are obtained from the neighbors in corresponding network but also the functional information is transferred from one network to another through the associations between the nodes in them. Compared with previous methods, our method takes extensive consideration of the structure and topo logical difference of the three networks and makes good use of the associations between them. We carry out experiments on S. cerevisiae (Baker's yeast) data. (1) For GO terms in MF, BP and CC categories, the maximum F-measure values of ThrRWare higher than that of DCS, ZhangDC, MRF, RLC, WAC and UBiRW. (2) On the whole, ThrRW has better performance on target proteins than other existing methods in terms of maximum F-measure and AUC values. (3) when less proteins with function annotations (up to 80% of protein without function annotation), ThrRW possesses more robust prediction performance than other exist methods. All of experimental results show that our method can effectively combine PIN, GO term functional similarity and protein domain information to predict protein functions.

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