MULTIOBJECTIVE EVOLUTIONARY ALGORITHM WITH GRAPHLET MEASURE FOR DETECTION OF COMPLEX TOPOLOGICAL AND BIOLOGICAL COMMUNITY STRUCTURE

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DEDICATION

To my father, who taught me that the best kind of knowledge to have is that which is learned for its own sake.

To my mother, who taught me that even the largest task can be accomplished if it is done one step at a time.

To my husband, who has been a constant source of support and encouragement during the challenges of doctoral study and life.

To my beloved sons, for their constant love and assistance.

I dedicate this thesis ...

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ABSTRACT

In the past few years, community structure detection has garnered much attention due to its significant role in analyzing complex network structures and functions. Detecting natural divisions in complex networks is proved to be an extremely Non-deterministic Polynomial-time hard (NP-hard) problem, which has been solved using evolutionary computation methods. Despite many efforts to design an effective community structure formula, the definition is still general, depending solely on the nodes' intra- and inter-connections. It lacks complete reflection of inherent topological properties, such as graphlet measure in terms of graphlet degree signatures and signature similarities, that can accurately detect complex communities' structure such as topological and biological community. The research proposes a new method termed MOEA_CGN (MultiObjective Evolutionary Algorithm based on Cooperation between Graphlet-based measure and Neighborhood relations) to improve the detection quality of complex topological and biological community structure in terms of accuracy and velocity. Thus, the contribution of this study is summarized in threefold. First, a new multiobjective optimization function is proposed to tackle the issue of a community structure definition. Second, a heuristic mutation operator is designed to enhance MOEA CGN performance to accurately detect complex topological community structure by tackling the resolution limit problem. Third, the heuristic mutation operator is improved to make the MOEA_CGN method identify and detect complex biological community structure accurately by tackling the heterogeneity issue of real-world networks. Systematic experiments on different realworld networks from various domains and synthetic networks of different complexities have demonstrated the proposed method's effectiveness and robustness to define the community detection problem. Specifically, the proposed method has achieved detection reliability with an average improvement of 6.7% in detecting complex topological communities and 9.17% in detecting complex biological communities compared with the state-of-the-art benchmark studies. Moreover, the proposed MOEA CGN method has demonstrated its ability to detect the optimal community structures in most complex networks faster than the competent multiobjective models based on community detection.

ABSTRAK

Dalam beberapa tahun kebelakangan ini, pengesanan struktur komuniti telah mendapat banyak perhatian kerana peranannya yang signifikan dalam menganalisis struktur dan fungsi rangkaian yang kompleks seperti komuniti topologi dan biologi. Mengesan pembahagian semula jadi dalam rangkaian kompleks terbukti menjadi masalah tegar polinomial-masa tidak deterministik (NP-tegar), yang telah diselesaikan dengan menggunakan kaedah pengkomputeran evolusi. Walaupun terdapat banyak usaha untuk merancang formula struktur komuniti yang berkesan, definisi ini masih umum, bergantung sepenuhnya pada hubungan intra dan inter nod. Ia kekurangan gambaran lengkap mengenai sifat topologi yang wujud, seperti ukuran grafik, dalam erti kata tandatangan darjah graflet dan persamaan tandatangan, yang dapat mengesan struktur komuniti yang kompleks dengan tepat. Penyelidikan ini mencadangkan kaedah baru yang dikenali sebagai MOEA_CGN (Algoritma Evolusi Multi Objektif berdasarkan Kerjasama antara Graphlet dan hubungan Kejiranan) untuk meningkatkan kualiti pengesanan struktur komuniti topologi dan biologi yang kompleks dari segi ketepatan dan halaju. Oleh itu, sumbangan kajian ini diringkaskan dalam tiga elemen berikut. Pertama, fungsi pengoptimuman multiobjektif baru dicadangkan untuk mengatasi masalah definisi struktur komuniti. Kedua, pengendalian mutasi heuristik dirancang untuk meningkatkan prestasi MOEA_CGN dalam mengesan struktur komuniti topologi yang kompleks dengan menangani masalah had penyelesaian. Ketiga, pengendali mutasi heuristik diperbaiki untuk menjadikan kaedah MOEA_CGN dapat mengenalpasti dan mengesan struktur komuniti biologi yang kompleks dengan tepat dalam menangani masalah heterogenitas rangkaian dunia nyata. Eksperimen sistematik pada rangkaian dunia nyata yang berbeza dari pelbagai domain dan rangkaian sintetik dengan kerumitan yang berbeza telah menunjukkan keberkesanan dan keteguhan kaedah yang dicadangkan untuk menentukan masalah pengesanan komuniti. Secara khusus, kaedah yang dicadangkan telah mencapai kebolehpercayaan pengesanan dengan peningkatan purata 6.7% dalam mengesan komuniti topologi kompleks dan 9.17% dalam mengesan komuniti biologi yang kompleks berbanding dengan kajian penanda aras terkini. Tambahan pula, kaedah MOEA_CGN yang dicadangkan telah menunjukkan kemampuannya untuk mengesan struktur komuniti yang optimum di rangkaian yang paling kompleks dengan lebih cepat daripada model multiobjektif yang kompeten berdasarkan pengesanan komuniti.

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LIST OF ABBREVIATIONS

ACO	-	Ant Colony Optimization
BA	-	Bat Algorithm
BCO	-	Bee Colony Optimization
BIAs	-	Bio-Inspired Approaches
CA	-	Cultural Algorithm
CAEA	-	Conical Area Evolutionary Algorithm
CC-GA	-	Clustering Coefficient-based Genetic Algorithm
CD	-	Community Detection
СО	-	Conductance
CPL	-	Characteristic Path Length
CR	-	Cut Ratio
CS	-	Cuckoo Search Algorithm
CS	-	Community Score
DE	-	Differential Evolution
DIMMOEA/D	-	Discrete Inverse Modelling-based Multi-Objective
		Evolutionary Algorithm with Decomposition
DPSO	-	Discrete Particle Swarm Optimization
EAs	-	Evolutionary Algorithms
EP	-	Exterior Population
EX	-	Expansion
FA	-	Firefly Algorithm
GA	-	Genetic Algorithm
GACD	-	Genetic Algorithm for Community Detection
GDV	-	Graphlet Degree Vector
GN	-	Girvan and Newman
GO	-	Gene Ontology
HTO	-	Heuristic Turbulence Operator
ID	-	Internal Density
KKM	-	Kernel K-Means
LFR	-	Lancichinetti-Fortunato-Radicchi

LMOEA	-	Local information based Multi-Objective Evolutionary
		Algorithm
MA	-	Memetic Algorithm
MCL	-	Markov Cluster algorithm
MCODE	-	Molecular Complex Detection
MDCL	-	Multi-objective Discrete Cuckoo search algorithm
		with Local search
MDPSO	-	Modified Discrete Particle Swarm Optimization
MGOC	-	Multiobjective Gene Ontology-based Clustering
MIPS	-	Munich Information Center for Protein Sequences
MOACO	-	Multi-Objective Ant Colony Optimization
MOACO/D-	-	Multi-Objective Ant Colony Optimization algorithm based
Net		on Decomposition
MOCD	-	Multi-Objective Community Detection Algorithm
MODAPROC	-	Multi-Objective Disease-Associated Protein Complex
MODPSO	-	MultiObjective Discrete Particle Swarm Optimization
MOEA/D	-	MultiObjective Evolutionary Algorithm Based on
		Decomposition
MOEA_CGN	-	MultiObjective Evolutionary Algorithm based on
		Cooperation between Graphlet-based measure and
		Neighborhood relations
MOEAs	-	MultiObjective Evolutionary Algorithms
MOEPGA	-	MultiObjective Evolutionary Programming Genetic
		Algorithm
MOGA_Net	-	MultiObjective Genetic Algorithms for networks
MOO	-	MultiObjective Optimization
MOP	-	Multiobjective Optimization Problem
MOPSO-Net	-	Multi-Objective Particle Swarm Optimization
NC	-	Normalized Cut
NMI	-	Normalized Mutual Information
NP-hard	-	Non-deterministic Polynomial-time hard
NNIA	-	Nondominated Neighbor Immune Algorithm
NRA	-	Negative Ratio Association

NS	-	Neighborhood Similarity
NSGA-II	-	Nondominated Sorting Genetic Algorithm II
S	-	Signature Similarity
OS	-	Overlapping Score
PCACD	-	Parallel Conical Area Community Detection
PF	-	Pareto Optimal Front
PGP	-	Pretty-Good Privacy
PPI	-	Protein-Protein Interaction network
PROCOMOSS	-	Protein Complex Detection using Multi-objective
		Evolutionary Approach based on Semantic Similarity
PSO	-	Particle Swarm Optimization
QDM-PSO	-	Quantum-based Discrete Multi-Objective Particle Swarm
		Optimization
RC	-	Ratio Cut
RMOEA	-	Reduction based- MultiObjective Evolutionary Algorithm
RNSC	-	Restricted Neighborhood Search Clustering
SCF	-	Scaled cost function
SOO	-	Single Objective Optimization
TS	-	Topological Similarity
US	-	United States
WNMI	-	Weighted Normalized Mutual Information
WOCDA	-	Whale Optimization-based Community Detection
		Algorithm
WOS		Web of Science
Х	-	Crossover

LIST OF SYMBOLS

Α	-	Adjacency or connection matrix
С	_	Cluster (group of vertices)
С	_	Detected partition
\mathcal{C}^*	-	True partition
Ε	-	Set of edges
Ι	-	Individual
G	-	Undirected graph
Κ	-	Number of clusters
т	-	Number of features
m(G)	-	Volume of graph
m(v)	-	Degree of any vertex
$m(\mathcal{C})$	-	Intra-cluster connections (Volume of cluster C)
$\overline{m}(\mathcal{C})$	-	Inter-cluster connections
Ν	-	Population size
n	-	Number of nodes
n(C)	-	Cardinality of cluster
\mathbb{P}	-	Population (set of individual)
Р	-	Current solution
p_c	-	Probability of crossover
p_{hm}	-	Probability of the proposed heuristic mutation
p_{ihm}	-	Probability of the proposed improved heuristic mutation
p_m	-	Probability of traditional mutation
Q	-	Modularity
r	-	Random number
S	-	Size of neighbors
gen	-	Generation
V	-	Set of nodes
${\mathcal N}$	-	Complex network
z^{*}	_	Best reference point

${\cal F}$	-	Fitness function
Ω	-	Solutions space
γ	-	Mixing parameter
λ	-	Weight vector
Г	-	Decoding function
α	-	Random number
С	-	Confusion matrix
g	-	Set of neighbors
Λ	-	Set of weight vectors
Χ	-	Decision variables vector
<i>X</i> *	-	Best solution
k	-	No. of objectives
Q	-	Modularity
Con	-	Contribution of a node to cluster
СС	-	Closeness centrality of a node to cluster
maxgen	-	Maximum number of generations
Ι'	-	Individual after applying heuristic mutation operator
S(u,v)	-	Signature similarity between two nodes' signature
D(u,v)	-	Distance between two nodes' signature

CHAPTER 1

INTRODUCTION

1.1 Introduction

Nowadays, many real complex systems from various fields of sociology, biology, engineering, and communication can be modelled and studied as complex networks of connected communities. In fact, complex networks are an effective formalism in representing the relationships among objects composing many real world systems. Protein interaction networks, neural networks, collaboration networks, world-wide-web networks, Internet network, communication networks, paper citation networks, transport networks, biological and metabolic networks are some examples of complex real-life networks (Pizzuti, 2018; Cheng et al., 2018; Pourkazemi and Keyvanpour, 2017). In general, complex networks can be represented as an undirected graph included all the given system's entities, wherein the vertices of the network correspond to the objects of the system, and the edge (or link) between a pair of objects corresponds to the activities between them. For instance, in biological networks, Protein-Protein Interaction (PPI) network is shaped by considering the collaboration between proteins, wherein the proteins represented the network cardinality (nodes), and the functional or physical interactions between proteins represented the network volume (edges) (Elmsallati et al., 2016; Guzzi and Milenković, 2017). In social complex networks, on the other hand, the objects or entities of the network can be people, and the edges of the network match the various social relations between people like friendship, familiarities, and everyday interests, etc.

Due to increasing the appearance of such complex systems and many other real networked systems, this has fostered the desire to solve and analyze them into organized-topological structures; under the name of modules, clusters, or communities using different mechanisms, in order to provide some organizational principles and fundamentals for real-world networks (Žalik and Žalik, 2018a; Pizzuti, 2018).

Detecting hidden communities in such complex networks has considered a crucial and proceeding challenge since lots of networked problems such as clustering, aligning and searching for relationships are corresponding to the subgraph isomorphism problem known in the literature as NP-hard (Non-deterministic Polynomial-time hard) that lately witnessed a considerable interest (Said *et al.*, 2018; Rao *et al.*, 2018; Elmsallati *et al.*, 2016; Cook, 1971). Research on complex networks analysis and community detection is of a prime interest and has a multidisciplinary nature coming from the graph theory, physics, statistics, and data mining. The problem has been widely addressed as a data analysis problem where Girvan and Newman formally stated it as a community structure detection problem or shortly, Community Detection (CD) problem (Girvan and Newman 2002; Newman and Girvan, 2004). Community detection, or community structure mining in complex networks, means partitioning a given complex network represented as an undirected sparse graph, into communities or groups of vertices (or nodes) having dense intra connections among them and sparse interconnections with the nodes of other clusters.

Thus, a community detection algorithm should be able to divide a complex network into communities with relatively sparse inter-connections and relatively dense intra-connections. This problem may not be accurately solved by using traditional methods due to its complexity and intractable computations where it has been classified as a highly combinatorial optimization NP-hard problem (Gach and Hao, 2012), so it solved using evolutionary computation methods, and thereby it is modelled in the literature as an optimization problem. In the last decade, multiobjective evolutionary algorithms have given a significant contribution in detecting complex community structure and outperforming the single objective evolutionary algorithms. A main characteristic of the multiobjective approach is that the set of Pareto optimal solutions reveals the hierarchical organization of the network. This peculiarity gives a great chance to analyze the network at various hierarchical levels and study communities with different modular levels. Hence, the decision-makers can make their decisions easily (Pizzuti, 2018; Pourkazemi and Keyvanpour, 2017).

All earlier community detection- based evolutionary algorithms focused on solving complex community detection by optimizing neighborhood relations in terms

of intra- and inter- community connections. But most of them, if not all, ignored employing graphlet measure in terms of nodes signature and nodes signature similarity along with the neighborhood relations in defining community structure in complex networks. Solving complex community detection problem by considering cooperation between graphlet-based measures and neighborhood relations has a significant impact in identifying ambiguous nodes to more suitable communities. Since it greatly helps to investigate the entire area of the node's vicinity by looking at all types of graphlet that a node can touch, and hence, the detection accuracy will be improved notably. In this study, a new multi objective method is proposed termed *MOEA_CGN* (MultiObjective Evolutionary Algorithm based on Cooperation between Graphlet-based measure and Neighborhood relations) to detect the structure of topological and biological communities more accurately than the earlier methods. The purpose of this chapter is to provide an overview of the research, including problem statement, the research goal, the objectives, the scope, and the significance of the research.

1.2 Problem Background

The last decade has witnessed the emergence of several novel evolutionary computation-based community detection approaches. In which several heuristics have been customized and developed using various types of optimizing objective functions, which either be single objective optimization or multiobjectives optimization. Based on the term of the optimization functions, only one objective function is optimized in the single objective optimization techniques. In contrast, many objective functions are simultaneously optimized in MultiObjective Optimization (MOO) techniques. Here, a few recent studies of MultiObjective Evolutionary Algorithm (MOEA) have been reviewed that achieved prominent performance in addressing the community detection problem and proved their ability to overcome the drawbacks of the single-objective evolutionary algorithm and the other traditional techniques.

The use of multiobjective frameworks to define the community structure in complex networks was first proposed by Pizzuti in 2009, 2012. The researcher used an NSGA-II framework for formulating MOGA - Net, a multiobjective model to

maximize two objective functions, namely, community score and community fitness. At the same year, Shi et al. (2012) defined the community structure as a multiobjective minimization model, called MOCD, wherein the modularity function (Q) was split into two terms. Based on the formulations given by Shi et al. (2012) and Pizzuti (2012), the emphasis was on neighborhood relations in terms of intra- community connections while the influence of the inter-community connections is either implicitly or indirectly optimized (Attea et al., 2016). The connections between the network nodes is one of the key concepts to define community detection problem, so it will be right to separate those connections that link set of nodes within a single cluster or community explicitly from those that link nodes with different clusters or communities by considering both inter- and intra- cluster connections and nodes' degree generalization (i.e., graphlet measures) to define community structure effectively.

Gong et al. (2012) followed a similar method to that of Shi et al. (2012) by splitting the *modularity density* formula into two terms, namely, Negative Ratio Association (NRA) and Ratio Cut (RC), to detect community structure in complex networks. Accordingly, they formulated the problem as a multiobjective minimization called *MOEA/D_Net* (multiobjective evolutionary model. algorithm with decomposition). After that, Gong et al. (2014) reformulated MOEA/D_Net model into an effective model termed MODPSO (multiobjective discrete particle swarm optimization based on decomposition), by changing the first objective from NRA into the Kernel K-Means (KKM), while RC remained as a second objective. Although the proposed models by Gong et al. (2012) and (2014) explicitly emphasized the impact of neighborhood relations in terms of intra- and inter- community connections, but their models did not able to detect the ideal community structure that describing main characteristics of all networks and their relationships in the best way. To effectively address the issue of community structure definition, this study has proposed a new multiobjective model based on cooperative between graphlet-based measures (in terms of nodes signature and nodes signature similarity) and neighborhood relations (in terms of intra- and inter- community connections).

On the other hand, in biological network, community or cluster structure definition has also been formulated by considering the topological objectives based on neighborhood relations only, which impacted on the developed methods' performance and restricted them from detecting a more accurate structure of complex biological community. Cao et al. (2015) proposed a new clustering algorithm termed MOEPGA (MultiObjective Evolutionary Programming Genetic Algorithm). In MOEPGA, several topological properties of the network, i.e. size, *CPL* (characteristic path length) and density have been integrated to detect meaningful protein complexes and conducting a systematic analysis to the problem with regards identifying complexes of protein in the benchmark PPI networks. Bandyopadhyay et al. (2015) introduced a multiobjective formulation to address the problem by optimizing three distinct criteria in a maximization language. The framework included two topological features of PPI networks that were formulated into two different quality functions which are the contribution of a node to cluster and closeness centrality of a node to cluster. Moreover, the semantic similarity of GO (Gene Ontology) was used as a third objective function. Ray et al. (2016) developed a method called MODAPROC (Multi-Objective Disease-Associated Protein Complex) based on a modified framework of NSGA - II. Three objective functions, namely, disease association, complex density, and outward interaction, were optimized in MODAPROC to discover and find diseasespecific gene complexes. A parallel optimization-based multiobjective method called DCRS was proposed by Sharma and Bhattacharyya (2018). The aim of developing DCRS was to detect protein complexes and identify their quality using the NSGA - IIframework. The method's name, DCRS, was derived from the four objective functions used in the system, which are density, contribution, reachability contribution, and semantic similarity.

Recently, several methods have been proposed to address community detection problem in complex networks effectively by employing the objective functions of either Pizzuti (2012), Shi *et al.* (2012), Gong *et al.* (2012), or Gong *et al.* (2014); and developing a local search operator to enhance the detection accuracy. Sani *et al.* (2018) introduced a new method named *MOACO* (Multi-Objective Ant Colony Optimization) to address the problem by applying Pareto theory (i.e., Pareto dominance and Pareto Archive) and Pearson Correlation measure as heuristic information along with the two objectives of Pizzuti (2012) (community score and community fitness). Rahimi et al. (2018) developed the *MOPSO – Net* method (Multi-Objective Particle Swarm Optimization) based upon a modified version of PSO that revolved around changing the particles' movement in the swarm. The technique used two competing objectives of Gong et al. (2014) (KKM and RC). Ji et al. (2019) proposed a multiobjective community detection method termed MOCD - ACO that combined the MultiObjective Evolutionary Algorithm based-Decomposition (MOEA/D) along with the local heuristic operator of ACO (Ant Colony Optimization). In the MOCD - ACO, two fitness functions of Gong et al. (2012) (NRA and RC) were simultaneously optimized. Besides, the search range was expanded by integrating a local search operator named weighted simulated annealing into the framework. As a result, the combined technique improved the search process by avoiding premature convergence during the optimization process and achieved better performance than other competent algorithms. Zou et al. (2019) proposed DIMMOEA/D (Discrete Inverse Modellingbased Multi-Objective Evolutionary Algorithm with Decomposition), a new algorithm to detect the embedded community structure in real and benchmark complex networks. By using the network topology properties, an inverse modelling strategy was applied to sample the area of objective space and produce a new offspring; and to measure the fitness quality of each generated solution, the authors used two conflicting criteria of Gong et al. (2012) (NRA and RC). Mu et al. (2019) developed MOACO/D - Net (Multi Objective Ant Colony Optimization algorithm based on Decomposition) to address main difficulties in the ACO algorithm based community detection problem. MOACO/D - Net solved the problem by simultaneously minimizing two objectives of Gong et al. (2012) (RC and NRA) in the optimization process. New solutions were constructing by the ants using the new proposed transition probability model. Then, an improvement operation was performed to enhance each solution based on the strong communities' concept.

Despite the increasing interest in developing effective local search operators based on general neighborhood relations, most of the developed methods are still suffering from the resolution limit problem and restricting the solution from going deep into the network structure to find accurate clusters. To address resolution limit problem effectively, this study proposed a new heuristic mutation operator based on cooperation between nodes signature similarity and neighborhood relations.

It is worth to note that all the above explored studies have mainly interested on addressing community detection problem in either: social complex networks with known ground-truth and real-complex networks with unknown ground-truth, or in PPI networks with known generic complexes. This means that there is a need to develop a new method addresses the heterogeneity issue of real-world networks to detect more accurate topological and biological community structure in complex networks derived from various domains.

To this end, the research aims to propose *MOEA_CGN* method to improve the predictive power of the evolutionary-based community detection algorithm. By addressing community detection challenges (which is community structure definition issue, resolution limit problem, and heterogeneity issue of real-world networks) and transcend the limitations in the earlier studies through exploiting neighborhood relations along with strong-theoretically grounded topological properties derived from a network (i.e., graphlet-based measures) in two main components of the adopted optimization method which are the objective functions and mutation operator.

1.3 Problem Statement

Community detection in complex networks is an ill-defined problem as there are no typical accepted protocols on the fundamental ingredients such as defining community itself (Fortunato and Hric, 2016; Javed *et al.*, 2018). The broad issue for the community detection problem in complex networks is the community structure definition. What this means in the context of an evolutionary algorithm is the development of a meaningful mathematical formula (objective functions) that effectively defines the topological structure of the hidden community in the complex networks. Many ideas have emerged to define the community structure, which in turn led to different definitions of single objective or multiobjective optimization functions. Most of the studies, if not all, defined the community structure in a complex network by solely considering the general neighborhood relations of the complex network and lacked complete reflection of inherent topological properties (i.e., graphlet-based measures in terms of nodes' signature and nodes' signature similarity) that can address the issue of a community structure definition effectively. Another limitation is that most of the studies aspired to the traditional or randomize explorative property only. They lacked to design any other heuristic evolutionary operator based on strong, systematic topological properties (i.e., graphlet-based measures in terms of nodes' signature similarity) to avoid resolution limit problem that restrict solutions from going deep into the network structure to find the precise complexes and accurately representing the domain knowledge. The growth of real-world networks from different domains (i.e., social and biological) is inevitable. But these real networks are characterized by topological heterogeneity and differed in some networked characteristics (volume and cardinality) depending on their domains, and this considered another discrete issue for the CD algorithm.

In summary, in this study, three main issues and challenges facing the community detection problem in complex networks have been considered, namely community structure definition issue, resolution limit problem, and heterogeneity issue of real-world networks. In view of that, this research has been guided by the following main research question:

How to design a multiobjective evolutionary algorithm based on cooperation between graphlet-based measure and neighborhood relations (MOEA_CGN) for detection of complex topological and biological community structure accurately?

This question will be fulfilled by answering detailed questions:

- 1. How a *MOEA_CGN* method with two new objective functions can be designed to define complex topological community structure?
- 2. How to improve *MOEA_CGN* method by making it more likely to converge to more accurate solutions? In other words, how to enhance *MOEA_CGN* method with a new heuristic mutation operator to avoid resolution limit problem?

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3. How to make the *MOEA_CGN* method regarded a reliable and dependable method in detecting complex biological communities accurately?

These questions can be answered by designing a CD method that invests the robust topological properties of networks and enhances the search properties in terms of intensification and diversification, as these properties considered essential to improve the ability of the adopted searching algorithm and detecting a more accurate community structure.

1.4 Research Goal

The goal of the study is to propose a new method termed *MOEA_CGN* (MultiObjective Evolutionary Algorithm based on Cooperation between Graphletbased measure and Neighborhood relations) to detect topological and biological community structure in complex networks. *MOEA_CGN* method takes into account addressing three main issues, namely, community structure definition issue, resolution limit problem, and heterogeneity issue of real-world networks, to improve the quality of community detection in terms of accuracy and velocity.

1.5 Research Objectives

The following are the objectives of the proposed study to detect topological and biological community structure in complex networks derived from different domains:-

1. To propose *MOEA_CGN* method with two new objective functions based on cooperation between neighborhood relations and strong, systematic topological measures (i.e., graphlet-based measures) to address the issue of community structure definition.

- 2. To enhance *MOEA_CGN* method with a new mutation operator based on a new qualitative definition of the topological similarity measure to address resolution limit issue.
- 3. To improve the proposed mutation operator based on the distance between the nodes' signature to make *MOEA_CGN* dependable method in detecting complex biological communities accurately.

1.6 Research Scope

The scope of the research is listed as below:

- i. This study has focused on detection topological and biological communities in complex networks derived from different domains.
- ii. The datasets used in this study are:
 - Synthetic-benchmark networks: five networks of GN: Girvan Newman, (2002) and sixteen networks of LFR: Lancichinetti-Fortunato-Radicchi, (2008) have been used.
 - Real-complex networks with known ground-truth: four standard realcomplex networks of various sizes have been used.
 - Real-complex networks with unknown ground-truth: eight standard realcomplex networks of various sizes have been used
 - Biological networks with known ground-truth: two Protein-Protein Interaction networks (PPI) have been used.
- iii. This study has proposed MOEA_CGN method based on MOEA/D (multiobjective evolutionary algorithm based on decomposition) framework of Zhang and Li (2007). MOEA/D is considered a powerful search and optimization mechanism as it providing an effective method to solve several NP-hard optimization problems. At the meanwhile, it never needs a high level of mathematical knowledge, and its computational complexity is low,

compared to other methods (Gong *et al.*, 2012; Cheng *et al.*, 2018; Zhang and Li, 2007; Zou *et al.*, 2019, Ying *et al.*, 2019). These features have made MOEA/D framework appropriate for solving the CD problem when a multiobjective evolutionary algorithm is needed.

- iv. The performance is measured according to detection velocity (with regards to the maximum number of generations required to get the optimal solution), and detection reliability (with regards to the average of the best value of the following measures: Modularity (*Q*), Normalized Mutual Information (*NMI*), Weighted Normalized Mutual Information (*WNMI*), Recall, Precision, and F-measure).
- v. The proposed method is simulated using Matlab R2016b. The experiments over small networks have been performed on a PC with an IntelR CoreTM i7-7700HQ CPU, 16 GB RAM under Windows 10 x64. While the experiments over large networks have been performed on a High Performance Computers (HPC) with 32-core 2.6GHz Intel Xeon E7-8895 server.

1.7 Research Significance

Community detection mainly aims at discovering the inherent structure of community within network or providing useful information on the organization of a network. Community detection allows us to focus on the areas having some degree of independence within a graph. It helps in the classification of the vertices according to their role in the communities to which they belong. For instance, it may be possible to distinguish entities fully embedded within groups from those on the boundary of the group that may act as an intermediary between units. Such boundary nodes can play an essential role in installing the units together and in the procedures of deploying the processes over the network (Chakraborty *et al.*, 2017; Fortunato and Hric, 2016). The growing demand for developing effective frameworks to discover such community structure in complex networks, for instance, organizations or individuals are bonded through several social contacts, profiles, or familial. Thus, it can be said that social

modularity represented detection a group of individuals linked with dense social ties. Detecting social modularity is useful in social network analysis, network summarization and privacy, i.e. member grouping and group segmentation (Karataş and Şahin, 2018, Javed *et al.*, 2018). In general, the presence of community structure in complex networks made available an assortment of applications for example targeted marketing, grouping social media subscribers for good advertising in addition to facilitating recommendations for readers, discovering fraudulent sites, discovering fraudulent communication networks activities, designing network protocols in delay tolerant networks, link prediction, refactoring software packages, dimensional reduction in pattern recognition, recommendation systems, skills acquisition in robotics (Karataş and Şahin, 2018; Rahimi *et al.*, 2018) and tracking bitcoin users (Remy *et al.*, 2017). With the increasing demand for these and many other real-world applications, the community structure seeks to model the basic features of these complex networked-systems by determining sub-structures and their topological features.

In biological networks, cell activity in PPI networks can be comprehended by analyzing those proteins that are organized as separate and interactable units. Hence, the PPI modularity refers to detection a set of proteins that physically or functionally interact to achieve a specific function. Additionally, detection of protein complexes in PPI networks can help in many significant therapeutic purposes, describing the evolutionary orthology signal (Jancura *et al.*, 2012), detecting cancer, and predicting the biological functions of yet unrecognized proteins (Pizzuti, 2014). On the other hand, a change in the pattern of proteins interaction is associated with many diseases and identification of such interactions through detecting protein complexes can aid in disease diagnosis (Lei *et al.*, 2018; Bandyopadhyay *et al.*, 2015). In fact, the network can be better understood by knowing the organization of the objects; due to it will provide better information which may be missed by considering the network as a whole.

1.8 Thesis Organization

This thesis is organized into 7 chapters. Chapter 2 reviews some basic concepts, the related works of this study and discusses the gaps that led to formulating the research problem. Chapter 3 presents the methodology that this research followed as well as exploring and discussing the details of the framework components and the datasets being used. The experimental results of the proposed MOEA_CGN method based on general MOEA/D framework are presented in Chapter 4. Chapter 5 presents the experimental results of the proposed *MOEA_CGN* method with a new heuristic mutation operator. In Chapter 6, the experimental results of the proposed *MOEA_CGN* method with an improved heuristic mutation operator are presented in order to detect complex biological communities accurately. Finally, Chapter 7 concludes the research, future works and some suggestions are provided in this chapter.

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