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ANALYSIS OF PARTICULAR COMPLEX NETWORKS USING TOPOLOGICAL INDICES

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Abstract- The concept of complex networks is a novel area in scientific research, describing a group of interconnected items and systems in nature and society, such as, the Internet, that represents a network of computers and routers connected to each other by physical links [2]. Indeed, social networks could be represented as complex networks by considering the accounts as vertices and the relationship between them as edges. In the last decades, social network analysis is getting growing attention in social sciences. The principal topic in the analysis of complex networks is studying the structures of a network and understanding the relationship between its components. The focus of this paper is on the topological indices as measure analysis, which belongs to topological descriptors 2D. A topological index is numeric values characterizing information relating to the topology and the structure of a molecular graph [27]. They have been used in the QSAR/QSPR models. In this paper, we are going to calculate the Degree distance as measure for some particular complex networks.

Keywords: Complex Network, Analysis of Topological Structures, QSPR/QSAR, Degree Distance Index, Social Networks Analysis.

1. INTRODUCTION

In recent years, the study of complex networks getting inspired by the analysis of real-world networks, which are all around us in different domains. Furthermore, researchers developed various methods and techniques to allow us to understand and predict the behavior of these networks [3] [4].

The word "complex network" refers to the fact that it is impossible to predict the behavior of these systems from their components [4].

The classification of complex networks relates to the nature of the relationship between the components of a network. There are several types of interaction between the different entities of a complex network, we note the physical relationships where the nodes are connected to each other by cables (e.g., internet), social relationships between human beings (e.g., friendship), geographic relationships where nodes represent regions (e.g. countries in a map) [5], [26].

Taking the example of social networks, they can be considered as complex networks. These vertices represent people with different nationalities, locations, ages ...etc., and the edges represent friendship or the relation between them. [3], [9], [10], [27].

The study of graph theory uses graphs to understand the standard for analyzing networks and detecting temporal changes in their structures. Graph theory uses graphs to model real-world situations in different domains such as mathematical chemistry, social sciences, computer sciences, industry, and others [10], [16], [25], [27].

The QSPR/QSAR are mathematical methods started with the representation of the information of molecule by using molecular descriptors. In other words, the QSAR/QSAR methods are based on the analysis of the relationship between the different components of a molecule [6], [28].

Molecular descriptors have an important role in the study of the QSAR/QSPR methods, which describe the information of a molecule, classified according to the dimensionality of the molecular representation [27], [28], [29]. In this work, our study is limited to the class of 2D descriptors that uses the representation of molecules as graphs. In this class, we find a category called topological indices [1], [27].

A topological index of a network is a numerical value characterizing information relating to the topology of a network. It is used to represent the structure of network with a graph [7], [8], [24], [27].

Let G be a connected graph composed of a set of vertices V and a set of edges E. The shortest path connecting two vertices in G is called the distance $d(u, v)$. The diameter $D(G)$ of a graph G is the longest distance between two vertices of this graph [29]. The degree of the vertex v, denoted by $\deg(v)$, is the number of edges incident to u [1], [29], [30].

The main purpose of topological indices is to measure the topological properties of a molecule, the oldest distance based topological index called the Wiener Index, introduced in 1947 by H. Wiener, which represent the sum of the distances between all the paires of vertices in a graph [8], [28], defined as: $W(G)=\sum_{\{u,v\}\subseteq V(G)} d(u,v)$, [27].

The Degree Distance index is the most popular degree-distance based topological index [27], [28], proposed in MTI (Molecular topological index) by Schultz [14]. It has been subject to many changes by Dobrynin and Kochetova [11] and Gutman [12], [13], [14].

In this article, we interested in the distance index of degree *DD*(*G*), particularly by its new formula based on the parameter $d_G^u(k)$, proposed in article [17].

The $d_G^u(k)$ is defined as the number of pairs of vertices of graph *G* which are far from *u* by *k* with (*k* <= *D* (*G*)). This parameter plays an important role in our method for analysing and understanding the structure of Complex Networks, after representing their entities as a set of vertices and the relation between them as a set of edges [13], [14], [15].

In [1], we introduced a method to analyze Complex networks and understand changes in their structures by using the *DD*(*G*) index. We proposed formulas to calculate the *DD*(*G*) index of networks connected to each other in different ways.

The main result of this article is to analyze three complex networks using the topological measure *DD*(*G*). The analysed networks will be simulated by three graphs named The Wheel vertex's graph, The Wheel edge's graph and The Wheel path's graph [1].

2. THE WHEEL VERTEX'S NETWORK

2.1. The Wheel Vertex's Graph

The Wheel vertex's graph, denoted by *WV*, is graph composed by *N* (*N*≥ 2) Wheel's graphs W_i connected by a common vertex *S* such that $|V(W_i)|\ n_w$ and $|E(W_i)|=m_w$ (Figure 1).

The Wheel vertex's graph has:

- The vertices number: $n=N(n_W-1)$
- The number of edges: $m=Nm_W$
- The vertices number of degree n_w-1: *N*
- The vertices number of degree 3: $N(n_W-2)$
- The vertices number of degree 6: 1;

2.2. The Main Result

Lemma 2.1: Let *WV* be a Wheel vertex's graph, previously described in (Section 2.1), we have:

- $DD(W_i)=7n_w^2-23n_w+16$, [22].
- For $u\in V(W_i)$, $i\in\{1,2,3,....,N\}$:

$$d_{W_i}^u(k)=\begin{cases}3(N-1) \text{ if } : k=2,\ d(u,s)=1\\ (n_w-4)(N-1) \text{ if } : k=3,\ d(u,s)=1\\ 3(N-1) \text{ if } : k=3,\ d(u,s)=2\\ (n_w-4)(N-1) \text{ if } : k=4\ ,d(u,s)=2\end{cases}$$

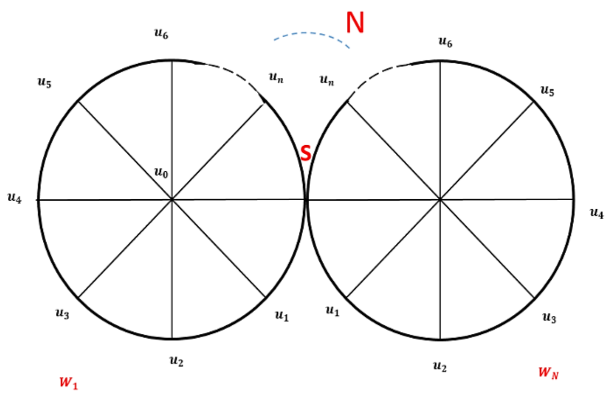

Figure 1. The Wheel vertex's graph *WV* composed of *N* Wheel graph W_i

Corollary 2.2: Let *WV* be a Wheel vertex's graph, previously described in (Section 2.1), The Degree Distance index of Wheel vertex's graph WV is:

$$DD(WV)=N[4(N-1)m_w(n_w-1)+\frac{7}{2}n^2{}_w(n^2{}_wN+1)- \\ -19n_wN-4n_w-4] \quad (1)$$

For proving our result, we use the Lemma 2.1 and the formula has proved in [1]:

$$DD(WV)\ =\ \sum_{i=1}^{N}[(DD(W_i))+\sum_{j=1}^{N}W_{ij}]$$

with:

$$W_{ij}\ =\ 4m_w(n_w-1)+\frac{1}{2}\sum_{u\in V(W_i)}\sum_{i=1}^{D(WV)}\deg(u)(k-2)d_{W_j}^v(k)$$

2.3. The Simulated Social Network

The Wheel vertex's graph represents a complex network, containing a common user account (vertex S) in a social network on the internet, which is a member in *N* groups of this social network (For example WhatsApp). Each group has n users, and each of them has at least 3 friendships (deg (*u*) = 3). The vertex in the center of each W_i graph represents the administrator of the group, who is the only one who had a direct relationship with all the members of the group (deg (*u*) = n_w–1).

The main result of subsection 2.2 describes the user importance by the degree in this complex network by using the $d_{W_i}^u(k)$ and the $\mathrm{dd}(u,W_i)$ where $(dd(u,W_i)=\sum_{k=1}^{D(W_i)}\deg(u)(k-2)d_{W_i}^u(k))$ [27], and describes the importance of social media groups using the *DD*(*WV*).

2.4. Application

As an application, we have tried to calculate the degree distance index for several cases by changing the important variables of our formula. The following Figure 2 shows the change in the value of the *DD*(*WV*) according to *N*, n_w, and m_w.

The result of this application shows the importance of the number of groups in a social network and its influence has a point, which is shown in the result of the *DD* (*WV*).

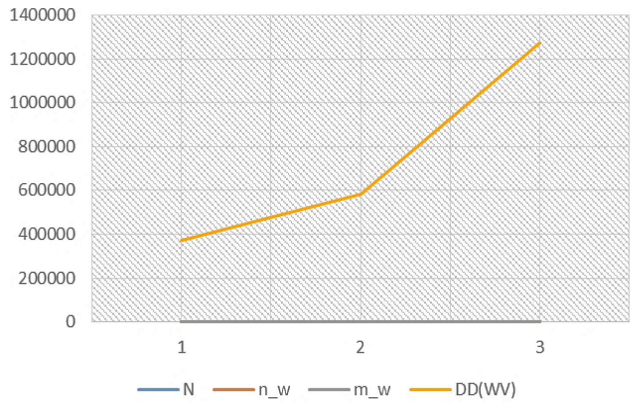

Figure 2. Application of the DD(WV) formula on different cases

3. THE WHEEL EDGE'S NETWORK

3.1. The Wheel Edge's Graph

The Wheel edge’s graph, denoted by *WE*, is graph composed by N ($N \geq 2$) Wheel's graphs W_i such that $|V(W_i)| = n_w$ and $|E(W_i)| = m_w$ connected by a common vertex s and a set of edges $\{s, u_i\}$, $i \in \{1,2,3,....,N\}$ see Figure 3.

The Wheel edge’s graph has:

- The vertices number: $n = Nn_W + 1$
- The number of edges: $m = N(n_W + 1)$
- The vertices number of degree 4: $N+1$
- The vertices number of degree 3: $N(n_W - 2)$
- The vertices number of degree $n_W - 1$: N;

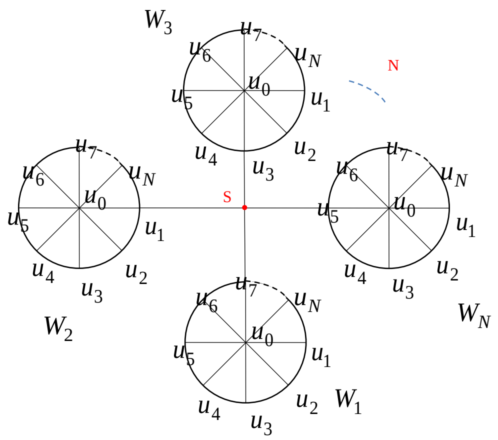

Figure 3. Wheel edge's graph *WE* composed of N Wheel's graph W_i

3.2. The Main Result

Lemma 3.1: Let *WV* be a Wheel edge’s graph, previously described in (Section 3.1), we have:

- $DD(W_i) = 7n_w^2 - 23n_w + 16$, [22].
- For $u \in V(W_i)$, $i \in \{1,2,3,....,N\}$:

$$d_{W_i}^u(k) = \begin{cases} N, \text{ if } : k=1,\ u=s \\ 3N, \text{ if } : k=2,\ u=s \\ N(n_w-4), \text{ if } : k=3,\ u=s \\ N-1, \text{ if } : k=2,\ d(u,s)=1 \\ 3(N-1), \text{ if } : k=3,\ d(u,s)=1 \\ (n_w-4)(N-1), \text{ if } : k=4,\ d(u,s)=1 \\ N-1, \text{ if } : k=3,\ d(u,s)=2 \\ 3(N-1), \text{ if } : k=4,\ d(u,s)=2 \\ (n_w-3)(N-1), \text{ if } : k=5,\ d(u,s)=2 \\ N-1, \text{ if } : k=4,\ d(u,s)=3 \\ 3(N-1), \text{ if } : k=5,\ d(u,s)=3 \\ (n_w-4)(N-1), \text{ if } : k=6,\ d(u,s)=3 \end{cases}$$

Corollary 3.2: Let WE be a Wheel edge’s graph, previously described in (Section 3.1), The Degree Distance index of Wheel edge’s graph *WE* is:

$$DD(WE) = N[4(N-1)n_w(m_w-1) + m_w + 7n^2{}_w + 19Nn_w + \frac{37}{2}n_w N - 40n_w + \frac{59}{2}] \tag{2}$$

For proving our result, we use the Lemma 3.1 and the formula has proved in [1]:

$$DD(WE) = \sum_{i=1}^{N}[(DD(W_i)) + dd_{W_i}(s) + \sum_{j=1}^{N} W_{ij}] + S$$

with:

$$W_{ij} = 4n_w(m_w+1) + \frac{1}{2}\sum_{u \in V(W_i)} \sum_{i=1}^{D(WE)} \deg(u)(k-2)d_{W_j}^{v}(k)]$$

and:

$$dd_{W_i}(s) = \sum_{i=1}^{D(W_i+1)} \deg(s)(k-2)d_{W_i}^{S}(k)$$

$$S = \sum_{i=1}^{N} n_w + \sum_{i=1}^{N} m_w$$

3.3. Simulated Social Network

The Wheel edge's graph represents another complex network, containing a user account S who is a member in N groups of a social network on the internet. These groups have one common user (vertex S) with a direct relationship with the administrators of the groups $(d(s,u)=1)$.

The principle of this simulation is to capture the notion of importance in a social network by identifying the most significant vertices in terms of degree. The result allows measuring how close a user is to all the other users in network via the $d_{W_i}^u(k)$, as well as its influence on the different parts of this network via the *DD* (*WE*).

3.4. Application

As an application, we have tried to calculate the degree distance index for several Wheel edge's networks by changing the important variables of our formula. The following Figure 4. shows the change in the value of the $DD(WE)$ according to N, n_w, and m_w.

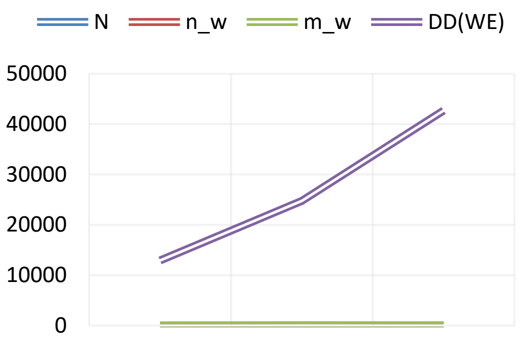

Figure 4. Application of the $DD(WE)$ formula on different cases

This application explains how sharing information by the different parts of a social network is important. This example shows us the influence of the transmission of information to the largest possible persons (the value of $DD(WE)$ increases).

4. THE WHEEL PATH'S NETWORK

4.1. The Wheel Path's Graph

The Wheel path's graph, denoted by WP, is graph composed by N ($N\geq 2$) Wheel's graphs W_i such that $|V(W_i)|=n_w$ and $|E(W_i)|=m_w$ connected by a vertex s_i, and a set of edges $\{s_i, s_{i+1}\}$, $i\in\{1,2,3,....,N\}$ (Figure 5).

The Wheel path's graph has:

- The vertices number: $n = Nn_W$
- The number of edges: $m = N(m_W+1)-1$
- The vertices number of degree 4 : 2
- The vertices number of degree 3: $N(n_W-2)$
- The vertices number of degree 5: $N-2$
- The vertices number of degree n_W-1 : N;

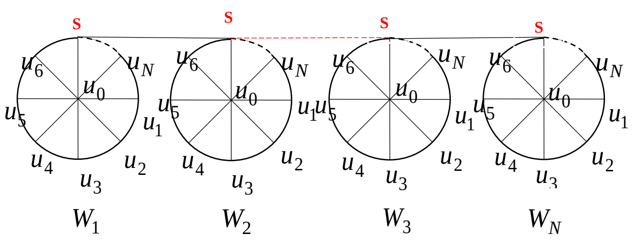

Figure 5. The Wheel path's graph WP composed by N Wheel graph W_i

4.2. The Main Result

Lemma 4.1: Let WP be a Wheel path's graph, previously described in (Section 4.1), we have:

- $DD(W_i)=7n_w^2-23n_w+16$, [22].
- For $s_i\in V(W_i)$:

$$d_{W_i}^{s_i}(k)=\begin{cases} N, \text{ if}: k=1,\ i=1,N \\ 4, \text{ if}: k=2,\ i=1,N \\ n_w, \text{ if}: k=\{3,.....,D(WP)-4\},\ i=1,N \\ n_w-1, \text{ if}: k=D(WP)-3,\ i=1,N \\ n_w-4, \text{ if}: k=D(WP)-2,\ i=1,N \\ 2, \text{ if}: k=1,\ i=2,N-1 \\ 7, \text{ if}: k=2,\ i=2,N-1 \\ 2n_w-5, \text{ if}: k=3,\ i=2,N-1 \\ n_w, \text{ if}: k=\{4,.....,D(WP)-5\},\ i=2,N-1 \\ n_w-1, \text{ if}: k=D(WP)-4,\ i=2,N-1 \\ n_w-4, \text{ if}: k=D(WP)-3,\ i=2,N-1 \\ 2, \text{ if}: k=1,\ i\neq 1,2,N-1,N \\ 8, \text{ if}: k=2,\ i\neq 1,2,N-1,N \\ 2n_w-1, \text{ if}: k=\{3,...,D(WP)-6\},\ i\neq 1,2,N-1,N \\ n_w-1, \text{ if}: k=D(WP)-5,\ i\neq 1,2,N-1,N \\ n_w-4, \text{ if}: k=D(WP)-4,\ i\neq 1,2,N-1,N \end{cases}$$

For $u\in V(W_i)$, $d(u,s_i)=1$:

$$d_{W_i}^{u}(k)=\begin{cases} 1, \text{ if}: k=2,\ i=1,N \\ 4, \text{ if}: k=3,\ i=1,N \\ n_w, \text{ if}: k=\{4,.....,D(WP)-3\},\ i=1,N \\ n_w-1, \text{ if}: k=D(WP)-2,\ i=1,N \\ n_w-4, \text{ if}: k=D(WP)-1,\ i=1,N \\ 2, \text{ if}: k=2,\ i=2,N-1 \\ 7, \text{ if}: k=3,\ i=2,N-1 \\ 2n_w-4, \text{ if}: k=4,\ i=2,N-1 \\ n_w, \text{ if}: k=\{5,....,D(WP)-4\},\ i=2,N-1 \\ n_w-1, \text{ if}: k=D(WP)-3,\ i=2,N-1 \\ n_w-4, \text{ if}: k=D(WP)-2,\ i=2,N-1 \\ 2, \text{ if}: k=2,\ i\neq 1,2,N-1,N \\ 8, \text{ if}: k=3,\ i\neq 1,2,N-1,N \\ 2n_w-1, \text{ if}: k=4,\ i\neq 1,2,N-1,N \\ 2n_w-4, \text{ if}: k=\{5,...,D(WP)-4\},\ i\neq 1,2,N-1,N \\ n_w-1, \text{ if}: k=D(WP)-3,\ i\neq 1,2,N-1,N \\ n_w-4, \text{ if}: k=D(WP)-2,\ i\neq 1,2,N-1,N \end{cases}$$

▪ For $u \in V(W_i)$, $d(u, s_i) = 2$:

$$d_{W_i}^u(k) = \begin{cases} 1, \text{ if}: k = 3,\ i = 1, N \\ 4, \text{ if}: k = 4,\ i = 1, N \\ n_w, \text{ if}: k = \{5, \ldots, D(WP) - 2\},\ i = 1, N \\ n_w - 1, \text{ if}: k = D(WP) - 1,\ i = 1, N \\ n_w - 4, \text{ if}: k = D(WP),\ i = 1, N \\ 2, \text{ if}: k = 3,\ i = 2, N - 1 \\ 7, \text{ if}: k = 4,\ i = 2, N - 1 \\ 2n_w - 4, \text{ if}: k = 5,\ i = 2, N - 1 \\ n_w, \text{ if}: k = \{6, \ldots, D(WP) - 3\},\ i = 2, N - 1 \\ n_w - 1, \text{ if}: k = D(WP) - 2,\ i = 2, N - 1 \\ n_w - 4, \text{ if}: k = D(WP) - 1,\ i = 2, N - 1 \\ 2, \text{ if}: k = 3,\ i \neq 1, 2, N - 1, N \\ 8, \text{ if}: k = 4,\ i \neq 1, 2, N - 1, N \\ 2n_w - 1, \text{ if}: k = 5,\ i \neq 1, 2, N - 1, N \\ 2n_w - 4, \text{ if}: k = 6,\ i \neq 1, 2, N - 1, N \\ n_w, \text{ if}: k = \{7, \ldots, D(WP) - 4\},\ i \neq 1, 2, N - 1, N \\ n_w - 1, \text{ if}: k = D(WP) - 3,\ i \neq 1, 2, N - 1, N \\ n_w - 4, \text{ if}: k = D(WP) - 2,\ i \neq 1, 2, N - 1, N \end{cases}$$

Corollary 4.2: Let WP be a Wheel path's graph, previously described in (Section 4.1), The Degree Distance index of Wheel path's graph WP is:

$$\begin{aligned} DD(WP) &= NDD(W_i) + 4N(N-1)\, n_w (m_w + 1) + \\ &+ \frac{5}{2} N^3 n_w^2 - \frac{11}{2} N^2 n_w^2 - \frac{17}{2} N^3 n_w - 16 n_w N^2 - \\ &- 8 n_w^2 N + 10 N^3 - p - \frac{375}{2} N^2 - 56 n_w^2 - \frac{481}{2} n_w N - \\ &- 188 n_w - 5N - 300 \end{aligned} \quad (3)$$

For proving our result, we use the Lemma 4.1 and the formula has proved in [1]:

$$DD(WV) = \sum_{i=1}^{N} [(DD(W_i)) + \sum_{j=1}^{N} W_{ij}] - P$$

with:

$$W_{ij} = 4n_w (m_w + 1) + \frac{1}{2} \sum_{u \in V(W_i)} \sum_{i=1}^{D(WP)} \deg(u)(k-2) d_{W_j}^v(k)$$

and:

$$P = 4(N-1)$$

4.3. Simulated Social Network

The Wheel Path's graph is a complex network that represents the connectivity between each user (vertex) of a social network and his neighbors.

This network contains users $(s_1, s_2, s_3, \ldots, s_N)$, which belong to N different groups, have at least four direct relationships ($d_{W_i}^u(1) = 4$), and each friend of the vertices $(s_1, s_2, s_3, \ldots, s_N)$ has other neighbors which give as a result $d_{W_i}^u(2)$. The principle of this complex graph is clearly explaining how two different groups can be linked via the interaction of the neighboring users by sharing mutual information in their groups. The result of this simulation shows us the influence of the transmission of information to the largest possible persons.

4.4. Application

As an application, we have tried to calculate the degree distance index for several Wheel path's networks by changing the important variables of our formula. The following Figure 6. shows the change in the value of the $DD(WP)$ according to N, n_w, and m_w.

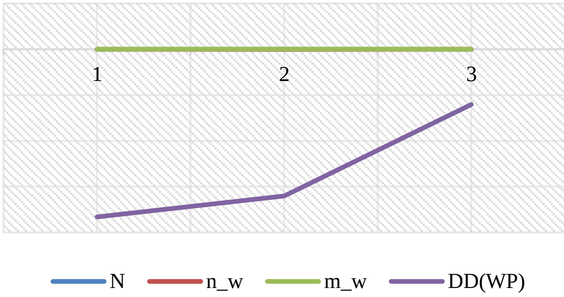

Figure 6. Application of the $DD(WP)$ formula on different cases

The result of this application shows us more we get users, the importance of a social network, its influence, and the transmission of information increases.

6. CONCLUSIONS

Graph theory has become a fundamental tool in analyzing complex networks. Understanding the relationship between structural properties of complex networks is an important key in the field of network science.

In this work, we described a method to model the structure of social networks using graph theory and topological indices as tools to understand changes in the structure of a network and analyze the relationship between its components by calculating the Degree Distance of certain complex networks connected to each other in different ways.

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