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ON THE TOPOLOGICAL PROPERTIES OF THE CERTAIN NEURAL NETWORKS

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Abstract

A topological index is a numeric quantity associated with a network or a graph that characterizes its whole structural properties. In [Javaid and Cao, *Neural Computing and Applications*, DOI 10.1007/s00521-017-2972-1], the various degree-based topological indices for the probabilistic neural networks are studied. We extend this study by considering the calculations of the other topological indices, and derive the analytical closed formulas for these new topological indices of the probabilistic neural network. Moreover, a comparative study using computer-based graphs has been carried out first time to clarify the nature of the computed topological descriptors for the probabilistic neural networks. Our results extend some known conclusions.

Keywords: neural network, topological indices, Graph theory

1 Introduction

During the past decades, various neural networks have been undergoing for a rapid development in the various areas of studies, such as neurochemistry, artificial intelligence, automatic control and informational sciences [1]. The neural networks are used for the calcium oscillation behavior in biological mathematical models [2], especially in the powerful brain-like "neural" computers [3]. In the studies of quantitative structure activity relationships (QSAR models) and quantitative structure property relationships (QSPR models), the physicochemical properties and topological indices are excellent tools to explore the biological and chemical activities of the chemical compounds [4, 5].

The numerical quantities which transform networks/compounds structures to a numerical number are called topological indices/descriptors. More precisely, a topological index $Top(G)$ is a function of a graph, in which if H is isomorphic to G, then $Top(H) = Top(G)$. In general, there are three major classes of topological indices which are distance-based topological indices, degree-based topological indices and counting related indices of graphs [6]. Topological indices are the useful tools provided by networks theory for theoretical study of networks properties.

Since the Sierpinski networks are the first non-trivial families of graphs, which have been extensively studied in the last few years. *M.Imran* et al. [7] had obtained the formulas for the *ABC* index, *GA* index and fourth and fifth version of the *ABC* and *GA* index in the Sierpinski networks in 2017. The further results of topological indices of the generalized tree and k-tree [8] have been presented by *S.H.Wang* et al. For the probabilistic neural networks, *M.Javaid* et al. [9] have investigated the degree based topological indices of them in 2017. More studies about topological indices of other networks, one may refer to [10, 11].

Motivated by a large number of applications on topological indices for the networks theory, the information regarding topological indices are obtained from the probabilistic neural networks (PNN's) which consist of three types of layers. Assume that first, second and third layers called by input, hidden and output layers have n nodes, k classes (each class contains m nodes) and k nodes, respectively [9]. In the construction of PNN, each node of an input layer is connected to all the nodes of each class of the hidden layer and all the nodes of each class of the hidden layer are connected to the unique corresponding node of the output layer. In Fig. 1, a PNN denoted by $PNN(n,k,m)$ is shown for $n=4, k=2$ and $m=3$.

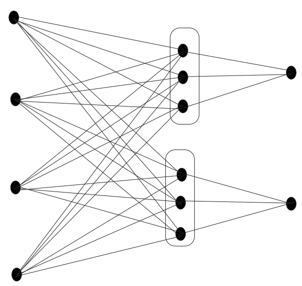


Figure 1. $PNN(4,2,3)$

The remaining of this paper is schematized as follows. Section 2 presents some preliminaries including the definitions and formulas. In Section 3, the main results are obtained for the TI's of the PNN and we conclude the whole paper in Section 4.

2 Preliminaries

A network is considered to be a connected graph having no multiple edges and no loops. We only consider finite and simple graphs here. Let $G=(V(G),E(G))$ be a graph with vertex-set $V(G)$ and edge-set $E(G)$. If $e \in E(G)$ has end vertices u and v, then we say that u and v are adjacent and this edge is denoted by uv. The cardinality of $V(G)$ is called the order of G. Let $d_i = d(v_i)$ be the degree of vertex v_i and $d(u,v)$ be the distance which is the length of the shortest path between u and v. The notations used in this article are mainly taken from the book [12].

The Wiener index of a connected graph G [13], denoted by $W(G)$, is recognized as the first proposed topological index, which is defined to be the sum of distances between every pair of vertices in G, i.e.,

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v).$$

The Harary index of a connected graph G, denoted by $H(G)$, is defined as

$$H(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)}.$$

During the past decades, it has received much attention [14]. Nowadays, several variants of Harary index are introduced from the theoretical or applied viewpoint [15]. There are some varying Harary indices, a part of these are listed below.

$$\begin{aligned} H_t(G) &= \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)+t}, \\ H_A(G) &= \sum_{\{u,v\}\subseteq V(G)} \frac{d(u)+d(v)}{d(u,v)}, \\ H_M(G) &= \sum_{\{u,v\}\subseteq V(G)} \frac{d(u)\times d(v)}{d(u,v)}. \end{aligned}$$

Moreover, for the additively weighted Harary index, there is another name which is reciprocal degree distance. And the name is from the celebrated topological index in chemical graph theory [16], which is called $DD(G)$ [17]. Furthermore, the definition of $DD(G)$ is given by

$$DD(G) = \sum_{\{u,v\}\subseteq V(G)} [d(u)+d(v)]d(u,v).$$

In the 1980s, *Narumi* and *Katayama* firstly considered the $NK(G)$ index [18], which is defined as

$$NK(G) = \prod_{v \in V(G)} d(v).$$

In [19], *Klein* and *Rosenfeld* investigated some properties of this topological index. In 1988, *H.Hosoya* introduced Hosoya polynomial as a counting polynomial. Later on, Hosoya polynomial for a vertex of a graph was introduced by *Gutman* [20], which is associated with Hosoya polynomial of the graph. As we know, its definition is given by

$$H(G,x) = \sum_{\{u,v\} \subseteq V(G)} x^{d(u,v)}.$$

Among the most significant molecular descriptors, the classically molecular invariants are named as Zagreb indices, which are expressed as expected formulas for the total π-electron energy of conjugated molecules [21]. As the known results and wide applications about Zagreb indices, we discuss the varying Zagreb indices, and they are given by

$$\overline{M_1}(G) = \sum_{u \neq v, uv \notin E(G)} [d(u) + d(v)],$$
$$\overline{M_2}(G) = \sum_{u \neq v, uv \notin E(G)} [d(u) \times d(v)].$$

Let $f(u)$ be any function of vertex u, and it is obeyed the following guidelines

$$\sum_{u \in V(G)} f(u) = \sum_{uv \in E(G)} [\frac{f(u)}{d((u)} + \frac{f(v)}{d(v)}].$$

It is worthy to mention that special case for $f(u) = d(u)^3$ is known as $F - coindex$ [22]. In this paper, we will discuss a varying $F - coindex$, which is given by [23]

$$\overline{F}(G) = \sum_{uv \notin E(G)} [d^2(u) + d^2(v)].$$

The irregularity index is the number of distinct terms of the degree sequence of G. It was introduced by *S.Mukwembi* [24] and its definition is given by

$$irr(G) = \sum_{uv \in E(G)} \mid d(u) - d(v) \mid .$$

For the first multiplication Zagreb index in details, one may refer to [25, 26, 27]. *Todeschini* et al. proposed the addition of additive graph invariants in the Zagreb index, and its definition is given by

$$\prod_1 (G) = \prod_{i=1}^{n} [d(v_i)]^2.$$

In 2000, *Ivanciuc* [28] and *Ivanciuc* et al. [29] firstly introduced the reciprocal complementary Wiener index, which is defined as

$$RCW(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d + 1 - d(u,v)},$$

where d is the diameter of G.

3 Main Results

This Section includes the main results of the present study.

Theorem 1 *Let $G \cong PNN(n,k,m)$, where n, k, $m \geq 1$. Then, the Wiener index of G is given as*

$$W(G) = n(n-1) + km(km + n + 3k - 3) + 2k(k + n - 1).$$

Proof. According to the definition of $W(G)$ in Section 2, $V(G)$ have the following six cases for calculating the distances between any two distinct vertices in $PNN(n,k,m)$.

(1) $u,v \in V_1$, (2) $u,v \in V_2$,
(3) $u,v \in V_3$, (4) $u \in V_1, v \in V_2$,
(5) $u \in V_1, v \in V_3$, (6) $u \in V_2, v \in V_3$.

Based on the above cases, one can get

$$\begin{aligned} W(G) &= \sum_{u,v \in V_1} d(u,v) + \sum_{u,v \in V_2} d(u,v) + \sum_{u,v \in V_3} d(u,v) \\ &+ \sum_{u \in V_1, v \in V_2} d(u,v) + \sum_{u \in V_1, v \in V_3} d(u,v) \\ &+ \sum_{u \in V_2, v \in V_3} d(u,v) \\ &= 2C_n^2 + 2C_{km}^2 + 4C_k^2 + kmn + 2kn \\ &+ km + 3km(k-1) \\ &= n(n-1) + km(km-1) + 2k(k-1) + kmn \\ &+ 2kn + km + 3km(k-1) \\ &= n(n-1) + km(km + n + 3k - 3) \\ &+ 2k(k + n - 1). \end{aligned}$$

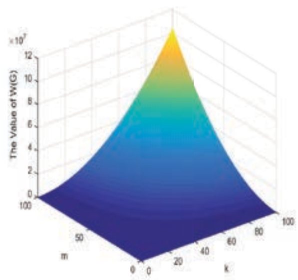
Theorem 2 *Let $G \cong PNN(n,k,m)$, where $n,k,m \geq 1$. Then, the Harary indices $H(G)$, $H_t(G)$, $H_A(G)$ and $H_M(G)$ are given as*

$H(G) = \frac{n(n-1)}{4} + \frac{km(km-1)}{4} + \frac{k(k-1)}{8} + \frac{kn}{2} + \frac{km(3n+k+2)}{3}$.

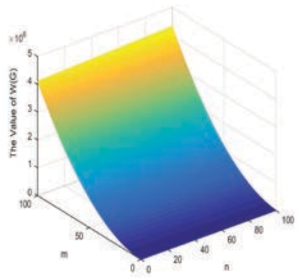
$H_t(G) = \frac{n(n-1)}{4+2t} + \frac{km(km-1)}{4+2t} + \frac{kn}{2+t} + \frac{k(k-1)}{8+2t} + \frac{km(n+1)}{1+t} + \frac{km(k-1)}{3+t}$.

$H_A(G) = \frac{kmn(n-1)}{2} + \frac{km(km-1)(n+1)}{2} + \frac{km(k-1)}{4} + kmn(km+n+1) + \frac{kmn(k+1)}{2} + \frac{km(m+n+1)(k+2)}{3}$.

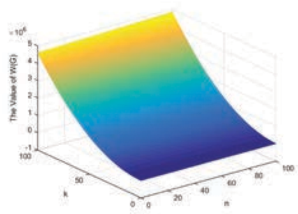
$H_M(G) = \frac{k^2m^2n(n-1)}{4} + \frac{km(km-1)(n+1)^2}{4} + \frac{km^2(k-1)}{8} + \frac{k^2m^2n(2n+3)}{2} + \frac{km^2(n+1)(k+2)}{3}$.



(a) n=100.



(b) k=20.



(c) m=20.

***Figure 2**. Computer-based comparative graph of the Wiener index for $PNN(n,k,m)$ and its expression is $W(G) = n(n-1) + km(km+n+3k-3) + 2k(k+n-1)$.*

Proof. According to the definition of *Harary* index, the distances between any two distinct vertices in $PNN(n,k,m)$ have the following six cases (1) $u,v \in V_1$, (2) $u,v \in V_2$, (3) $u,v \in V_3$, (4) $u \in V_1, v \in V_2$, (5) $u \in V_1, v \in V_3$, (6) $u \in V_2, v \in V_3$.

Based on the above cases, we can obtain

$$\begin{aligned} H(G) &= \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)} \\ &= \sum_{u,v\in V_1} \frac{1}{d(u,v)} \\ &+ \sum_{u,v\in V_2} \frac{1}{d(u,v)} + \sum_{u,v\in V_3} \frac{1}{d(u,v)} \\ &+ \sum_{u\in V_1, v\in V_2} \frac{1}{d(u,v)} \\ &+ \sum_{u\in V_1, v\in V_3} \frac{1}{d(u,v)} + \sum_{u\in V_2, v\in V_3} \frac{1}{d(u,v)} \\ &= \frac{1}{2}C_n^2 + \frac{1}{2}C_{km}^2 + \frac{1}{4}C_k^2 \\ &+ kmn + \frac{1}{2}kn + km + \frac{km(k-1)}{3} \\ &= \frac{n(n-1)}{4} + \frac{km(km-1)}{4} + \frac{k(k-1)}{8} \\ &+ \frac{kn}{2} + \frac{km(3n+k+2)}{3}. \end{aligned}$$

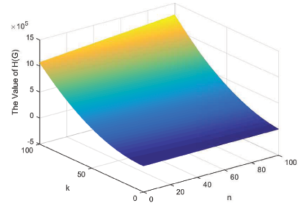
Under the definition of a varying Harary index, by the comparable approach as used in the $H(G)$, we can obtain the result as follows

$$H_t(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)+t}$$

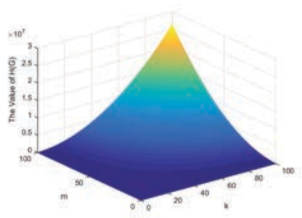
$= \sum_{u,v\in V_1} \frac{1}{d(u,v)+t} + \sum_{u,v\in V_2} \frac{1}{d(u,v)+t} + \sum_{u,v\in V_3} \frac{1}{d(u,v)+t} + \sum_{u\in V_1,v\in V_2} \frac{1}{d(u,v)+t} + \sum_{u\in V_1,v\in V_3} \frac{1}{d(u,v)+t} + \sum_{u\in V_2,v\in V_3} \frac{1}{d(u,v)+t}$

$= \frac{1}{2+t}C_n^2 + \frac{1}{2+t}C_{km}^2 + \frac{1}{4+t}C_k^2 + \frac{1}{1+t}kmn + \frac{1}{2+t}kn + \frac{1}{1+t}km + \frac{1}{3+t}km(k-1)$

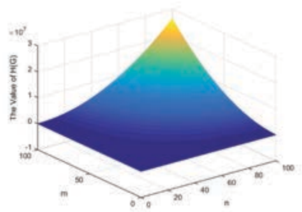
$= \frac{n(n-1)}{4+2t} + \frac{km(km-1)}{4+2t} + \frac{k(k-1)}{8+2t} + \frac{kmn}{1+t} + \frac{kn}{2+t} + \frac{km}{1+t} + \frac{km(k-1)}{3+t}$.



(a) m=20.

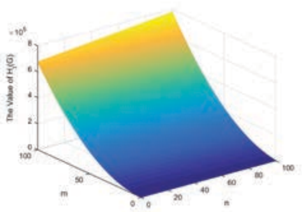


(b) n=100.

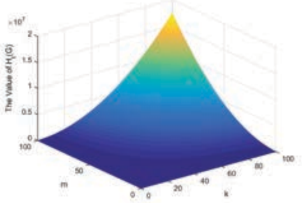


(c) k=20.

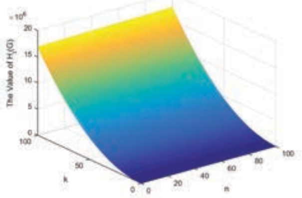
Figure 3. Computer-based comparative graph of the Harary index for $PNN(n,k,m)$ and its expression is $H(G) = \frac{n(n-1)}{4} + \frac{km(km-1)}{4} + \frac{k(k-1)}{8} + \frac{kn}{2} + \frac{km(3n+k+2)}{3}$.



(a) k=20, t=1.



(b) n=100, t=1.



(c) m=20, t=1.

Figure 4. Computer-based comparative graph of the $H_t(G)$ index for $PNN(n,k,m)$ and its expression is $H_t(G) = \frac{n(n-1)}{4+2t} + \frac{km(km-1)}{4+2t} + \frac{kn}{2+t} + \frac{k(k-1)}{8+2t)} + \frac{km(n+1)}{1+t} + \frac{km(k-1)}{3+t}$.

Especially, in the next two situations (based on the $H_t(G)$), let $t = 1$ or 2, respectively. Then we can obtain

$$\begin{aligned}
H_1(G) &= \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)+1} \\
&= \sum_{u,v\in V_1} \frac{1}{d(u,v)+1} + \sum_{u,v\in V_2} \frac{1}{d(u,v)+1} \\
&+ \sum_{u,v\in V_3} \frac{1}{d(u,v)+1} \\
&+ \sum_{u\in V_1, v\in V_2} \frac{1}{d(u,v)+1} \\
&+ \sum_{u\in V_1, v\in V_3} \frac{1}{d(u,v)+1} + \sum_{u\in V_2, v\in V_3} \frac{1}{d(u,v)+1} \\
&= \frac{1}{2+1}C_n^2 + \frac{1}{2+1}C_{km}^2 + \frac{1}{4+1}C_k^2 \\
&+ \frac{1}{1+1}kmn + \frac{1}{2+1}kn \\
&+ \frac{1}{1+1}km + \frac{1}{3+1}km(k-1) \\
&= \frac{n(n-1)}{6} + \frac{km(km-1)}{6} + \frac{k(k-1)}{10} \\
&+ \frac{km(n+1)}{2} + \frac{kn}{3} + \frac{km(k-1)}{4}.
\end{aligned}$$

And

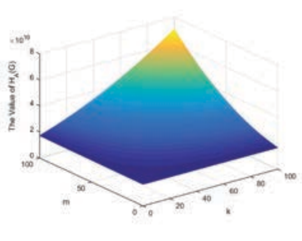
$$\begin{aligned}
H_2(G) &= \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)+2} \\
&= \sum_{u,v\in V_1} \frac{1}{d(u,v)+2} + \sum_{u,v\in V_2} \frac{1}{d(u,v)+2} \\
&+ \sum_{u,v\in V_3} \frac{1}{d(u,v)+2} \\
&+ \sum_{u\in V_1, v\in V_2} \frac{1}{d(u,v)+2} \\
&+ \sum_{u\in V_1, v\in V_3} \frac{1}{d(u,v)+2} + \sum_{u\in V_2, v\in V_3} \frac{1}{d(u,v)+2} \\
&= \frac{1}{2+2}C_n^2 + \frac{1}{2+2}C_{km}^2 \\
&+ \frac{1}{4+2}C_k^2 + \frac{1}{1+2}kmn + \frac{1}{2+2}kn \\
&+ \frac{1}{1+2}km + \frac{1}{3+2}km(k-1) \\
&= \frac{n(n-1)}{8} + \frac{km(km-1)}{8} + \frac{k(k-1)}{12} \\
&+ \frac{km(n+1)}{3} + \frac{kn}{4} + \frac{km(k-1)}{5}.
\end{aligned}$$

Based on the definition of $H_A(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{d(u)+d(v)}{d(u,v)}$, the distances between any two distinct vertices in $PNN(n,k,m)$ have the following six cases

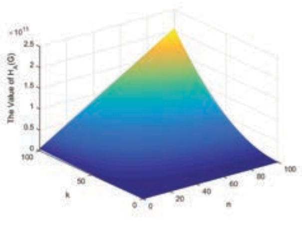
(1) $u,v \in V_1$, (2) $u,v \in V_2$,
(3) $u,v \in V_3$, (4) $u \in V_1, v \in V_2$,
(5) $u \in V_1, v \in V_3$, (6) $u \in V_2, v \in V_3$.

Based on the above cases, one can get

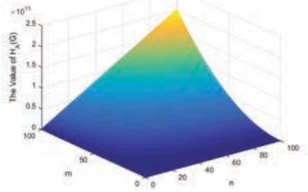
$$
\begin{aligned}
&H_A(G)\\
&= \sum_{u,v\in V_1} \frac{d(u)+d(v)}{d(u,v)} + \sum_{u,v\in V_2} \frac{d(u)+d(v)}{d(u,v)}\\
&+ \sum_{u,v\in V_3} \frac{d(u)+d(v)}{d(u,v)} + \sum_{u\in V_1, v\in V_2} \frac{d(u)+d(v)}{d(u,v)}\\
&+ \sum_{u\in V_1, v\in V_3} \frac{d(u)+d(v)}{d(u,v)} + \sum_{u\in V_2, v\in V_3} \frac{d(u)+d(v)}{d(u,v)}\\
&= \frac{2km}{2} C_n^2 + \frac{2(n+1)}{2} C_{km}^2\\
&+ \frac{2m}{4} C_k^2 + kmn(km+n+1) + \frac{km+m}{2} kn\\
&\quad + km(1+m+n) + \frac{m+n+1}{3} km(k-1)\\
&= \frac{kmn(n-1)}{2} + \frac{km(km-1)(n+1)}{2} +\\
&\frac{km(k-1)}{4} + kmn(km+n+1)\\
&\quad + \frac{kmn(k+1)}{2} + \frac{km(m+n+1)(k+2)}{3}.
\end{aligned}
$$



(a) n=100.



(b) m=20.

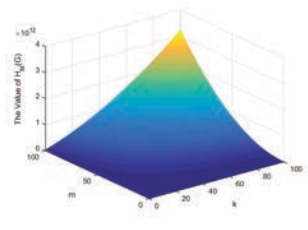


(c) k=20.

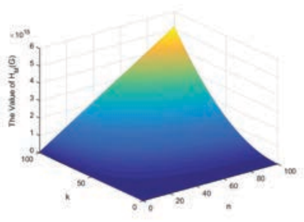
Figure 5. Computer-based comparative graph of the $H_A(G)$ index for $PNN(n,k,m)$ and its expression is $H_A(G) = \frac{kmn(n-1)}{2} + \frac{km(km-1)(n+1)}{2} + \frac{km(k-1)}{4} + kmn(km+n+1) + \frac{kmn(k+1)}{2} + \frac{km(m+n+1)(k+2)}{3}$.

Similarly, according to the definition of $H_M(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{d(u)\times d(v)}{d(u,v)}$, and its situations are same as $H_A(G)$, then we have

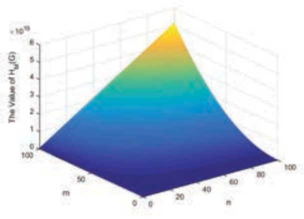
$$
\begin{aligned}
&H_M(G)\\
&= \sum_{u,v\in V_1} \frac{d(u)\times d(v)}{d(u,v)} + \sum_{u,v\in V_2} \frac{d(u)\times d(v)}{d(u,v)}\\
&\quad + \sum_{u,v\in V_3} \frac{d(u)\times d(v)}{d(u,v)} + \sum_{u\in V_1, v\in V_2} \frac{d(u)\times d(v)}{d(u,v)}\\
&\quad + \sum_{u\in V_1, v\in V_3} \frac{d(u)\times d(v)}{d(u,v)} + \sum_{u\in V_2, v\in V_3} \frac{d(u)\times d(v)}{d(u,v)}\\
&= \frac{k^2m^2}{2} C_n^2 + \frac{(n+1)^2}{2} C_{km}^2 + \frac{m^2}{4} C_k^2 + kmn[km(n+1)] +\\
&\frac{km^2}{2} kn + km[m(n+1)] + \frac{m(n+1)}{3} km(k-1)\\
&= \frac{k^2m^2n(n-1)}{4} + \frac{km(km-1)(n+1)^2}{4} + \frac{km^2(k-1)}{8}\\
&\quad + \frac{k^2m^2n(2n+3)}{2} + \frac{km^2(n+1)(k+2)}{3}.
\end{aligned}
$$



(a) n=100.



(b) m=20.



(c) k=20.

Figure 6. Computer-based comparative graph of the $H_M(G)$ index for $PNN(n,k,m)$ and its expression is
$H_M(G) = \frac{k^2m^2n(n-1)}{4} + \frac{km(km-1)(n+1)^2}{4} + \frac{km^2(k-1)}{8} + \frac{k^2m^2n(2n+3)}{2} + \frac{km^2(n+1)(k+2)}{3}$.

Theorem 3 *Let $G \cong PNN(n,k,m)$, where $n,k,m \geq 1$. Then the expression of $DD(G)$ is given as $DD(G) = kmn(km+2k+3n+1)+2km(km-1)(n+1)+4km(k-1)+km(m+n+1)(3k-2)$.*

Proof. As a celebrated topological index in chemical graph theory, the distances between any two distinct vertices in $PNN(n,k,m)$ have the following six cases

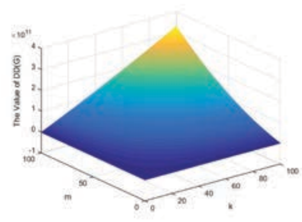
(1) $u,v \in V_1$,	(2) $u,v \in V_2$,
(3) $u,v \in V_3$,	(4) $u \in V_1, v \in V_2$,
(5) $u \in V_1, v \in V_3$,	(6) $u \in V_2, v \in V_3$.

Based on the definition of $DD(G) = \sum_{\{u,v\} \subseteq V(G)} [d(u)+d(v)]d(u,v)$, we have

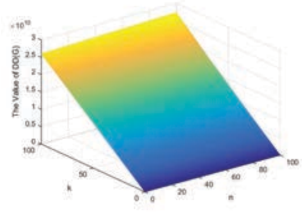
$DD(G) = \sum_{u,v \in V_1} [d(u)+d(v)]d(u,v) + \sum_{u,v \in V_2} [d(u)+d(v)]d(u,v) + \sum_{u,v \in V_3} [d(u)+d(v)]d(u,v) + \sum_{u \in V_1, v \in V_2} [d(u)+d(v)]d(u,v) + \sum_{u \in V_1, v \in V_3} [d(u)+d(v)]d(u,v) + \sum_{u \in V_2, v \in V_3} [d(u)+d(v)]d(u,v)$

$= 4kmC_n^2 + 4(n+1)C_{km}^2 + 8mC_k^2 + kmn(km+n+1) + 2kmn(k+1) + km(m+n+1) + 3km(k-1)(m+n+1)$

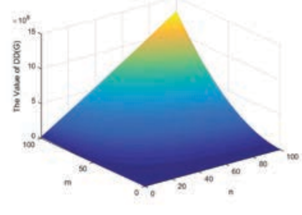
$= kmn(3n+km+2k+1) + 2km(km-1)(n+1) + 4km(k-1) + km(m+n+1)(3k-2)$.



(a) n=100.



(b) m=20.



(c) k=20.

Figure 7. Computer-based comparative graph of the $DD(G)$ index for $PNN(n,k,m)$ and its expression is
$DD(G) = kmn(km+2k+3n+1)+2km(km-1)(n+1)+4km(k-1)+km(m+n+1)(3k-2)$.

Theorem 4 *Let $G \cong PNN(n,k,m)$, where $n,k,m \geq 1$. Then the expression of $H(G,x)$ is given as*

$H(G,x) = \frac{k(k-1)}{2}x^4 + km(k-1)x^3 + knx^2 + \frac{n(n-1)}{2}x^2 + \frac{km(km-1)}{2}x^2 + kmx(n+1)$.

Proof. Obviously, the distances between any two distinct vertices in $PNN(n,k,m)$ have the following six cases:

(1) $u,v \in V_1$,	(2) $u,v \in V_2$,
(3) $u,v \in V_3$,	(4) $u \in V_1, v \in V_2$,
(5) $u \in V_1, v \in V_3$,	(6) $u \in V_2, v \in V_3$.

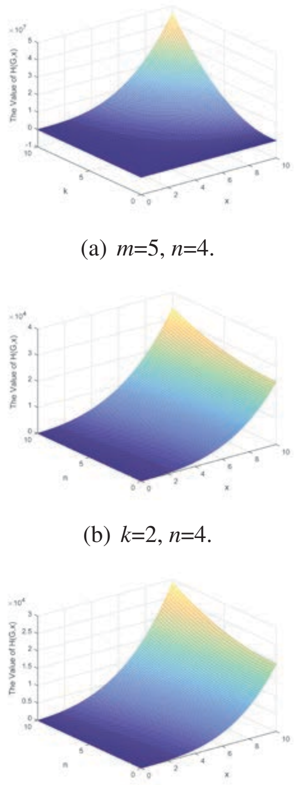
Under the definition of $H(G,x) = \sum_{\{u,v\} \subseteq V(G)} x^{d(u,v)}$ and the above cases, one can get

$H(G,x) = \sum_{u,v \in V_1} x^{d(u,v)} + \sum_{u,v \in V_2} x^{d(u,v)} + \sum_{u,v \in V_3} x^{d(u,v)} + \sum_{u \in V_1, v \in V_2} x^{d(u,v)} + \sum_{u \in V_1, v \in V_3} x^{d(u,v)} + \sum_{u \in V_2, v \in V_3} x^{d(u,v)}$

$= C_n^2 x^2 + C_{km}^2 x^2 + C_k^2 x^4 + C_n^1 C_{km}^1 x + C_n^1 C_k^1 x^2 + kmx + km(k-1)x^3$

$= \frac{n(n-1)}{2}x^2 + \frac{km(km-1)}{2}x^2 + \frac{k(k-1)}{2}x^4 + kmnx + knx^2 + kmx + km(k-1)x^3$

$= \frac{k(k-1)}{2}x^4 + km(k-1)x^3 + knx^2 + \frac{n(n-1)}{2}x^2 + \frac{km(km-1)}{2}x^2 + kmx(n+1).$



(a) m=5, n=4.

(b) k=2, n=4.

(c) k=2, m=3.

Figure 8. Computer-based comparative graph of the $H(G,x)$ index for $PNN(n,k,m)$ and its expression is $H(G,x) = \frac{k(k-1)}{2}x^4 + km(k-1)x^3 + knx^2 + \frac{n(n-1)}{2}x^2 + \frac{km(km-1)}{2}x^2 + kmx(n+1)$.

Theorem 5 *Let $G \cong PNN(n,k,m)$, where $n,k,m \geq 1$. Then, the first Zagreb index and second Zagreb index are as follows*

$$\overline{M_1}(G) = km[n^2 + (n+1)(k+km-1) - 1].$$

$$\overline{M_2}(G) = \frac{k^2m^2n(n+1)}{2} + \frac{km(km-1)(n+1)^2}{2} + \frac{km^2(k-1)}{2}.$$

Proof. Noting the definitions of $\overline{M_1}(G)$ and $\overline{M_2}(G)$, $V(G)$ have the following four cases for calculating $\overline{M_1}(G)$ and $\overline{M_2}(G)$. Moreover, based on the following cases, any two distinct vertices u and v are not adjacent:

(1) $u,v \in V_1$, (2) $u,v \in V_2$,
(3) $u,v \in V_3$, (4) $u \in V_1, v \in V_3$.

In $PNN(n,k,m)$, we firstly consider the $\overline{M_1}(G) = \sum_{u \neq v, uv \notin E(G)}[d(u)+d(v)]$. Then, we have

$$\begin{aligned}
&\overline{M_1}(G)\\
&= \sum_{u,v \in V_1}[d(u)+d(v)] + \sum_{u,v \in V_2}[d(u)+d(v)]\\
&\quad + \sum_{u,v \in V_3}[d(u)+d(v)] + \sum_{u \in V_1, v \in V_3}[d(u)+d(v)]\\
&= 2kmC_n^2 + 2(n+1)C_{km}^2 + 2mC_k^2 + C_n^1 C_k^1 (km+m)\\
&= km[n^2 + (n+1)(k+km-1) - 1].
\end{aligned}$$

Similarly, according to the definition of $\overline{M_2}(G) = \sum_{u \neq v, uv \notin E(G)}[d(u) \times d(v)]$, and its situations are same as $\overline{M_1}(G)$, then we can obtain

$\overline{M_2}(G) = \sum_{u,v \in V_1}[d(u) \times d(v)] + \sum_{u,v \in V_2}[d(u) \times d(v)] + \sum_{u,v \in V_3}[d(u) \times d(v)] + \sum_{u \in V_1, v \in V_3}[d(u) \times d(v)]$

$= C_n^2 km \cdot km + C_{km}^2 (n+1)(n+1) + C_k^2 m \cdot m + C_n^1 C_k^1 km \cdot m$

$= k^2m^2 \cdot \frac{n(n-1)}{2} + (n+1)^2 \cdot \frac{km(km-1)}{2} + m^2 \cdot \frac{k(k-1)}{2} + k^2m^2n$

$= \frac{k^2m^2n(n+1)}{2} + \frac{km(km-1)(n+1)^2}{2} + \frac{km^2(k-1)}{2}.$

Theorem 6 *Let $G \cong PNN(n,k,m)$ $n,k,m \geq 1$. Then, the expression of $\overline{F}(G)$ is given as*

$\overline{F}(G) = km^2(kn^2 - kn + k - 1) + km(km-1)(n+1)^2 + km^2n(k^2+1).$

Proof. According to the definition of $\overline{F}(G)$ in Section 2, there are the following four cases

(1) $u,v \in V_1$, (2) $u,v \in V_2$,
(3) $u,v \in V_3$, (4) $u \in V_1, v \in V_3$.

Based on the $\overline{F}(G) = \sum_{uv \notin E(G)}[d^2(u)+d^2(v)]$ and the above cases, one can get

$\overline{F}(G) = \sum_{u,v \in V_1}[d^2(u)+d^2(v)] + \sum_{u,v \in V_2}[d^2(u)+d^2(v)] + \sum_{u,v \in V_3}[d^2(u)+d^2(v)] + \sum_{u \in V_1, v \in V_3}[d^2(u)+d^2(v)]$

$= 2k^2m^2C_n^2 + 2(n+1)^2C_{km}^2 + 2m^2C_k^2 + kn[(km)^2+m^2]$

$= n(n-1)k^2m^2 + km(km-1)(n+1)^2 + k(k-1)m^2 + nk[m^2(k^2+1)]$

$= km^2(kn^2-kn+k-1)+km(km-1)(n+1)^2+km^2n(k^2+1).$

Theorem 7 *Let $G \cong PNN(n,k,m)$, where $n,k,m \geq 1$. Then the expression of $irr(G)$ is given as*

$$irr(G) = nkm \mid km-n-1 \mid + mk \mid n+1-m \mid .$$

Proof. According to the definition of $irr(G)$, just only two cases are known

$$(1) u \in V_1, v \in V_2, (2) u \in V_2, v \in V_3.$$

Based on the above cases and the $irr(G) = \sum_{uv \in E(G)} \mid d(u)-d(v) \mid$, we can arrive at

$irr(G) = \sum_{uv \subseteq E(G)} \mid d(V_1)-d(V_2) \mid + \sum_{uv \subseteq E(G)} \mid d(V_2)-d(V_3) \mid$

$= C_n^1C_{km}^1 \mid km-n-1 \mid + C_{km}C_k^1 \mid n+1-m \mid$

$= nkm \mid km-n-1 \mid + k^2m \mid n+1-m \mid .$

Theorem 8 *Let $G \cong PNN(n,k,m)$, where $n,k,m \geq 1$. Then, the first multiplication Zagreb index is given as*

$$\prod_1(G) = (km)^{2n}(n+1)^{2km}m^{2k}.$$

Theorem 9 *Let $G \cong PNN(n,k,m)$, where $n,k,m \geq 1$. Then the expression of $NK(G)$ is given as*

$$NK(G) = (km)^n(n+1)^{km}m^k.$$

Theorem 10 *Let $G \cong PNN(n,k,m)$, where $n,k,m \geq 1$. Then the reciprocal complementary Wiener index is given as*

$$RCW(G) = \frac{n(2k+n-1)}{6} + \frac{km(2km+3n+6k-5)}{12} + \frac{k(k-1)}{2}.$$

Proof. Based on the definition of $RCW(G)$ in Section 2, there are the following six cases

(1) $u,v \in V_1$, (2) $u,v \in V_2$,
(3) $u,v \in V_3$, (4) $u \in V_1, v \in V_2$,
(5) $u \in V_1, v \in V_3$, (6) $u \in V_2, v \in V_3$.

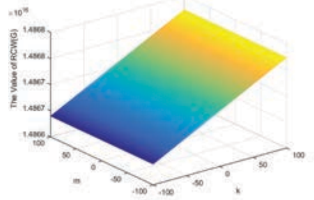
According to the above cases and $RCW(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d+1-d(u,v)}$, we have

$RCW(G) = \sum_{u,v \in V_1} \frac{1}{d+1-d(u,v)} + \sum_{u,v \in V_2} \frac{1}{d+1-d(u,v)} + \sum_{u,v \in V_3} \frac{1}{d+1-d(u,v)} + \sum_{u \in V_1, v \in V_2} \frac{1}{d+1-d(u,v)} + \sum_{u \in V_1, v \in V_3} \frac{1}{d+1-d(u,v)} + \sum_{u \in V_2, v \in V_3} \frac{1}{d+1-d(u,v)}$

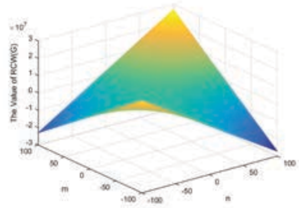
$= \frac{1}{d+1-2}C_n^2 + \frac{1}{d+1-2}C_{km}^2 + \frac{1}{d+1-4}C_k^2 + \frac{1}{d+1-1}kmn + \frac{1}{d+1-2}kn + \frac{1}{d+1-1}km + \frac{1}{d+1-3}km(k-1)$

$= \frac{n(n-1)}{6} + \frac{km(km-1)}{6} + \frac{k(k-1)}{2} + \frac{kmn}{4} + \frac{kn}{3} + \frac{km}{4} + \frac{km(k-1)}{2}$

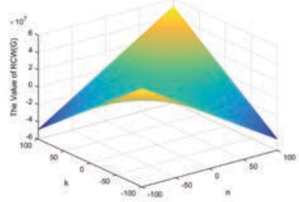
$= \frac{n(2k+n-1)}{6} + \frac{km(2km+3n+6k-5)}{12} + \frac{k(k-1)}{2}.$



(a) n=100.



(b) k=5.



(c) m=10.

Figure 10. Computer-based comparative graph of the $RCW(G)$ index for $PNN(n,k,m)$ and its expression is $RCW(G) = \frac{n(2k+n-1)}{6} + \frac{km(2km+3n+6k-5)}{12} + \frac{k(k-1)}{2}$.

4 Conclusion

In this paper, we calculated the degree-based topological indices (TI's) as well as distanced-based TI's of $PNN(n,k,m)$. Furthermore, the analytical closed formulas of degree-based and distance-based indices for the network were manifested, which will help the scholars to understand and explore the underlying topologies of $PNN(n,k,m)$, which are working in network science and physical features. In order to help us to know the properties of topological indices, which we had already computed, we plotted the three-dimensional graphics of the $W(G)$, $H(G)$, $H_t(G)$, $H_A(G)$, $H_M(G)$, $DD(G)$, $H(G,x)$, $NK(G)$ and $RCW(G)$ with the help of space cartesian coordinate system.

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6 Conflict of Interest

The authors declare that they have no conflict of interest.

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