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M-POLYNOMIAL METHOD FOR TOPOLOGICAL INDICES OF 3-LAYERED PROBABILISTIC NEURAL NETWORKS

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Abstract. A molecular network can be uniquely identified by a number, polynomial or matrix. A topological index (TI) is a number that characterizes a molecular network completely which is used to predict the physical features of the certain changes such as bioactivities and chemical reactivities in the chemical compound. Javaid and Cao [Neural Comput. and Applic., 30(2018), 3869-3876] studied the first Zagreb index, second Zagreb index, general Randic index, and augmented Zagreb index for the 3-layered probabilistic neural networks (PNN). In this paper, we prove the M-polynomial of the 3-layered PNN and use it as a latest developed tool to compute the certain degree based TI's. At the end, a comparison is also shown to find the better one among all the obtained results.
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1. Motivation and Introduction

In Neurochemistry, we study the processes which occur in nerve tissue or nervous system and a computer system model on the nerve tissue and nervous system is called a neural network. The probabilistic neural networks are studied to solve a number of problems in the different areas of engineering, medical, chemistry, computer and mathematics, see [38]. In particular, for the enhancement of the email security systems and the intrusion detection systems [39, 40], to verify the signature [2], to identify damage localization for bridges and the effectiveness for ships [28, 30], to predict the stability number of armor blocks of breakwaters [25], for detecting resistivity to antibiotics and diagnosing hepatitis [6, 8], for the segmentation and quantification of brain tissues from the certain type of

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images [42], and for the characterization of genetic variations in metabolic responses [20]. These networks are also applied in the environmental sciences, see [37]. Moreover, to know about the different properties of the probabilistic neural networks, we refer [23].

More recently, certain topological properties of 3-layered probabilistic neural networks are studied to find the physical changes of the bioactivities and chemical reactivities in these networks being significantly useful in the in chemical industry, particulary in pharmaceutical, see [22, 16]. In the present study, we prove M-polynomial of the 3-layered probabilistic neural networks and apply it as a latest developed technique to find the various topological indices (TI's) in the continuation of the progressive study of these networks.

In 1935, Polya defined the concept of a counting polynomial with remarkable applications in various areas of mathematics and chemistry [32]. Later on, Wiener (1947) introduced the first topological index as a boiling point of the paraffin [41]. A topological index is a numeric quantity that characterizes the whole structure of a molecular graph of the chemical compound and remains invariant for the isomorphic structures. With the help of the computed counting polynomials and the topological indices (TI's), we study the physical features, chemical reactivities and boiling activities of the chemical compound in the molecular graph, for example vapor pressure, surface tension, chromatographic retention times, heat of evaporation, heat of formation, melting point and boiling point [7, 24, 35].

Moreover, the topological indices are used to predict the bioactivity of the chemical compounds in the studies of quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) [14]. In particular, these are used to solve the problems related to optimisation procedure, molecular van der Waals volumes or areas, anticancer drugs, solubility, purification, extraction, liquids densities, enthalpies of combustion and vaporization for the acids ($C_2H_4O_2 - C_{20}H_{40}O_2$) [16, 17, 27, 29, 36, 44].

In the literature, degree-based TI's are most studied, see survey [15]. In particular, Gutman and Trinajsti (1972) [13] derived the first and the second Zagreb indices for the total energy of conjugated molecules. Later on these have been used as the branching indices [10, 9]. These are also used in the studies of the quantitative structure-activity relationship (QSAR) and the quantitative structure-property relationship (QSPR) [14]. Milan Randic (1975) [34] defined the TI which is called by Randic index. Bollobas and Erdos (1998) [5], and Amic et al. (1998) [1] defined the generalized Randic index independently. In 2010, the augmented Zagreb index is defined by Furtula et al. [12].

Many computational results of the topological indices (TI's) are also obtained on the various chemical structures, for example silicate network, hexagonal network, honeycomb network, fullerenes, carbon nanotube networks, rhombus silicate network and rhombus oxide network [3, 4, 21, 33]. For further study, we refer [9, 10, 14, 45, 26].

Moreover, Hosoya polynomial is a key polynomial in the area of distance-based TI's. The Wiener index can be obtained as the first derivative of the Hosoya polynomial at numeric value 1. Similarly, the hyper-Wiener index and the Tratch-Stankevich-Zefirov can be computed from the Hosoya polynomial. Recently, Deutsch and Klavzar (2015) [11] introduced the concept of M-polynomial and showed that its role for the degree-based TI's is parallel to the role of the Hosoya polynomial for the distance-based TI's. The M-polynomials of the polyhex nanotubes are studied in [31].

In this paper, we prove the M-polynomial of the 3-layered probabilistic neural networks. Then, by the use of this M-polynomial, we compute the topological indices based on the degree of vertices such as first Zagreb (M_1), second Zagreb (M_2), second modified Zagreb (MM_2), general Randic (R_α), reciprocal general Randic (RR_α), symmetric division deg (SDD), harmonic, inverse sum and the augmented Zagreb are computed for the 3-layered probabilistic neural networks. At the end, a comparison is also shown between all the obtained indices. The rest of the paper is organised as, in Section 2, we present definitions and formulas. Section 3 include the main results for the M-polynomial and topological indices. In Section 4, we present a comparison for all the obtained results.

2. Preliminaries

Let $\Gamma = (V(\Gamma), E(\Gamma))$ be a molecular graph with $V(\Gamma) = \{w_1, w_2, ..., w_n\}$ as a vertex-set and $E(\Gamma)$ as an edge-set such that the vertices (nodes) denote atoms and edges denote bonds between that atoms of the underlying chemical structure. If there is a connection between each pair of vertices, the graph is called a connected graph. The number of vertices that are connected to v by the edges is degree of v ($d(v)$). In this paper, we assume that a network is a simple (without multiple edges and loops) and finite connected graph. For the further study of the graph theory terminologies, we refer [18, 43].

Definition 2.1. Let Γ be a molecular graph. Then, first Zagreb index ($M_1(\Gamma)$), second Zagreb index ($M_2(\Gamma)$), general Randic index ($R_\alpha(\Gamma)$, whereα is a real number), symmetric division deg index (SDD) harmonic index ($HI(\Gamma)$), inverse sum index ($IS(\Gamma)$), and augmented Zagreb index ($AZI(\Gamma)$) of Γ are defined as follows.

$$M_1(\Gamma) = \sum_{v\in V(\Gamma)} [d(v)]^2 = \sum_{vw\in E(\Gamma)} [d(v)+d(w)],$$

$$M_2(\Gamma) = \sum_{vw\in E(\Gamma)} [d(v)\times d(w)], \;\; R_\alpha(\Gamma) = \sum_{vw\in E(\Gamma)} [d(v)\times d(w)]^\alpha,$$

$$SDD(\Gamma) = \sum_{vw\in E(\Gamma)} [\frac{min(d(v),d(w))}{max(d(v),d(w))}+\frac{max(d(v),d(w))}{min(d(v),d(w))}],$$

$$H(\Gamma) = \sum_{vw\in E(\Gamma)} \frac{2}{d(v)+d(w)} \;, IS(\Gamma) = \sum_{vw\in E(\Gamma)} \frac{d(v)\times d(w)}{d(v)+d(w)} \text{ and}$$

$$AZI(\Gamma) = \sum_{vw\in E(\Gamma)} [\frac{d(v)\times d(w)}{d(v)+d(w)-2}]^3.$$

Definition 2.2. Let Γ be a molecular graph and $E_{i,j}(\Gamma); i,j \geq 1$ be the sets which make the partition of the edge-set of Γ such that $\{d(u), d(v)\} = \{i, j\}$ for the edge uv. Then, M-polynomial of Γ is defined as

$$M(\Gamma, x, y) = \sum_{i\leq j} [E_{i,j}(\Gamma)x^i x^j].$$

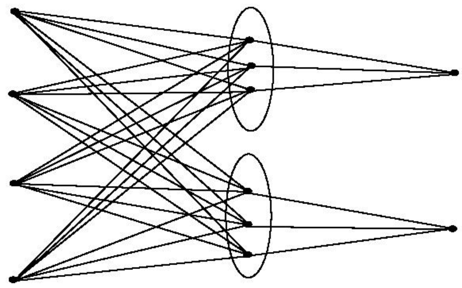

FIGURE 1. $PNN(4,2,3)$

Table 1:

Indices	$f(x,y)$	Derivation from $M(\Gamma,x,y)$
M_1	$x+y$	$(D_x+D_y)(M(\Gamma,x,y))\|_{x=1=y}$
M_2	xy	$(D_xD_y)(M(\Gamma,x,y))\|_{x=1=y}$
MM_2	$\frac{1}{xy}$	$(S_xS_y)(M(\Gamma,x,y))\|_{x=1=y}$
R_α	$(xy)^\alpha$, $\alpha \in N$	$(D_x^\alpha D_y^\alpha)(M(\Gamma,x,y))\|_{x=1=y}$
RR_α	$\frac{1}{(xy)^\alpha}$, $\alpha \in N$	$(S_x^\alpha S_y^\alpha)(M(\Gamma,x,y))\|_{x=1=y}$
SDD	$\frac{x^2+y^2}{xy}$	$(D_xS_y+D_yS_x)(M(\Gamma,x,y))\|_{x=1=y}$
H	$\frac{2}{x+y}$	$2S_xJ(M(\Gamma,x,y))\|_{x=1}$
IS	$\frac{xy}{x+y}$	$S_xQ_2JD_xD_y(M(\Gamma,x,y))\|_{x=1}$
AZI	$(\frac{xy}{x+y-2})^3$	$S_x^3JD_x^3D_y^3(M(\Gamma,x,y))\|_{x=1}$

In Table. 1, the relations between the aforesaid TI's and M-polynomial are defined. Moreover, MM_2 is second modified Zagreb, RR_α is reciprocal general Randić, $D_x = \frac{\partial(f(x,y))}{\partial(x)}$, $D_y = \frac{\partial(f(x,y))}{\partial(y)}$, $S_x = \int_0^x \frac{f(t,y)}{t}\,dt$, $S_y = \int_0^y \frac{f(x,t)}{t}\,dt$. $J(f(x,y)) = f(x,x)$ and $Q_\alpha(f(x,y)) = x^\alpha f(x,y)$, where $\alpha \neq 0$.

Now, we construct the 3-layered probabilistic neural network consisting on 3 layers of vertices. Suppose that there are n vertices in the first-layer (input-layer), k classes in the second-layer (hidden-layer) with m vertices in each class and k vertices in the third-layer (output-layer) such that each vertex of the first-layer is linked with all the vertices of each class of the second-layer and all the vertices of each class of the second-layer are linked to the unique vertex lying in the third-layer. Thus a 3-layered probabilistic neural network denoted by $PNN(n,k,m)$ has $n+k(m+1)$ vertices and $km(n+1)$ edges, where n, k and m are integers. Figure 1 presents $PNN(n,k,m)$ for $n=4$, $k=2$ and $m=3$.

3. MAIN RESULTS

In this section, we compute the M-polynomial of the 3-layered probabilistic neural network. Moreover, find the mathematical expressions for the certain degree-based TI's with the help of the M-polynomial.

Theorem 3.1. Let $\Gamma \cong PNN(n,k,m)$ be a 3-layered probabilistic neural network, where $n \geq 1$, $m,k \geq 2$, $n+1 \geq m$ and $km \geq n+1$. Then, the M-polynomial of Γ is
$M(\Gamma,x,y) = (km)x^my^{n+1} + (nkm)x^{n+1}y^{km}$.

Proof. From Fig. 1, we note that Γ has three types of vertices such as

$$V_1 = \{w \in V(\Gamma) | d(w) = \ km\},$$

$$V_2 = \{w \in V(\Gamma) | d(w) = n+1\},$$

and $$V_3 = \{\ w \in V(\Gamma) | d(w) =\ \ m\},$$

where $|V_1| = n$, $|V_2| = km$ and $|V_3| = k$. Consequently, $|V(PNN(n,k,m))| = v = |V_1| + |V_2| + |V_3| = n + k(m+1)$. Moreover, Γ has two types of edges such as

$$E_1 = E_{\{m,n+1\}} = \{vw \in E(\Gamma) | d(v) = m, d(w) = n+1\},$$

and $E_2 = E_{\{n+1,km\}} = \{vw \in E(\Gamma) | d(v) = n+1, d(w) = km\}$. Thus, we obtain the Tables 2 and 3.

Vertex partitions	V_1	V_2	V_3
Cardinality	n	km	k

Table.2: Vertex-partition sets.

Edge partitions	$E_1 = E_{\{m,n+1\}}$	$E_2 = E_{\{n+1,km\}}$
Cardinality	km	nkm

Table.3 Edge-Partition sets.

Now, by the use of Definition 2.2 and the Tables 2 and 3, we obtain

$M(\Gamma, x, y) = \sum\limits_{i \le j} [E_{i,j}(\Gamma) x^i y^j],$

$= \sum\limits_{m \le n+1} [E_{\{m,n+1\}}(\Gamma) x^m y^{n+1}] + \sum\limits_{n+1 \le km} [E_{\{n+1,km\}}(\Gamma) x^{n+1} y^{km}],$

$= |E_1| x^m y^{n+1} + |E_2| x^{n+1} y^{km},$

$= (km) x^m y^{n+1} + (nkm) x^{n+1} y^{km}.$

Theorem 3.2. Let $\Gamma \cong PNN(n,k,m)$ be the 3-layered probabilistic neural network and $M(\Gamma, x, y) = (km)x^m y^{n+1} + (nkm)x^{n+1} y^{km}$ be its M-polynomial, where $n \ge 1$, $m, k \ge 2$, $n+1 \ge m$ and $km \ge n+1$. Then, first Zagreb index ($M_1(\Gamma)$) and General Randic index, ($R_\alpha(\Gamma)$, where $\alpha \in N$) obtained from M-polynomial are as follows.

$(i) M_1(\Gamma) = mk[m(nk+1) + (n+1)^2],$

$(ii) R_\alpha(\Gamma) = (km)(1 + nk^\alpha)[m(n+1)]^\alpha.$

Proof. If $f(x,y) = M(\Gamma, x, y)$ then $f(x,y) = (km)x^m y^{n+1} + (nkm)x^{n+1} y^{km}$. Now, the required partial derivatives are obtained as

$D_x(f(x,y)) = m(km)x^{m-1} y^{n+1} + km(nkm)x^{n+1} y^{km-1},$

$D_y(f(x,y)) = (n+1)(km)x^m y^n + (km)(nkm)x^{n+1} y^{km-1},$

$D_x(D_y(f(x,y))) = m(n+1)(km)x^{m-1} y^n + (n+1)(km)(nkm)x^n y^{km-1},$

$D_x^\alpha(D_y^\alpha(f(x,y))) = (m(n+1))^\alpha (km)x^{m-1} y^n + (km(n+1))^\alpha (nkm)x^n y^{km-1}.$

Now, we obtain

$D_x(f(x,y))|_{x=1=y} = m(km) + km(nkm) = km^2 + nk^2 m^2,$

$D_y(f(x,y))|_{x=1=y} = (n+1)(km) + (km)(nkm) = km(n+1) + nk^2 m^2,$

$D_x(D_y(f(x,y)))|_{x=1=y} = m(n+1)(km) + (n+1)(km)(nkm),$

$D_x^\alpha(D_y^\alpha(f(x,y)))|_{x=1=y} = (m(n+1))^\alpha (km) + (km(n+1))^\alpha (nkm).$

Consequently,

$(i) M_1(\Gamma) = (D_x + D_y)(f(x,y))|_{x=1=y} D_x(f(x,y))|_{x=1=y} + D_y(f(x,y))|_{x=1=y},$

$= (km^2 + nk^2 m^2) + (km(n+1) + nk^2 m^2),$

$= mk[m(nk+1)+(n+1)^2]$,

$(ii) R_\alpha(\Gamma) = (D_x^\alpha D_y^\alpha)(f(x,y))|_{x=1=y}$,

$= (m(n+1))^\alpha(km)+(km(n+1))^\alpha(nkm)$,

$= (km)(1+nk^\alpha)[m(n+1)]^\alpha$.

In Corollary 3.3, we obtain the second Zagreb index by replacing $\alpha = 1$ in Theorem 3.2.

Corollary 3.3. Let $\Gamma \cong PNN(n,k,m)$ and $M(\Gamma,x,y) = (km)x^m y^{n+1} + (nkm)x^{n+1}y^{km}$, where $n \geq 1$, $m,k \geq 2$, $n+1 \geq m$ and $km \geq n+1$. Then, second Zagreb index of Γ is $M_2(\Gamma) = (D_x D_y)(f(x,y))|_{x=1=y} = (n+1)(km^2)(1+nk)$.

Theorem 3.4. Let $\Gamma \cong PNN(n,k,m)$ be the 3-layered probabilistic neural network and $M(\Gamma,x,y) = (km)x^m y^{n+1} + (nkm)x^{n+1}y^{km}$ be its M-polynomial, where $n \geq 1$, $m,k \geq 2$, $n+1 \geq m$ and $km \geq n+1$. Then, the reciprocal General Randic, ($RR_\alpha(\Gamma)$, where $\alpha \in N$) is obtained by the M-polynomial as follows.

$$RR_\alpha(\Gamma) = [1+\frac{n}{(k)^\alpha}]\frac{km}{[m(n+1)]^\alpha}.$$

Proof. If $f(x,y) = M(\Gamma,x,y)$ then $f(x,y) = (km)x^m y^{n+1} + (nkm)x^{n+1}y^{km}$. Now, the required integrals are obtained as

$$S_x(f(x,y)) = (\frac{km}{m})x^m y^{n+1} + (\frac{nkm}{n+1})x^{n+1}y^{km},$$

$$S_y(f(x,y)) = (\frac{km}{n+1})x^m y^{n+1} + (\frac{nkm}{km})x^{n+1}y^{km},$$

$$S_x S_y(f(x,y)) = (\frac{km}{m(n+1)})x^m y^{n+1} + (\frac{nkm}{km(n+1)})x^{n+1}y^{km},$$

$$S_x^\alpha S_y^\alpha(f(x,y)) = (\frac{km}{(m(n+1))^\alpha})x^m y^{n+1} + (\frac{nkm}{(km(n+1))^\alpha})x^{n+1}y^{km}.$$

Now, we obtain

$$S_x^\alpha S_y^\alpha(f(x,y))|_{x=1=y} = \frac{km}{(m(n+1))^\alpha} + \frac{nkm}{(km(n+1))^\alpha}.$$

Consequently,

$(v) RR_\alpha(\Gamma) = (S_x^\alpha S_y^\alpha)(f(x,y))|_{x=1=y}$,

$= [1+\frac{n}{(k)^\alpha}]\frac{km}{[m(n+1)]^\alpha}$.

The second modified Zagreb index ($MM_2(\Gamma)$) can be obtain using $\alpha = 1$ in Theorem 3.4 as stated in Corollary 3.5.

Corollary 3.5. Let $\Gamma \cong PNN(n,k,m)$ be the 3-layered probabilistic neural network and $M(\Gamma,x,y) = (km)x^m y^{n+1} + (nkm)x^{n+1}y^{km}$ be its M-polynomial, where $n \geq 1$, $m,k \geq 2$, $n+1 \geq m$ and $km \geq n+1$. Then, the second modified Zagreb is
$MM_2(\Gamma) = (S_x S_y)(f(x,y))|_{x=1=y} = S_x(S_y(f(x,y)))|_{x=1=y} = \frac{k}{n+1}[1+\frac{n}{k}]$.

Theorem 3.6. Let $\Gamma \cong PNN(n,k,m)$ be the 3-layered probabilistic neural network and $M(\Gamma,x,y) = (km)x^m y^{n+1} + (nkm)x^{n+1}y^{km}$ be its M-polynomial, where $n \geq 1$, $m,k \geq 2$, $n+1 \geq m$ and $km \geq n+1$. Then, the symmetric division degree index ($SDD(\Gamma)$) is obtained by the M-polynomial as follows.

$$SDD(\Gamma) = \frac{1}{n+1}[(n+1)^2(n+k)+km^2(1+nk)].$$

Proof. If $f(x,y) = M(\Gamma,x,y)$ then $f(x,y) = (km)x^m y^{n+1} + (nkm)x^{n+1}y^{km}$. Now, the required expressions are

$S_x(f(x,y)) = (k)x^m y^{n+1} + (\frac{nkm}{n+1})x^{n+1}y^{km}$,

$S_y(f(x,y)) = (\frac{km}{n+1})x^m y^{n+1} + (n)x^{n+1}y^{km}$,

$D_yS_x(f(x,y)) = (n+1)(k)x^m y^n + n(\frac{k^2m^2}{n+1})x^{n+1}y^{km-1}$,

$D_xS_y(f(x,y)) = (\frac{km^2}{n+1})x^{m-1}y^{n+1} + n(n+1)x^n y^{km}$.

Now, we obtain

$D_yS_x(f(x,y))|_{x=1=y} = (n+1)(k) + n(\frac{k^2m^2}{n+1})$,

$D_xS_y(f(x,y))|_{x=1=y} = (\frac{km^2}{n+1}) + n(n+1)$.

Consequently,

$SDD(\Gamma) = (D_xS_y + D_yS_x)(f(x,y)) = (D_xS_y)(f(x,y)) + (D_yS_x)(f(x,y))$,

$= D_x(S_y(f(x,y))) + D_y(S_x(f(x,y)))$,

$= [(n+1)(k) + n(\frac{k^2m^2}{n+1})] + [(\frac{km^2}{n+1}) + n(n+1)]$,

$= (n+1)(n+k) + (\frac{km^2}{n+1})(1+nk) = \frac{1}{n+1}[(n+1)^2(n+k) + km^2(1+nk)]$.

Theorem 3.7. Let $\Gamma \cong PNN(n,k,m)$ be the 3-layered probabilistic neural network and $M(\Gamma,x,y) = (km)x^m y^{n+1} + (nkm)x^{n+1}y^{km}$ be its M-polynomial, where $n \geq 1$, $m,k \geq 2$, $n+1 \geq m$ and $km \geq n+1$. Then, harmonic index ($H(\Gamma)$) obtained from M-polynomial is as follows.

$H(\Gamma) = 2km[\frac{m(k+n) + (n+1)^2}{(km+n+1)(m+n+1)}]$.

Proof. If $f(x,y) = M(\Gamma,x,y)$ then $f(x,y) = (km)x^m y^{n+1} + (nkm)x^{n+1}y^{km}$. Now, the required expressions are obtained as

$J(f(x,y)) = (km)x^{m+n+1} + (nkm)x^{km+n+1}$,

$S_x(Jf(x,y)) = (\frac{km}{m+n+1})x^{m+n+1} + (\frac{nkm}{km+n+1})x^{km+n+1}$.

Now, we obtain

$S_x(Jf(x,y))|_{x=1=y} = \frac{km}{m+n+1} + \frac{nkm}{km+n+1}$.

Consequently,

$H(\Gamma) = 2S_x(Jf(x,y))|_{x=1=y}$,

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

Theorem 3.8. Let $\Gamma \cong PNN(n,k,m)$ be the 3-layered probabilistic neural network and $M(\Gamma,x,y) = (km)x^m y^{n+1} + (nkm)x^{n+1}y^{km}$ be its M-polynomial, where $n \geq 1$, $m,k \geq 2$,

$n+1 \geq m$ and $km \geq n+1$. Then, inverse sum index ($IS(\Gamma)$) obtained from M-polynomial is

$$IS(\Gamma) = \frac{km^2(n+1)^2[k(m+n)+1]}{(m+n+1)(km+n+1)},$$

Proof. If $f(x,y) = M(\Gamma, x, y)$ then $f(x,y) = (km)x^m y^{n+1} + (nkm)x^{n+1}y^{km}$. Now, the required expressions are obtained as

$$J(D_x(D_y(f(x,y)))) = m(n+1)(km)x^{m+n-1} + (n+1)(km)(nkm)x^{Km+n-1},$$

$$Q_2 J(D_x(D_y(f(x,y)))) = m(n+1)(km)x^{m+n+1} + (n+1)(km)(nkm)x^{Km+n+1},$$

$$S_x Q_2 J(D_x(D_y(f(x,y)))) = \tfrac{m(n+1)(km)}{m+n+1}x^{m+n+1} + \tfrac{(n+1)(km)(nkm)}{km+n+1}x^{Km+n+1}.$$

Consequently,

$$IS(\Gamma) = S_x Q_2 J(D_x(D_y(f(x,y))))|_{x=1=y}$$
$$= \frac{km^2(n+1)^2[k(m+n)+1]}{(m+n+1)(km+n+1)}.$$

Theorem 3.9. Let $\Gamma \cong PNN(n,k,m)$ be the 3-layered probabilistic neural network and $M(\Gamma, x, y) = (km)x^m y^{n+1} + (nkm)x^{n+1}y^{km}$ be its M-polynomial, where $n \geq 1$, $m, k \geq 2$, $n+1 \geq m$ and $km \geq n+1$. Then, augmented Zagreb index ($AZI(\Gamma)$) obtained from M-polynomial is

$$AZI(\Gamma) = [(km+n-1)^3 + nk^3(m+n-1)^3]\frac{(km)[m(n+1)]^3}{(m+n-1)^3(km+n-1)^3}.$$

Proof. Let $f(x,y) = M(\Gamma, x, y)$ be the M-polynomial of the 3-layered probabilistic neural network. Then $f(x,y) = (km)x^m y^{n+1} + (nkm)x^{n+1}y^{km}$. Now, the required expressions are obtained as

$$(D_x^3(D_y^3(f(x,y)))) = (m(n+1))^3(km)x^{m-1}y^n + (km(n+1))^3(nkm)x^n y^{km-1},$$
$$J(D_x^3(D_y^3(f(x,y)))) = (m(n+1))^3(km)x^{m+n-1} + (km(n+1))^3(nkm)x^{km+n-1},$$
$$S_x J(D_x^3(D_y^3(f(x,y))))$$
$$= (km)\frac{(m(n+1))^3}{m+n-1}x^{m+n-1} + (nkm)\frac{(km(n+1))^3}{km+n-1}x^{km+n-1},$$
$$S_x^3 J(D_x^3(D_y^3(f(x,y)))),$$
$$= (km)\frac{(m(n+1))^3}{(m+n-1)^3}x^{m+n-1} + (nkm)\frac{(km(n+1))^3}{(km+n-1)^3}x^{km+n-1}.$$

Now, we obtain

$$S_x^3 J(D_x^3(D_y^3(f(x,y))))|_{x=1=y} = (km)\frac{(m(n+1))^3}{(m+n-1)^3} + (nkm)\frac{(km(n+1))^3}{(km+n-1)^3}.$$

Consequently,

$$AZI(\Gamma) = S_x^3 J(D_x^3(D_y^3(f(x,y))))|_{x=1=y},$$

$$= [(km+n-1)^3 + nk^3(m+n-1)^3]\frac{(km)[m(n+1)]^3}{(m+n-1)^3(km+n-1)^3}.$$

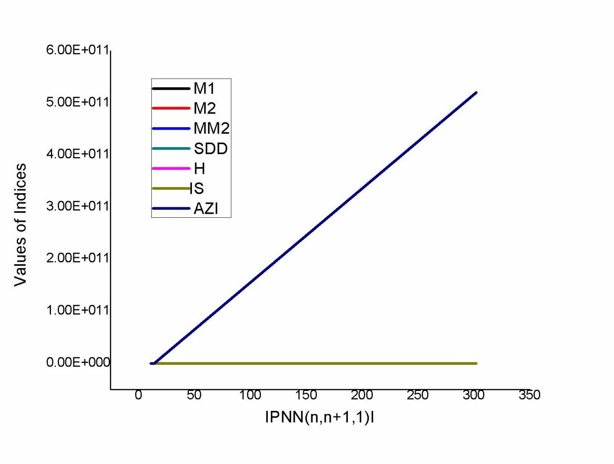

FIGURE 2. Comparison of degree-based TI's of $PNN(n, n+1, 1)$

4. Conclusion

To make an easy comparison of the computed results, we take $PNN(n, n+1, 1)$ with $v = 3n + 2$. In Figure 2, we take the values of v and the obtained topological indices of $PNN(n, n+1, 1)$ along the horizontal and vertical line respectively. It is easy to observe that all the topological indices M_1, M_2, MM_2, SDD, H and IS coincide with a constant rate such that IS remains dominant. Moreover, AZI is better one which increases with increasing v.

Now, we close our discussion stating the significant determination of these results. In this paper, the M-polynomial of the 3-layered Probabilistic neural network is proved and applied to study the the certain degree-based topological indices that will help to understand the physical changes of this network. These results also have remarkable applications in the pharmaceutical industry [19, 15]. In particular these are used for the preparation of the anticancer drugs, see [16, 17].

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6. Conflict of Interest

The authors have no conflict of interest.

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