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Research Article

Computing Topological Indices of 3-Layered Artificial Neural Network

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Abstract: Let η be a network graph with vertex and edge sets $P(\eta)$ and $E(\eta)$, respectively. This study aims to find the expected value (obtained during training and testing data) for Artificial Neural Networks (*ANN*) through indices. A three-layer artificial neural network is considered here, which we call $ANN(m, n, o)$. Moreover, a comparison is given between the topological indices (TI) of ANN with topological indices (TI) of the Probabilistic Neural Network (*PNN*). By comparing the indices, we can assess the effect of network structure on *ANN* model accuracy. The comparison between the two approaches helps us understand the accuracy and performance of *ANN* and *PNN* models. We can also gain insights into the differences between *ANN* and *PNN* in terms of their ability to learn and generalize.

***Keywords*:** artificial neural network, probabilistic neural network, topological indices, network graph

MSC: 05C90, 05C92, 68M10

1. Introduction

An artificial neural network [1] consists of neural tissue and a computer system similar to a nervous system. This computer system will form a multiprocessor computer system. The characteristics of this system are that it is a system with simple processing elements, essential scalar messages, a high degree of interconnection and adaptive communication between units. *ANN*, which is made up of many layers of neurons. The input layer of neurons and an output layer of neurons are connected through one or more hidden layers. The inter connectivity between neuron layers is composed of connection weights. Using the Back Propagation algorithm and by assigning weights to the training phase of *ANN* neurons minimizes the errors between the projected result and the actual output. An *ANN* is trained using the training data and evaluated against the test data to obtain the best topology and weights and using validation data the accuracy of the model is verified. In [2, 3], *ANN* provides a reasonably fast and flexible way of modeling, and is, therefore, suitable for rainfall-runoff prediction. Bias refers to the weight given to a neuron directly without being connected to the previous neuron under certain conditions. Multilayer perceptron (MLP) is the most common type of neuron in *ANN*. It consists of one or more hidden layers in a feed-forward neural network. Since most articles compare the performance of *ANN* models in the discipline of chemistry, chemistry-information technologies, pharmaceutical and biotechnology research [4]. It investigates the relationship between quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR), which are employed in the prediction of biological activity and characteristics of chemical compounds, as well as to design new biotechnological products.

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To explore the expected accuracy rate (The value which we are obtaining during training data and test data) of *ANN* many methods are available. Those methods include many levels of training which consume more time and are expensive. However, identifying the expected value via the topological index approach reduces the training time and cost. This approach also investigates QSAR/QSPR studies. Topological indices (TI) are graph invariants computed usually by means of degrees or neighborhood degrees of vertices of a graph. Here, the artificial neural networks are considered as a graph variant, and then the topological indices (TI) approach is used to find the expected value. Degreebased TIs' are widely used since this approach is more consistent [5]. In [6, 7] 5^{th} and 4^{th} topological indices of nano-star dendrimers are explored. Rajan et al. [8] discussed various TI on silicate, honeycomb, and hexagonal networks. The connectivity index is examined for modeling the enthalpy formation of alkanes by Estrada et al. [2]. Gutman and Trinajstic [9] identified the dependence of the Huckel total π-electron energy on the molecular topology. Baca et al. [10] calculated some TIs' for carbon nanotube network in 2015. Budak and Beyli in 2011 [11] classified the accuracy of resistivity for the three antibiotics namely ampicillin, chloramphenicol disks and trimethoprim-sulfamethoxazole with the help of *PNN*. Also, *PNN* is used to diagnose hepatitis [12] and segment brain tissues from MR images [13]. Javaid and Jinde [14] have formulated topological indices of the *PNN*(n, k, m) and it is related to the physical features of this same network. Jia et al. [15] have computed the degree-based and distanced-based topological indices (TI's) of *PNN*(n, k, m) and the obtained TI's are viewed in terms of 3D graphs. In [14] and [15] the authors identified different TI's under the sum version of *PNN*(n, k, m) but in [16] and [17] authors have identified the research gap and they have proposed new multiplicative version Zagreb index and Randic version discrete adriatic indices of the probabilistic neural network respectively. Javaid et al. [18] analyzed the physical changes of the 3-layered probabilistic neural network and explored certain degree-based M-polynomial TIs' of the same network. In 2020, Kang et al. [19] identified irregularity indices and viewed those indices in terms of graphs for the *PNN*. Many authors have contributed the research for analyzing the physical features of *PNN* in terms of TI but not for the *ANN*(a, b, c). We have motivated in this direction to present the topological indices of *ANN*(a, b, c) because in *ANN*(a, b, c) each a input neuron connecting with each b hidden layer neuron and each b hidden layer neuron connecting with each c output layer neuron. Since in *PNN*(n, k, m) out of n input neuron each neuron connecting with each k class of m hidden neuron and each k class of m hidden neuron is not connecting with each m output neuron except $m = 1$, because of this reason we interested to find an expected accuracy rate of topological indices of *ANN*(a, b, c) which has not been identified in *PNN*(n, k, m). Further, we explore the application of topological indices of *ANN*(a, b, c) in primary liver cancer surgery. In [20] the authors attempted to compare the accuracy rate with the *ANN* and LR model in predicting hospital mortality after primary liver cancer surgery and the authors identified that the accuracy rate of *ANN* and LR model for a given clinical data also it is validated that the accuracy rate of the *ANN* model is more consistent than its LR model. In this connection, we also initiate our work to compare and identify the significant accuracy rate between the *ANN* model and the various TIs' of *ANN*(a, b, c) [20]. Additionally, we give a comparison of the obtained TIs' of *ANN*(a, b, c) with the existing TIs' of *PNN*(n, n, 1) [14].

For the artificial neural network, on the basis of vertex degree, we compute topological indices such as general Randic, first general Zagreb, generalised Zagreb, atom-bond connectivity (*ABC*), geometric-arithmetic (*GA*), augmented Zagreb index (*AZI*), and symmetric division deg (*SDD*) index. This paper is organized as follows. Section 2 deals with some basic ideas and formulas. In section 3 some main results of *ANN*(a, b, c) in the direction of topological indices are studied and in section 4 the analyzed tabular results of *ANN*(a, b, c) and also compared TI's graph of *ANN*(a, b, c) with TI's of *PNN*(n, n, 1). Finally, section 5 has given concluding remarks.

2. Preliminaries

A network graph $\eta = (P(\eta), E(\eta))$ stands for any network structure, where $P(\eta) = \{p_1, p_2, p_3, ..., p_n\}$ stands for set of vertices (nodes), and $E(\eta)$ stands for set of edges. In chemical graphs, atoms are represented by the nodes (vertices), and bonds between those atoms are represented by the edges. In neural networks we consider, the layer of neurons denotes a set of vertices and edges denote the connection between layers of neurons. The order and size of the graph of *ANN* are denoted by $|P(\eta)| = p$ and $|E(\eta)| = e$ respectively. If there is a connection between any two vertices in a network, it is said to be connected. The number of edges connected to p is the degree of a vertex p, which is denoted by d_p. The neighborhood degree of vertex p is given by $S_p = \sum_{p \in N_{(\eta(p))}} (d_p)$, where $N_\eta(p)$ is the collection of all neighborhoods of a vertex p.

In this study, a network graph is defined as a connected finite graph with no loops or multiple edges. A topological index of a graph is a numerical quantity that is invariant of the graph. We use several topological indices as a tool in *ANN* to quantify the expected accuracy rate (The value which we are obtaining during training data and test data) and physical features of *ANN*. Gutman and Trinajstic developed the first and second Zagreb indices for the π-total energy of conjugated molecules in 1972 [9]. Many indices were introduced and used as branching indices [21, 22] shortly after these indices were introduced and utilized. Zagreb indices are primarily used in molecular structure research [23, 24]. The first and second Zagreb indices are

$$M_1(\eta) = \sum_{pq \in E(\eta)} (d_p + d_q) \text{ and } R_1(\eta) = M_2(\eta) = \sum_{pq \in E(\eta)} (d_p \times d_q)$$

respectively.

Bollobas and Erdos [25], as well as Amic et al. [26] independently derived the generalized Randic index in 1998. Several significant features and results of the Randic index have been proposed in detail by theoretical chemists and mathematicians in [27]. The general Randic index $R_\alpha(\eta)$ for $\alpha \in \mathbb{R}$ is,

$$R_\alpha(\eta) = \sum_{pq \in E(\eta)} (d_p \times d_q)^\alpha$$

then $\alpha = \frac{-1}{2}, \frac{1}{2}$ and 1 are called Randic index, reciprocal Randic index and second Zagreb index respectively.

Li et al. [28] characterized the first general Zagrab index ($M_1^\alpha(\eta)$).

$$M_1^\alpha(\eta) = \sum_{p \in P(\eta)} (d_p^\alpha), \text{ for } \alpha \in \mathbb{R}$$

Azari [29, 30] described the generalized Zagreb index ($M_{r,s}(\eta)$).

$$M_{r,s}(\eta) = \sum_{pq \in E(\eta)} (d_p^r d_q^s + d_q^r d_q^s), \text{ for } r, s \in \mathbb{Z}^+$$

The atom-bond connectivity index (*ABC*) is proposed by Estrada et al. [2] in 1998, which has been used to investigate alkane stability and cycloalkane strain energy. Vukicevic and Furtula established [31] the geometric arithmetic ($GA(\eta)$) index in 2009, which categorises all of them as

$$ABC(\eta) = \sum_{pq \in E(\eta)} \left(\sqrt{\frac{d_p + d_q - 2}{d_p \times d_q}} \right) \text{ and } GA(\eta) = \sum_{pq \in E(\eta)} \left(\frac{2\sqrt{d_p \times d_q}}{d_p + d_q} \right)$$

Furtula et al. [32] initiated the augmented Zagreb index ($AZI(\eta)$) in 2010, which is a modified version of the *ABC* index. A few years ago, Vukicevic et al. [33, 13] suggested the Adriatic indices but just a few of them have emerged as possibly useful in forecasting physiochemical features of molecules in particular symmetric division deg index ($SDD(\eta)$) [34, 35]

$$AZI(\eta) = \sum_{pq \in E(\eta)} \left(\left(\frac{d_p \times d_q}{d_p + d_q - 2} \right)^3 \right) \text{ and } SDD(\eta) = \sum_{pq \in E(\eta)} \left(\frac{d_p^2 + d_q^2}{d_q \times d_p} \right)$$

Later, Ghorani and Hosseinzadeh (2010) and Graovac et al. (2011) [7] defined the 4^{th} version of the atom-bond connectivity (ABC_4) index and the 5^{th} version of geometricarithmetic (GA_5) index, respectively.

$$ABC_4(\eta) = \sum_{pq \in E(\eta)} \sqrt{\frac{S_p + S_q - 2}{S_q \times S_p}} \text{ and } GA_5(\eta) = \sum_{pq \in E(\eta)} 2\frac{\sqrt{S_p \times S_q}}{S_q + S_p}$$

Hosamani (2016) [36] developed the Sanskruti index (*SI*), which was inspired by the augmented Zagreb index. These are listed as,

$$SI(\eta) = \sum_{pq \in E(\eta)} \left[\frac{S_p \times S_q}{S_q + S_p - 2} \right]^3$$

Let us discuss the framework of an artificial neural network. In this topic, we discuss completely connected multiple-layer (3-layer) neural networks. We consider some examples of artificial neural networks, including the Autoencoder artificial neural network shown in Figure 1, 2. The single-layer neural networks have two layers the first layer contains a number of neurons and the second layer contains b number of neurons. We consider the neuron's degree as a weight for a vertex of the network. The several types of single-layer networks are presented as input and output layer, input and hidden layer, hidden and output layer. Multiple-layer (3-layer) neural networks have three layers namely an input layer, hidden layer and an output layer with a, b and c number of neurons respectively. In $ANN(a, b, c)$ network each input layer a neuron is connected with each hidden layer b neuron and each hidden layer b neuron is connected with each output layer c neuron. These multiple-layer are often used to calculate the accuracy rate of $ANN(a, b, c)$.

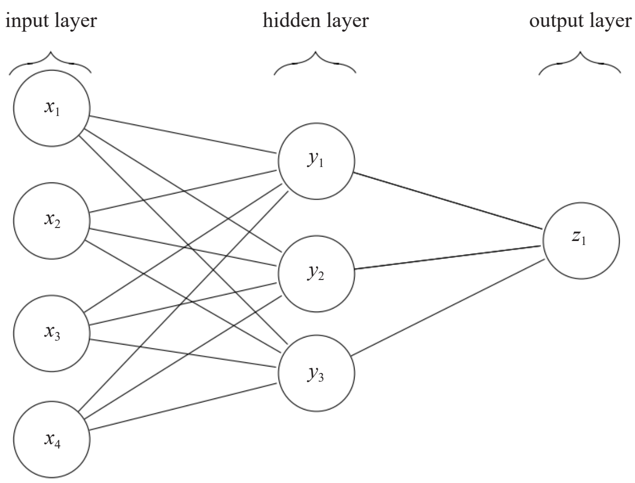

Figure 1. $ANN(4, 3, 1)$

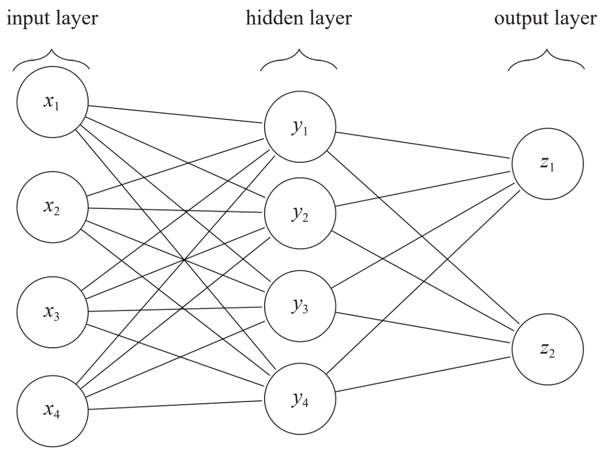

Figure 2. *ANN*(4, 4, 2)

3. Main result

In this section, we discuss an artificial neural network of a single-layer ($ANN(a, b)$) and multiple-layer ($ANN(a, b, c)$) where a, b, and c are input, hidden and output layers of neuron respectively. The total number of neurons in a layer is a vertex set, and the link between layers of neurons is an edge set. A single-layer network has two types of vertices ($ANN(a, b)$). We have $|P_1| = a$, $|P_2| = b$ in consequence, $|P(ANN(a, b))| = |P_1| + |P_2| = a + b = p$ (total number of neurons in all layers) where

$$P_1 = \{p \in P(ANN(a,b)) | \ d_p = b\} \text{ and } P_2 = \{p \in P(ANN(a,b)) | \ d_p = a\}.$$

In a single-layer network, we have only one type of edge with respect to degrees of end vertices in $ANN(a, b)$. $E_1 = \{pq \in E(ANN(a, b) \mid d_p = b, d_q = a\}$. Then the cardinality of an edge set is ab. The multiple-layer networks ($ANN(a, b, c)$) have three types of vertices.

$$P_1 = \{p \in P(ANN(a,b,c)) | \ d_p = b\}, P_2 = \{p \in P(ANN(a,b,c)) | \ d_p = a+c\},$$

$$\text{and } P_3 = \{p \in P(ANN(a,b,c)) | \ d_p = b\}.$$

$|P_1| = a$, $|P_2| = b$, $|P_3| = c$ in consequence, $|P(ANN(a, b, c))| = p = |P_1| + |P_2| + |P_3| = a + b + c$. The cardinality of Multiple-layer network edges is $b(a + c)$.

The edge set is divided into the corresponding sum of the degrees of end vertices. It is divided into two sets. $E_1 = \{pq \in E(ANN(a, b, c)) \mid d_p = b, d_q = a + c\}$. The cardinality of the edge set E_1 is ab. $E_2 = \{pq \in E(ANN(a, b, c)) \mid d_p = a + c, d_q = b\}$. The cardinality of the edge set E_2 is bc.

Theorem 1 Let η be an $ANN(a, b)$ graph for $a, b \geq 1$, then its Randic index ($R_{-1/2}(\eta)$), reciprocal Randic index ($R_{1/2}(\eta)$) and second Zagreb index ($R_1(\eta)$) are $R_{-\frac{1}{2}} = \sqrt{ab}$, $R_{\frac{1}{2}} = (ab)^{3/2}$ and $R_1 = (ab)^1$ respectively.

Proof. In order to calculate the required indices of η isomorphic to $ANN(a, b)$, we consider degree based $E_1 = \{pq \in E(ANN(a, b) \mid d_p = b, d_q = a\}$ edge partition of $ANN(a, b)$ with their cardinality ab. Then we have the general Randic index of $ANN(a, b)$

$$R_\alpha(\eta) = \sum_{pq \in E(\eta)} (d_p \times d_q)^\alpha = (ab)(ab)^\alpha = (ab)^{\alpha+1}$$

by putting $\alpha = \frac{-1}{2}$ in general Randic index, we have Randic index of *ANN*(*a*, *b*)

$$R_{\frac{-1}{2}}(\eta) = \sum_{pq \in E(\eta)} (d_p \times d_q)^{\frac{-1}{2}} = (ab)^{\frac{1}{2}}$$

by putting $\alpha = \frac{1}{2}$ in the general Randic index, we have a reciprocal Randic index of *ANN*(*a*, *b*)

$$R_{\frac{1}{2}}(\eta) = \sum_{pq \in E(\eta)} (d_p \times d_q)^{\frac{1}{2}} = (ab)^{\frac{3}{2}}$$

by putting $\alpha = 1$ in the general Randic index, we have a second Zagreb index of *ANN*(*a*, *b*)

$$R_1(\eta) = \sum_{pq \in E(\eta)} (d_p \times d_q)^1 = (ab)^2$$

□

Theorem 2 Let η be an *ANN*(*a*, *b*) graph for *a*, $b \geq 1$, then its first general Zagreb ($M_1^\alpha(\eta)$) and the generalized Zagreb indices ($M_{r,s}(\eta)$) are $M_1^\alpha(\eta) = ab(b^{\alpha-1} + a^{\alpha-1})$ and $M_{r,s}(\eta) = ab(b^r a^s + a^r b^s)$ respectively.

Proof. In order to calculate the required indices of η isomorphic to *ANN*(*a*, *b*), we consider degree based $E_1 = \{pq \in E(ANN(a, b) \mid d_p = b, d_q = a\}$ edge partition of *ANN*(*a*, *b*) with their cardinality given *ab*. We have the first general Zagreb indices

$$M_1^\alpha(\eta) = \sum_{p \in P(\eta)} (d_p^\alpha) = ab^\alpha + ba^\alpha = ba(b^{\alpha-1} + a^{\alpha-1})$$

also, we have the generalized Zagreb indices

$$M_{r,s}(\eta) = \sum_{pq \in E(\eta)} (d_p^r d_q^s + d_q^r d_q^s) = ab(b^r a^s + a^r b^s)$$

□

Corollary 1 Assume that η is single layer *ANN*(*a*, *b*) graph for *a*, $b \geq 1$, then the forgotten index ($F(\eta)$) and hyper Zagreb index ($HM(\eta)$) are $F(\eta) = \sum_{pq \in E(\eta)} (d_p^2 + d_q^2) = ab(b^2 + a^2)$ and $HM(\eta) = \sum_{pq \in E(\eta)} (d_p + d_q)^2 = ab(a+b)^2$ respectively.

Proof. This proof is similar to Theorem 2. □

Theorem 3 Let η be an *ANN*(*a*, *b*) graph for *a*, $b \geq 1$, then atom-bond connectivity ($ABC(\eta)$), geometric-arithmetic ($GA(\eta)$), augmented Zagreb ($AZI(\eta)$), and symmetric division deg ($SDD(\eta)$) indices are $ABC(\eta) = (\sqrt{ab})(\sqrt{b+a-2})$, $GA(\eta) = \frac{2\sqrt{b^3a^3}}{b+a}$, $AZI(\eta) = \frac{(ab)^4}{(a+b-2)^3}$ and $SDD(\eta) = \frac{ab^3 + a^3b}{a \times b}$ respectively.

Proof. In order to calculate the required indices of η isomorphic to *ANN*(*a*, *b*), we consider degree based $E_1 = \{pq \in E(ANN(a, b) \mid d_p = b, d_q = a\}$ edge partition of *ANN*(*a*, *b*) with their cardinality *ab*. Then the *ABC* index of *ANN*(*a*, *b*) is

$$ABC(\eta) = \sum_{pq \in E(\eta)} \left(\sqrt{\frac{d_p + d_q - 2}{d_p \times d_q}} \right) = ab \left(\sqrt{\frac{b+a-2}{ba}} \right) = \sqrt{ab}\sqrt{b+a-2}$$

The GA index of $ANN(a, b)$ is

$$GA(\eta) = \sum_{pq \in E(\eta)} \left(\frac{2\sqrt{d_p \times d_q}}{d_p + d_q} \right) = ab \left(\frac{2\sqrt{ba}}{b+a} \right) = \frac{2\sqrt{b^3 a^3}}{b+a}$$

The AZI index of $ANN(a, b)$ is

$$AZI(\eta) = \sum_{pq \in E(\eta)} \left(\frac{d_p \times d_q}{d_p + d_q - 2} \right)^3 = ab \left(\frac{ab}{b+a-2} \right)^3 = \frac{(ab)^4}{(a+b-2)^3}$$

Finally the SDD index of $ANN(a, b)$ is

$$SDD(\eta) = \sum_{pq \in E(\eta)} \left(\frac{d_p^2 + d_q^2}{d_q \times d_p} \right) = ab \left(\frac{b^2 + a^2}{a \times b} \right) = \frac{ab^3 + a^3 b}{a \times b}$$

□

Remark 1 In Theorem 1-3, we explored the expected accuracy rate (The value which we obtained during training data and test data) of a 2-layer artificial neural network.

Theorem 4 Let η be an $ANN(a, b, c)$ graph for $a, b, c \geq 1$, then the Randic index ($R_{-1/2}(\eta)$), reciprocal Randic index ($R_{1/2}(\eta)$), second Zagreb index ($R_1(\eta)$) are $R_{\frac{-1}{2}} = \sqrt{(a+c)b}$, $R_{\frac{1}{2}} = ((a+c)n)^{3/2}$ and $R_1 = (b(a+c))^2$ respectively.

Proof. In order to calculate the required indices of η isomorphic to $ANN(a, b, c)$, we consider degree based edge partitions $E_1 = \{pq \in E(ANN(a, b, c)) \mid d_p = b, d_q = a + c\}$ and $E_2 = \{pq \in E(ANN(a, b, c)) \mid d_p = a + c, d_q = b\}$ of $ANN(a, b, c)$ with their cardinality ab and bc respectively. We have the general Randic index of $ANN(a, b, c)$

$$R_\alpha(\eta) = \sum_{pq \in E(\eta)} (d_p \times d_q)^\alpha$$

$$= \sum_{pq \in E(b, a+c)} (d_p \times d_p)^\alpha + \sum_{pq \in E(b, a+c)} (d_p \times d_q)^\alpha$$

$$= ab(b \times (a+c))^\alpha + bc((a+c) \times b)^\alpha = b(a+c)(b(a+c))^\alpha$$

In general Randic index by putting $\alpha = \frac{-1}{2}$, we have Randic index of $ANN(a, b, c)$

$$R_{\frac{-1}{2}}(\eta) = \sum_{pq \in E(\eta)} (d_p \times d_q)^{\frac{-1}{2}}$$

$$= \sum_{pq \in E(b, a+c)} (d_p \times d_p)^{\frac{-1}{2}} + \sum_{pq \in E(b, a+c)} (d_p \times d_q)^{\frac{-1}{2}} = \sqrt{b(a+c)}$$

In general Randic index by putting $\alpha = \frac{1}{2}$, we have reciprocal Randic index of $ANN(a, b, c)$

$$R_{\frac{1}{2}}(\eta) = \sum_{pq\in E(\eta)} (d_p \times d_q)^{\frac{1}{2}}$$

$$= \sum_{pq\in E(b,a+c)} (d_p \times d_p)^{\frac{1}{2}} + \sum_{pq\in E(b,a+c)} (d_p \times d_q)^{\frac{1}{2}} = (b(a+c))^{\frac{3}{2}}$$

In general Randic index by putting $\alpha = 1$, we have second Zagreb index of $ANN(a, b, c)$

$$R_1(\eta) = \sum_{pq\in E(\eta)} (d_p \times d_q)^1$$

$$= \sum_{pq\in E(n,m+o)} (d_p \times d_p)^1 + \sum_{pq\in E(b,a+c)} (d_p \times d_q)^1 = (b(a+c))^2$$

□

Theorem 5 Let η be an $ANN(a, b, c)$ graph for $a, b, c \geq 1$, then first general Zagreb ($M_1^\alpha(\eta)$) and the generalized Zagreb indices ($M_{r,s}(\eta)$) are $M_1^\alpha(\eta) = b^\alpha(a + c)^\alpha((a + c)^{\alpha-1} + n^{\alpha-1})$ and $M_{r,s}(\eta) = b((a + c)(b^r(a + c)^s + b^s(a + c)^r))$ respectively.

Proof. In order to calculate the required indices of η isomorphic to $ANN(a, b, c) \geq 1$, we consider degree based edge partitions $E_1 = \{pq \in E(ANN(a, b, c)) \mid d_p = b, d_q = a + c\}$ and $E_2 = \{pq \in E(ANN(a, b, c)) \mid d_p = a + c, d_q = b\}$ of $ANN(a, b, c)$ with their cardinality ab and bc respectively. We have the first general Zagreb indices

$$M_1^\alpha(\eta) = \sum_{p\in P(\eta)} (d_p^\alpha) = b^\alpha (a+c)^\alpha ((a+c)^{1-\alpha} + b^{1-\alpha})$$

also, we have the generalized Zagreb indices

$$M_{r,s}(\eta) = \sum_{pq\in E(\eta)} (d_p^r d_q^s + d_q^r d_q^s) = ab(b^r (a+c)^s + (a+c)^r b^s) + bc((a+c)^r b^s$$

$$+ b^r (a+c)^s) = b((a+c)(b^s (a+c)^r + b^r (a+c)^s)$$

□

Corollary 2 Assume that η is a multiple layer $ANN(a, b, c)$ for $a, b, c \geq 1$. Forgotten index ($F(\eta)$) and Hyper Zagreb index ($HM(\eta)$) are $F(\eta) = \sum_{pq\in E(\eta)} (d_p^2 + d_q^2) = (a+c)b[(a+c)^2 + (b)^2]$ and $HM(\eta) = \sum_{pq\in E(\eta)} (d_p + d_q)^2 = (a + b + c)^2[b(a + c)]$ respectively.

Proof. This proof is similar to Theorem 5. □

Theorem 6 Let η be an $ANN(a, b, c)$ graph for $a, b, c \geq 1$, then atom-bond connectivity ($ABC(\eta)$), geometric-arithmetic ($GA(\eta)$), augmented Zagreb ($AZI(\eta)$), symmetric division deg ($SDD(\eta)$), fourth version of the atom-bond connectivity ($ABC_4(\eta)$), fifth version of geometric-arithmetic ($GA_5(\eta)$) and Sanskruti ($SI(\eta)$) indices are

$(i)\ ABC(\eta) = (\sqrt{(a+c)b})(\sqrt{b+a+c-2})$,

$(ii)\ GA(\eta) = \dfrac{2b(a+c)\sqrt{b(a+c)}}{b+a+c}$,

$(iii)\ AZI(\eta) = \dfrac{(b(a+c))^4}{(a+b+c-2)^3}$,

$(iv)\ SDD(\eta) = b^2 + (a+c)^2$,

$(v)\ ABC_4(\eta) = \frac{(ab+bc)\sqrt{2(ab+bc-1)}}{ab+bc}$,

$(vi)\ GA_5(\eta) = ab+bc$, and

$(vii)\ SI(\eta) = \frac{(ab+bc)^4}{(ab+bc-2)^3}$ respectively.

Proof. In order to calculate the required indices of η isomorphic to $ANN(a, b, c)$, we consider degree based on edge partitions of $E_1 = \{pq \in E(ANN(a, b, c)) \mid d_p = b, d_q = a + c\}$ and $E_2 = \{pq \in E(ANN(a, b, c)) \mid d_p = a + c, d_q = b\}$ of $ANN(a, b, c)$ with their cardinality ab and bc respectively.

Then the ABC index of $ANN(a, b, c)$ is

$$ABC(\eta) = \sum_{pq \in E(\eta)} \left(\sqrt{\frac{d_p + d_q - 2}{d_p \times d_q}} \right)$$

$$= ab\left(\sqrt{\frac{b+a+c-2}{b(a+c)}} \right) + bc\left(\sqrt{\frac{a+b+c-2}{(a+c)b}} \right)$$

$$= \sqrt{b(a+c)}\sqrt{a+b+c-2}$$

The GA index of $ANN(a, b, c)$ is

$$GA(\eta) = \sum_{pq \in E(\eta)} \left(\frac{2\sqrt{d_p \times d_q}}{d_p + d_q} \right)$$

$$= ab\left(\frac{2\sqrt{b(a+c)}}{b+a+c} \right) + bc\left(\frac{2\sqrt{(a+c)b}}{a+c+b} \right)$$

$$= \frac{2b(a+c)\sqrt{b(a+c)}}{b+a+c}$$

The AZI index of $ANN(a, b, c)$ is

$$AZI(\eta) = \sum_{pq \in E(\eta)} \left(\left(\frac{d_p \times d_q}{d_p + d_q - 2} \right)^3 \right)$$

$$= ab(\frac{b(a+c)}{b+a+c-2})^3 + bc(\frac{(a+c)b}{a+c+b-2})^3 = \frac{(b(a+c))^4}{(a+b+c-2)^3}$$

Finally the SDD index of $ANN(a, b, c)$ is

$$SDD(\eta) = \sum_{pq \in E(\eta)} \left(\frac{d_p^2 + d_q^2}{d_q \times d_p} \right)$$

$$= ab\left(\frac{b^2+(a+c)^2}{b(a+c)}\right)+bc\left(\frac{(a+c)^2+b^2}{b(a+c)}\right)=b^2+(a+c)^2$$

For calculating $ABC_4(\eta)$, $GA_5(\eta)$ & $SI(\eta)$ the edge partitions are the sum of the degrees of the neighborhoods of the end vertices. That is the neighborhood edge partition of S_p and S_q is $E_{\{Sp,Sq\}} = E_{\{ab+bc,ab+bc\}}$ with cardinalities ab and bc, where S_p & S_q are the neighborhood vertices of p & q respectively.

The ABC_4 index is the neighborhood degree of ABC index of $ANN(m, n, o)$

$$ABC_4(\eta)=\sum_{pq\in E(\eta)}\sqrt{\frac{S_p+S_q-2}{S_q\times S_p}}$$

$$= ab\left(\sqrt{\frac{(ab+bc)+(ab+bc)-2}{(ba+bc)^2}}\right)+bc\left(\sqrt{\frac{(ab+bc)+(ab+bc)-2}{(ba+bc)^2}}\right)$$

$$=\frac{(ab+bc)\sqrt{2(ab+bc-1)}}{ab+bc}$$

The GA_5 index is neighborhood degree of GA index of $ANN(a, b, c)$

$$GA_5(\eta)=\sum_{pq\in E(\eta)}2\frac{\sqrt{S_p\times S_q}}{S_q+S_p}$$

$$= ab\left(2\frac{\sqrt{(ab+bc)\times(ab+bc)}}{2(ba+bc)}\right)+bc\left(2\frac{\sqrt{(ab+bc)\times(ab+bc)}}{(ba+bc)2}\right)$$

$$= ab+bc\left(2\frac{\sqrt{(ab+bc)\times(ab+bc)}}{(ba+bc)2}\right)$$

Finally the SI index is neighborhood degree of AZI index of $ANN(a, b, c)$

$$SI(\eta)=\sum_{pq\in E(\eta)}\left[\frac{S_p\times S_q}{S_q+S_p-2}\right]^3$$

$$= ab\left[\frac{ab+bc}{ab+bc-2}\right]^3+bc\left[\frac{ab+bc}{ab+bc-2}\right]^3=\frac{(ab+bc)^4}{(b+bc-2)^3}$$

□

Remark 2 We explored the expected value for the 3-layer artificial neural network in Theorem 4-6. From Table 1, the GA index has the better expected accuracy rate among all the other indices. Where $GA(\eta)=\frac{2b(a+c)\sqrt{b(a+c)}}{b+a+c}$, for a, b, $c \geq 1$.

Table 1. Topological indices of *ANN*(*a*, *b*, *c*) predicting hospital mortality of thousand pairs after primary liver cancer surgery

Topological Indices (TI)	Accuracy rate for TI of *ANN*(*a*, *b*, *c*) [%]	P value
$AZI\ (\eta)$	100.001	< 0.001
$ABC\ (\eta)$	100.001	< 0.001
$M_1\ (\eta)$	100.001	< 0.001
$R_1\ (\eta)$	100.003	< 0.001
$F\ (\eta)$	100.004	< 0.001
$GA\ (\eta)$	100.000	< 0.001
$SDD\ (\eta)$	100.003	< 0.001
$GA_5\ (\eta)$	100.003	< 0.001

4. Comparison and discussion

In this section, we have estimated the expected accuracy rate of *ANN*(*a*, *b*, *c*) in terms of TIs' and compared the obtained TIs' of *ANN*(*a*, *b*, *c*) with the expected accuracy rate of *ANN* [20] in predicting the hospital mortality of primary liver cancer surgery and we discussed the stem graph of *PNN*(*n*, *n*, 1) [14] and *ANN*(*a*, *b*, *c*).

In Figure 3 and 4, *x* and *y*-axes represent the number of neurons in the 3 layered *ANN*(*a*, *b*, *c*) and the values of the obtained degree sum and neighborhood degree sum TIs' of *ANN*(*a*, *b*, *c*) respectively. The graph shows all the obtained TIs' namely $ABC(\eta)$, $GA(\eta)$, $AZI(\eta)$, $SDD(\eta)$, $M_1(\eta)$, $R_1(\eta)$, $F(\eta)$, $GA_5(\eta)$, $ABC_4(\eta)$ and $SI(\eta)$ in terms of stem plot using Matlab tool, also those values are considered as expected accuracy rate of *ANN*(*a*, *b*, *c*). Moreover, the topological index $GA(\eta)$ recites best expected accuracy rate of *ANN*(*a*, *b*, *c*) among all other TIs'. In neighborhood degree index $GA_5(\eta)$ depicts best expected accuracy rate of *ANN*(*a*, *b*, *c*) for other neighborhood degree indices.

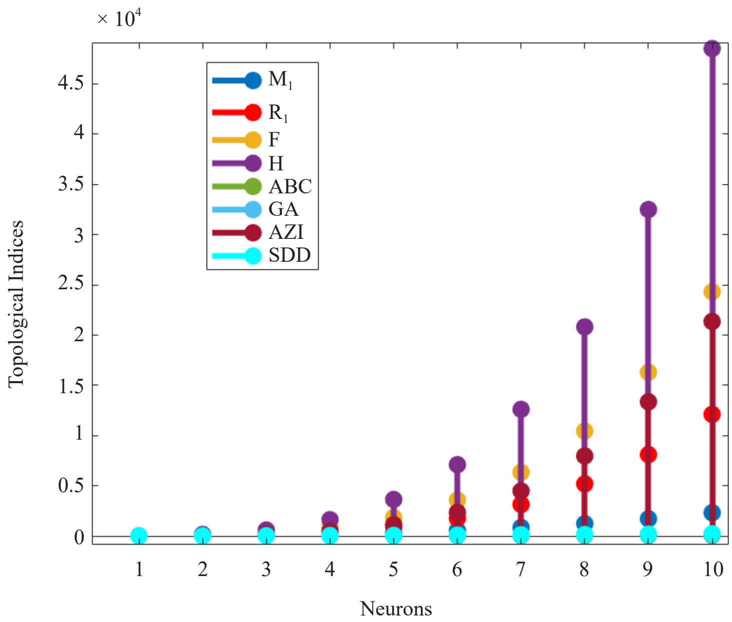

Figure 3. Graph for degree sum Topological Indices of *ANN*(*a*, *b*, *c*)

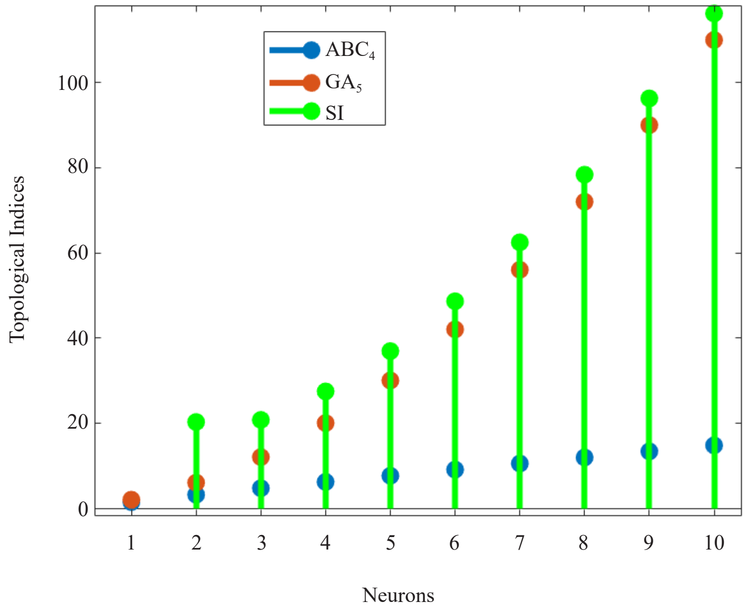

Figure 4. Graph for neighborhood degree sum Topological Indices of *ANN*(*a*, *b*, *c*)

Comparing Table 1 and 2, it is noted that the prediction of hospital mortality of primary liver cancer surgery, after some training the expected accuracy rate is obtained which is significantly better in the *ANN* model [20]. But in the proposed model the expected accuracy rate is obtained with the minimum number of data points by using the topological indices without any training.

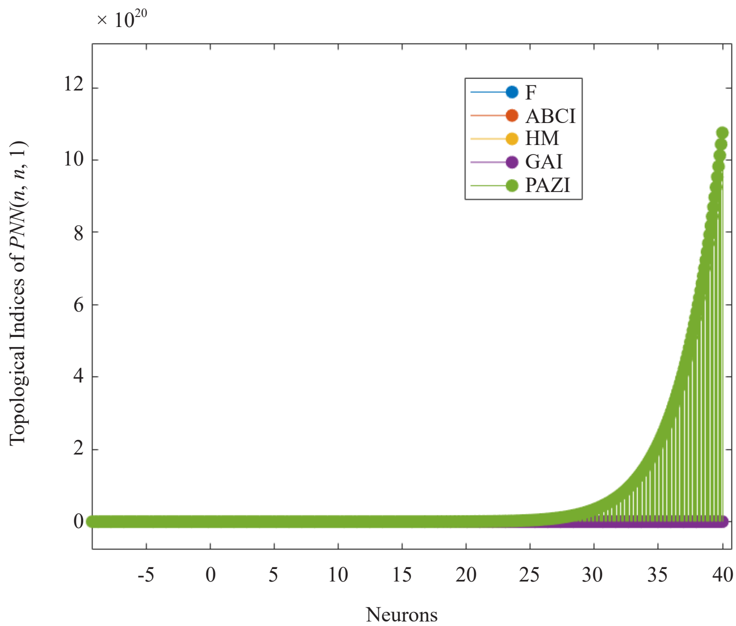

Figure 5. Graph for degree sum Topological Indices of *PNN*(*n*, *n*, 1)

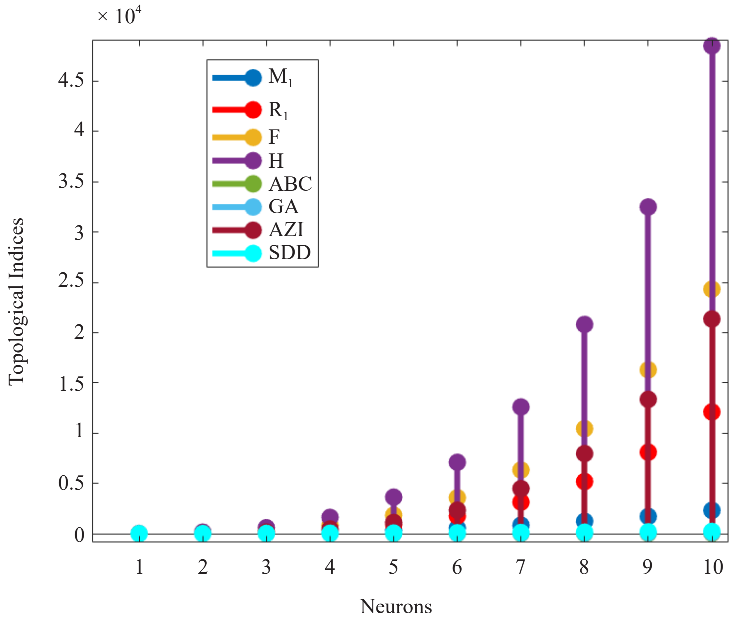

Figure 6. Graph for degree sum Topological Indices of *ANN*(*a*, *b*, *c*)

Table 2. ANN predicting hospital mortality of thousand pairs after primary liver cancer surgery [20]

Performance indices	ANN [%]	P value
Accuracy rate	97.28	< 0.001

Further, the degree sum topological indices of *PNN*(*n*, *n*, 1) and *ANN*(*a*, *b*, *c*) are shown in Figure 5 and 6 respectively with the help of Matlab. The *PNN*(*n*, *k*, *m*) does not depict the expected accuracy rate compared with *ANN*(*a*, *b*, *c*), since *PNN*(*n*, *k*, *m*) has *n* neurons in the input layer, the hidden layer consists of *k* classes such that each class has *m* neurons and the output layer has *m* neurons [14] and each hidden layer of *m* neurons with *k* classes is not linked with all the *m* output neurons in *PNN*(*n*, *k*, *m*) except for $k = n$ and $m = 1$.

5. Concluding remarks

Many countries in the world are giving more importance to *ANN* model research because it provides a better expected accuracy rate. In particular the *ANN* model plays a major role in the medical field in predicting hospital mortality in the treatment of deadly diseases such as cancer. In this context, this study has provided an expected accuracy rate of *ANN*(*a*, *b*, *c*) by the degree and neighborhood degree of topological indices. In degree sum and neighborhood degree TIs', $GA(\eta)$ and $GA_5(\eta)$ give a better expected accuracy rate respectively. Without training the data, this proposed method has successfully predicted a better accuracy rate than the *ANN* model. Moreover, compared with the topological indices of *PNN*(*n*, *n*, 1) a better accuracy rate is arrived at by computing topological indices of *ANN*(*a*, *b*, *c*). It is also determined the physical features of an *ANN*(*a*, *b*, *c*) network with the help of certain TIs'. In this sequel, the topological indices of *ANN*(*a*, *b*, *c*) with more parameters of other graph structures like bipartite graphs will be investigated for other complex fatal disease treatments in the near future.

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Conflict of interest

The authors declare that they have no conflict of interest.

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