Research Article

Computing Topological Invariants of Deep Neural Networks

Xiujun Zhang, 1 Nazeran Idrees, 2 Salma Kanwal, 3 Muhammad Jawwad Saif, 4 and Fatima Saeed 2

1 School of Computer Science, Chengdu University, Chengdu, China
2 Department of Mathematics, Government College University Faisalabad, Faisalabad 38000, Pakistan
3 Department of Mathematics, Lahore College for Women University, Lahore 54000, Pakistan
4 Department of Applied Chemistry, Government College University Faisalabad, Faisalabad 38000, Pakistan

Correspondence should be addressed to Nazeran Idrees; nazeraiidrees@gcuf.edu.pk and Salma Kanwal; salma.kanwal055@gmail.com

Received 8 May 2022; Revised 27 July 2022; Accepted 12 September 2022; Published 7 October 2022

Copyright © 2022 Xiujun Zhang et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

A deep neural network has multiple layers to learn more complex patterns and is built to simulate the activity of the human brain. Currently, it provides the best solutions to many problems in image recognition, speech recognition, and natural language processing. The present study deals with the topological properties of deep neural networks. The topological index is a numeric quantity associated to the connectivity of the network and is correlated to the efficiency and accuracy of the output of the network. Different degree-related topological indices such as Zagreb index, Randić index, atom-bond connectivity index, geometric-arithmetic index, forgotten index, multiple Zagreb indices, and hyper-Zagreb index of deep neural network with a finite number of hidden layers are computed in this study.

1. Introduction

Neural networks are not only studied in artificial intelligence but also have got great applications in intrusion detection systems, image processing, localization, medicine, and chemical and environmental sciences [1–3]. Neural networks are used to model and learn complex and nonlinear relationships, which is very important in real life because many of the relationships of inputs and outputs are nonlinear and complex. Artificial neural networks are the backbone of robotics, defense technology, and neural chemistry. Neural networks are not only being widely used as a tool for predictive analysis but also trained successfully to model processes including crystallization, adsorption, distillation, gasification, dry reforming, and filtration in neural chemistry [4–8].

Bollobás and Erdős [10] introduced the general Randić index given by equation (1). The first and second Zagreb indices were introduced by Gutman and Trinajstić [11] in 1972, which appeared during the analysis of π-electron energy of atoms. The multiplicative version of these Zagreb indices (the first multiplicative Zagreb index and the second multiplicative Zagreb index) of a graph were formulated by Ghorbani and Azimi [12]. Shiri et al. [13] introduced a new version of Zagreb indices named as the hyper-Zagreb index. The widely used atom-bond connectivity (ABC) index is
introduced by Estrada et al. [14]. Zhou and Trinajstić [15] gave the idea of the sum-connectivity index (SCI). The geometric-arithmetic index was introduced by Vukičević and Furtula [16]. Javaid et al. [17] investigated the degree-based topological indices for the probabilistic neural networks in 2017. Topological indices for multilayered probabilistic neural networks and recurrent neural networks have also been computed recently [18–21]. For more work-related to computation and bounds of topological indices, see [22–29].

Consider a graph \( G \) having a set of nodes \( V \) and a set of edges \( E \). Degree of a node \( v \), denoted by \( d_v \), is the number of nodes connected to \( v \) via an edge. A degree-based topological indices of a graph \( G \) are defined as follows:

Randić index

\[
\chi(G) = \sum_{u,v \in E} \left( \frac{1}{\sqrt{d_u d_v}} \right).
\]

General Randić index

\[
R_\alpha(G) = \sum_{u,v \in E} (d_u d_v)^\alpha.
\]

First Zagreb index

\[
M_1(G) = \sum_{u,v \in E} [d_u + d_v].
\]

Second Zagreb index

\[
M_2(G) = \sum_{u,v \in E} [d_u d_v].
\]

First multiple Zagreb index

\[
PM_1(G) = \prod_{u,v \in E} [d_u + d_v].
\]

Second multiple Zagreb index

\[
PM_2(G) = \prod_{u,v \in E} [d_u d_v].
\]

Hyper-Zagreb index

\[
HM(C[m,n]) = \sum_{u,v \in E} (d_u + d_v)^2.
\]

Atom-bond connectivity index

\[
ABC(G) = \sum_{u,v \in E} \sqrt{d_u + d_v - 2d_u d_v}.
\]

Sum connectivity index

\[
SCI(G) = \sum_{u,v \in E} \left( \frac{1}{\sqrt{d_u + d_v}} \right).
\]

Geometric-arithmetic index

\[
GA(G) = \sum_{u,v \in E} \left( 2 \sqrt{d_u d_v} / d_u + d_v \right).
\]

2. Methodology

A deep neural network (DNN) can be represented by a graph \( Z = (V, E) \), where \( V \) denotes the nodes of the network and \( E \) denotes the set of edges between the nodes. We consider a DNN with an input layer having \( M \) nodes, \( r \) hidden layers each layer having \( N_i \), \( i = 1, 2, \ldots, r \) number of nodes such that the first layer has \( N_1 \) nodes, the second layer has \( N_2 \) nodes, and similarly, the \( r \)-th layer has \( N_r \) nodes, which can also be expressed as \( DNN(N_1 N_2 \ldots N_r) \). The output layer of DNN has \( N \) nodes. Each node of every layer is connected to all nodes of the next layer. For instance, Figure 1 shows a DNN with an input layer having four nodes, an output layer with three nodes, and five hidden layers.

We first partition the edges of the graph of DNN according to the degree of end vertices of the graph. We analyze the structure of the graph by considering the connectivity of vertices of each layer to the next layer. In DNN, each node of every layer is connected to all nodes of the next layer. This fact is employed to count the degree of each vertex. Consider a deep neural network \( DNN(N_1 N_2 \ldots N_r) \). Each node in the input layer has a degree \( N_1 \) because every input node is connected to each node of a first hidden layer having \( N_1 \) nodes. In the first hidden layer, all node \( (N_1) \) has the same degree, i.e., \( M + N_2 \). Nodes of the second layer have degree \( N_1 + N_3 \). Similarly, the nodes of \( i \)-th hidden layer have degree \( N_{r-1} + N_{i+1} \). The nodes of the output layer have degree \( N_r \).

We will compute topological indices using the edge partition method. We will classify the edges on basis of degrees of end-nodes of the edges. The number of edges connecting the input layer to the first hidden layer is \( N_1 \), whose end-nodes have degrees \( N_1 \) and \( M + N_2 \). The edges connecting \( i \)-th hidden layer to \( i + 1 \)-st layer have end-nodes having degrees \( N_{r-1} + N_{i+1} \) and \( N_i + N_{i+2} \) and the number of such edges is \( N_i N_{i+1} \). Similarly, the \( N_i N_r \) edges connecting the last hidden layer to the output layer have degrees \( N_{r-1} + N \) and \( N_r \) of end-nodes. These findings are summarized in Table 1 below, which will be further helpful in computing the topological indices.

3. Results and Discussions

In this section, we have derived the expressions to compute the topological indices of the deep neural network. These results are related to the connectivity of nodes of DNN.

Theorem 1. Let \( Z = DNN(N_1 N_2 \ldots N_r) \) be a deep neural network. Then the Randić index \( R_{(1/2)}(Z) \) and general Randić index \( R_\alpha(Z) \) of DNN are given as

(i) \( R_{(1/2)}(Z) = (MN_1) \sqrt{(N_1)(M + N_2)} + (N_1 N_2) \sqrt{(M + N_2)(N_1 + N_3)} + \sum_{i=2}^{r-1} N_i N_{i+1} ((N_{i+1} + N_{i+2})^{(1/2)} + (N_{i+1} N_i) \sqrt{(N_{r-2} + N_r)(N_{r-1} + N)} + (N_i N_r) \sqrt{(N_{r-1} + N)(N_r)} \).

(ii) \( R_\alpha(Z) = (MN_1) ((N_1)(M + N_2))^{\alpha} + (N_1 N_2) ((M + N_2)(N_1 + N_3))^{\alpha} + \sum_{i=2}^{r-1} N_i N_{i+1} ((N_{i+1} + N_{i+2})^{\alpha} + (N_{i+1} N_i) ((N_{r-2} + N_r)(N_{r-1} + N))^{\alpha} + (N_i N_r) ((N_{r-1} + N)(N_r))^{\alpha} \).
Proof. We calculated the degrees of end nodes of every edge for DNN \((N_1 N_2 \ldots N_r)\). By using the definitions and values from Table 1, we get the following results:

\[
R_{(1/2)}(Z) = \sum_{uv \in E(Z)} \sqrt{d_u d_v} = \sum_{d_u, d_v} \sqrt{d_u d_v} + \sum_{u \in V} \sum_{v \in V \setminus \{u\}} \sqrt{d_u d_v} + \sum_{v \in V} \sum_{u \in V \setminus \{v\}} \sqrt{d_u d_v} + \sum_{u \in V} \sum_{v \in V \setminus \{u\}} \sqrt{d_u d_v} + \sum_{v \in V} \sum_{u \in V \setminus \{v\}} \sqrt{d_u d_v}
\]

Substituting values from Table 1, we get

\[
R_{(1/2)}(Z) = (MN_1) \sqrt{(N_1)(M + N_2)} + (N_1 N_2) \sqrt{(M + N_2)(N_1 + N_3)} + (N_2 N_3) + \ldots + (N_{r-2} N_{r-1}) \sqrt{(N_{r-3} + N_{r-4})(N_{r-2} + N_r)} + (N_{r-3} N_{r-2}) \sqrt{(N_{r-3} + N_{r-4}) (N_{r-2} + N_r)} + (N_{r-2} N_{r-1}) \sqrt{(N_{r-3} + N_{r-4}) (N_{r-2} + N_r)} + (N_{r-1} N_r) \sqrt{(N_{r-1} + N_r) (N_r)}.
\]

This can be expressed as follows:

\[
R_{(1/2)}(Z) = (MN_1) \sqrt{(N_1)(M + N_2)} + (N_1 N_2) \sqrt{(M + N_2)(N_1 + N_3)} + (N_2 N_3) + \ldots + (N_{r-2} N_{r-1}) \sqrt{(N_{r-3} + N_{r-4})(N_{r-2} + N_r)} + (N_{r-3} N_{r-2}) \sqrt{(N_{r-3} + N_{r-4}) (N_{r-2} + N_r)} + (N_{r-2} N_{r-1}) \sqrt{(N_{r-3} + N_{r-4}) (N_{r-2} + N_r)} + (N_{r-1} N_r) \sqrt{(N_{r-1} + N_r) (N_r)}.
\]

Table 1: The edge partition of DNN \((N_1 N_2 \ldots N_r)\) based on degrees of end nodes.

| (\(d_u, d_v\)), \(uv \in E(Z)\) | Number of edges of the form \((d_u, d_v)\) |
|---|---|
| \((N_1, M + N_2)\) | \(MN_1\) |
| \((M + N_2, N_1 + N_3)\) | \(N_1 N_2\) |
| \((N_1 + N_3, N_2 + N_4)\) | \(N_2 N_3\) |
| \(\ldots\) | \(\ldots\) |
| \((N_{r-3} + N_{r-4}, N_{r-2} + N_{r-1})\) | \(N_{r-2} N_{r-1}\) |
| \((N_{r-2} + N_{r-1} + N)\) | \(N_{r-1} N_r\) |
| \((N_{r-1} + N, N_r)\) | \(N_r N\) |

Figure 1: A deep neural network with five hidden layers of DNN \((4, 4, 5, 6, 4, 3, 3)\).
Theorem 2. Let $Z \equiv DNN(N_1, N_2, \ldots, N_r)$ be a deep neural network. Then, first Zagreb index ($M_1(Z)$), second Zagreb index ($M_2(Z)$), first multiplicative Zagreb ($PM_1(Z)$) index, and second multiplicative Zagreb index ($PM_2(Z)$) of DNN are given as follows:

(i) $M_1(Z) = (MN_1)(N_1 + M + N_2) + (N_1N_2)(M + N_2) + \sum_{i=2}^{r-2} N_i(N_{i-1} + N_{i+1} + N_i)$

(ii) $M_2(Z) = (MN_1)[(N_1)(M+N_2)] + (N_1N_2)(M+N_2 + N_1 + N_3) + \sum_{i=2}^{r-2} N_i(N_{i-1} + N_{i+1} + N_i)$

(iii) $PM_1(Z) = (N_1 + M + N_2)MN_1 \times (M + N_2 + N_1)\times \prod_{i=1}^{r-2} (N_{i-1} + N_{i+1} + N_i)$

(iv) $PM_2(Z) = [(N_1)(M + N_2)]MN_1 \times [(M + N_2)N_1 + N_3] \times \prod_{i=1}^{r-2} (N_{i-1} + N_{i+1} + N_i)$

Proof. To compute the topological indices of DNN, we use the edge partition method. In Table 1, we have calculated the degrees of end-nodes of each edge for $DNN(N_1, N_2, \ldots, N_r)$. Now, by using the definitions and values from Table 1, we have the following results:

(i) $M_1(Z) = \sum_{uv \in E} [d_u + d_v] = \sum_{uv \in E} [d_u + d_v] + \sum_{uv \in E} [d_u + d_v] + \sum_{uv \in E} [d_u + d_v] + \sum_{uv \in E} [d_u + d_v]$

Substituting values from Table 1, we get

$M_1(Z) = (MN_1)(N_1 + M + N_2) + (N_1N_2)(M + N_2) + \sum_{i=2}^{r-2} N_i(N_{i-1} + N_{i+1} + N_i) + (N_r)(N_{r-1} + N + N_r)$

It can be expressed as follows:

$M_1(Z) = (MN_1)(N_1 + M + N_2) + (N_1N_2)(M + N_2 + N_1 + N_3) + \sum_{i=2}^{r-2} N_i(N_{i-1} + N_{i+1} + N_i) + (N_r)(N_{r-1} + N + N_r)$

$M_2(Z) = \sum_{uv \in E} [d_u + d_v] = \sum_{uv \in E} [d_u + d_v] + \sum_{uv \in E} [d_u + d_v] + \sum_{uv \in E} [d_u + d_v] + \sum_{uv \in E} [d_u + d_v]$

Substituting values from Table 1, we have
Using Table 1, we get
\[ E_{uv}(N_r) = \sum_{i=1}^{r-2} N_i N_{i+1} + N_r N_{i+2}, \quad \text{for } r > 3 \]
(18)

Substituting the values from Table 1, we get
\[ PM_2(Z) = \prod_{u \in E \setminus \{u \mid d_u = 1\}} [d_u \times d_v] + \prod_{u \in E \setminus \{u \mid d_v = 1\}} [d_u \times d_u] + \prod_{u \in E \setminus \{u \mid d_v = 1\}} [d_u \times d_u] \]
(21)

The above expression can be expressed as follows:
\[ PM_2(Z) = \prod_{u \in E \setminus \{u \mid d_u = 1\}} [d_u \times d_v] + \prod_{u \in E \setminus \{u \mid d_v = 1\}} [d_u \times d_u] + \prod_{u \in E \setminus \{u \mid d_v = 1\}} [d_u \times d_u] \]
(22)

Theorem 3. Let \( Z \equiv \text{DNN}(N_1, N_2, \ldots, N_r) \) be a deep neural network. Then the forgotten Zagreb index (\( F(Z) \)) and hyper-Zagreb index (\( HM(Z) \)) of DNN are given as follows:

\[ F(Z) = \left( MN_1 \right) \left( N_1 \right)^2 + \left( MN_2 \right) \left( N_1 + N_2 \right)^2 + \left( N_1^3 \right) \left( N_2 + N_3 \right)^2 + \sum_{i=1}^{r-2} N_i N_{i+1} (N_{i+1} + N_{i+2})^2 + (N_{i+1} + N_{i+2})^2 \]
(23)

Proof. To compute the topological indices of DNN, we use the edge partition method. In Table 1, we have calculated the degrees of end nodes of every edge for \( \text{DNN}(N_1, N_2, \ldots, N_r) \).
Now, by using the definitions and values from Table 1, we get the results given below

(i) \( F(Z) = \sum_{u \in E} [d_u^2 + d_v^2] = \sum_{u \in E \cap \{N_i + M + N_j\}} d_u^2 + d_v^2 \)

\[ + \sum_{u \in E \cap \{M + N_i + N_j\}} [d_u^2 + d_v^2] + \sum_{u \in E \cap \{N_i + N_j + N_k\}} [d_u^2 + d_v^2] \]

\[ + \sum_{u \in E \cap \{N_{r-1} + N_{r-1} + N_j\}} [d_u^2 + d_v^2] \]

\[ + \sum_{u \in E \cap \{N_{r-1} + N_j + N_{r+1}\}} [d_u^2 + d_v^2] \]

Using Table 1, the above relation becomes

\[ F(Z) = (MN_i)(N_i)^2 + (M + N_j)^2 \]

\[ + (N_1 N_2)(M + N_j)^2 + (N_1 + N_j)^2 \]

\[ + \sum_{i=1}^{r-1} N_i N_{r+i} [(N_{r+i} + N_{r+i})^2 + (N_i + N_{r+i})^2] \]

\[ + (N_i N_j) (N_{r-1} + N_j + N_{r-1} + N)^2 + (N_1 N_i) (N_{r-1} + N)^2 + (N_i)^2 \]

This can be summarized as follows:

\[ F(Z) = (MN_i)(N_i)^2 + (M + N_j)^2 \]

\[ + (N_1 N_2)(M + N_j)^2 + (N_1 + N_j)^2 \]

\[ + \sum_{i=1}^{r-1} N_i N_{r+i} [(N_{r+i} + N_{r+i})^2 + (N_i + N_{r+i})^2] \]

\[ + (N_i N_j) (N_{r-1} + N_j + N_{r-1} + N)^2 + (N_1 N_i) (N_{r-1} + N)^2 + (N_i)^2 \]

(ii) \( HM(Z) = \sum_{u \in E} (d_u + d_v) = \sum_{u \in E \cap \{N_i + M + N_j\}} [d_u + d_v] \)

\[ + \sum_{u \in E \cap \{M + N_i + N_j\}} [d_u + d_v] \]

\[ + \sum_{u \in E \cap \{N_i + N_j + N_k\}} [d_u + d_v] \]

\[ + \sum_{u \in E \cap \{N_{r-1} + N_{r-1} + N_j\}} [d_u + d_v] \]

\[ + \sum_{u \in E \cap \{N_{r-1} + N_j + N_{r+1}\}} [d_u + d_v] \]

\[ + \sum_{u \in E \cap \{N_{r-1} + N_j + N_{r+1} + N\}} [d_u + d_v] \]

Substituting values from Table 1, we get

\[ HM(Z) = (MN_i)(N_i + M + N_j)^2 \]

\[ + (N_1 N_2)(M + N_j + N_i + N_j)^2 \]

\[ + (N_1 N_3)(N_1 + N_3 + N_2 + N_j)^2 + \ldots \]

\[ + (N_r N_{r+1}) (N_{r-1} + N_{r+1} + N_{r+2} + N_j)^2 + (N_{r-1} N_r) (N_{r-2} + N_r + N_{r-1} + N)^2 \]

\[ + (N_1 N_i) (N_{r-1} + N + N_i)^2 \]

The above expression can be further summarized as follows:

\[ HM(Z) = (MN_i)(N_i + M + N_j)^2 \]

\[ + (N_1 N_2)(M + N_2 + N_1 + N_j)^2 \]

\[ + \sum_{i=1}^{r-2} N_i N_{r+i} (N_i + N_{r+i} + N + N_i + N_{r+i})^2 \]

\[ + (N_{r-1} N_r) (N_{r-2} + N_r + N_{r-1} + N)^2 \]

\[ + (N_1 N_i) (N_{r-1} + N + N_i)^2 \]

Theorem 4. Let \( Z \equiv DNN(N_1 N_2 \ldots N_r) \) be a deep neural network. The atom-bond connectivity index \( (ABC(Z)) \), geometric-arithmetic index \( (GA(Z)) \), sum connectivity index \( (SCI(Z)) \), and augmented Zagreb index \( (AZI(Z)) \) of DNN are given as follows:

(i) \( ABC(Z) = (MN_i)(\sqrt{N_i + M + N_j - 2} / (N_i)(M + N_j)) \)

\[ + (N_1 N_2)(\sqrt{M + N_j + N_1 + N_j - 2} / (M + N_j)) \]

\[ + (N_1 N_3)(N_1 + N_3 + N_2 + N_j - 2) / (M + N_j) \]

\[ + (N_1 N_i) (N_{r-1} + N_i + N_{r-1} + N - 2) / (N_{r-1} + N) \]

\[ + (N_i N_j) / (N_i + N + N_i + N - 2) / (N_i + N) \]

(ii) \( GA(Z) = (2(MN_i)(\sqrt{(N_i)(M + N_j)} / (N_i + M + N_j))) + \sqrt{N_i N_j} / (M + N_j) \)

\[ + 2(N_i N_2)(\sqrt{(M + N_j)(N_i + N_j)} / (M + N_j + N_i + N_j)) + \sqrt{N_i N_j} / (N_i + N_i + N_i + N_i + N_i + N_i + N_i + N_j) \]

\[ + 2(N_i N_2)(\sqrt{(N_{r-1} + N_i + N_{r-1} + N - 2)} / (N_{r-1} + N_r + N_{r-1} + N)) + \sqrt{(N_{r-1} + N_r + N_{r-1} + N)} \]

\[ + 2(N_i N_j) / (N_{r-1} + N_j + N_{r-1} + N + N_j) \]

(iii) \( SCI(Z) = (M(N_i)^{1/2}) / (M + N_j) + (N_1 N_2) / (\sqrt{M + N_j}) \)

\[ + (N_1 N_3) / (N_i + N_i + N_i + N_i + N_i + N_i + N_i + N_i) \]

\[ + (N_1 N_i) / (N_{r-1} + N_i + N_{r-1} + N + N_i) \]

\[ + (N_i N_j) / (N_{r-1} + N_j + N_{r-1} + N + N_j) \]

\[ + (N_i N_i) / (N_{r-1} + N_i + N_{r-1} + N + N_i) \]

\[ + (N_i N_j) / (N_{r-1} + N_i + N_{r-1} + N + N_i) \]

(iv) \( AZI(Z) = (MN_i)(N_i)(M + N_j) / (N_i + M + N_j + N_i + M + N_j) \)

\[ + (N_1 N_2)(M + N_j) / (N_i + M + N_j + N_i + M + N_j) \]

\[ + (N_1 N_3)(N_i + N_i + N_i + N_i + N_i + N_i + N_i + N_i) / (N_i + M + N_j + N_i + M + N_j) \]

\[ + (N_1 N_i) / (N_{r-1} + N_i + N_{r-1} + N + N_i + M + N_j) \]

\[ + (N_i N_j) / (N_{r-1} + N_i + N_{r-1} + N + N_i + M + N_j) \]

\[ + (N_i N_i) / (N_{r-1} + N_i + N_{r-1} + N + N_i + M + N_j) \]

\[ + (N_i N_j) / (N_{r-1} + N_i + N_{r-1} + N + N_i + M + N_j) \]

\[ + (N_i N_i) / (N_{r-1} + N_i + N_{r-1} + N + N_i + M + N_j) \]

\[ + (N_i N_j) / (N_{r-1} + N_i + N_{r-1} + N + N_i + M + N_j) \]

\[ + (N_i N_i) / (N_{r-1} + N_i + N_{r-1} + N + N_i + M + N_j) \]

\[ + (N_i N_j) / (N_{r-1} + N_i + N_{r-1} + N + N_i + M + N_j) \]

\[ + (N_i N_i) / (N_{r-1} + N_i + N_{r-1} + N + N_i + M + N_j) \]
Proof

(i) $\text{ABC}(Z) = \sum_{uv \in E} (d_u + d_v - 2d_ud_v) = \sum_{uv \in E(M+N1+N2)} (d_u + d_v - 2d_ud_v) + \sum_{uv \in E(M+N1+N3)} (d_u + d_v - 2d_ud_v) + \ldots + \sum_{uv \in E(M+N1+N2)} (d_u + d_v - 2d_ud_v) + \sum_{uv \in E(M+N1+N2)} (d_u + d_v - 2d_ud_v)$

Using edge partition in Table 1, we have

\[
\text{ABC}(Z) = (MN_1) \sqrt{\frac{(N_1 + M + N_2 - 2)}{(N_1)(M+N_2)}} + (N_1N_2) \sqrt{\frac{(M + N_2 + N_1 + N_3 - 2)}{(M+N_2)(N_1 + N_3)}} + (N_2N_3) \sqrt{\frac{(N_1 + N_3 + N_2 + N_4 - 2)}{(N_1 + N_3)(N_2 + N_4)}} + \ldots
\]

\[
+ (N_{r-2}N_{r-1}) \sqrt{\frac{(N_{r-3} + N_{r-2} + N_{r-1} + N - 2)}{(N_{r-3} + N_{r-2})(N_{r-2} + N)}} + (N_{r-1}N_r) \sqrt{\frac{(N_{r-1} + N + N_r - 2)}{(N_{r-1} + N)(N_r)}}.
\]

which can be shortened as follows:

\[
\text{ABC}(Z) = (MN_1) \sqrt{\frac{(N_1 + M + N_2 - 2)}{(N_1)(M+N_2)}} + (N_1N_2) \sqrt{\frac{(M + N_2 + N_1 + N_3 - 2)}{(M+N_2)(N_1 + N_3)}} + \sum_{i=2}^{\infty} N_iN_{i+1} \sqrt{\frac{(N_{i-1} + N_i + N_i - 2)}{(N_{i-1} + N_i)(N_i + N_{i+2})}}
\]

\[
+ (N_{r-1}N_r) \sqrt{\frac{(N_{r-2} + N_r + N_{r-1} + N - 2)}{(N_{r-2} + N_r)(N_{r-1} + N)}} + (N_rN) \sqrt{\frac{(N_{r-1} + N + N_r - 2)}{(N_{r-1} + N)(N_r)}}
\]
(ii) \( GA(Z) = \sum_{uv \in E} (2\sqrt{d_u d_v} / d_u + d_v) = \sum_{uv \in E(N_i, M+N_z)} (2\sqrt{d_u d_v} / d_u + d_v) + \sum_{uv \in E(M+N_i, N_z)} (2\sqrt{d_u d_v} / d_u + d_v) + \sum_{uv \in E(N_z, N_z, M+N_z)} (2\sqrt{d_u d_v} / d_u + d_v) + \ldots + \sum_{uv \in E(N_i, N_z, N_i, N_z)} (2\sqrt{d_u d_v} / d_u + d_v) + \sum_{uv \in E((N_i, M+N_z), N_z, N_z, M+N_z)} (2\sqrt{d_u d_v} / d_u + d_v) + \sum_{uv \in E(N_i, N_i, M+N_z)} (2\sqrt{d_u d_v} / d_u + d_v)

Using Table 1, we get:

\[
GA(Z) = 2(MN_1) \sqrt{(N_1)(M+N_z)} / (N_1 + M+N_z)
\]

\[+ 2(N_1N_2) \sqrt{(M+N_2)(N_1 + N_3)} / (M+N_2 + N_1 + N_3)
\]

\[+ 2(N_1N_3) \sqrt{(N_1 + N_3)(N_2 + N_4)} / (N_1 + N_3 + N_2 + N_4)
\]

\[+ 2(N_2N_3) \sqrt{(N_1 + N_3)(N_2 + N_4)} + \ldots
\]

\[+ 2(N_{r-2}N_{r-1}) \sqrt{(N_{r-3} + N_{r-1})(N_{r-2} + N_r)} / (N_{r-3} + N_{r-1} + N_{r-2} + N_r)
\]

\[+ 2(N_{r-1}N_r) \sqrt{(N_{r-2} + N_r)(N_{r-1} + N)} / (N_{r-2} + N_r + N_{r-1} + N)
\]

\[+ 2(N_rN) \sqrt{(N_{r-1} + N)(N_r)} / (N_{r-1} + N + N_r)
\]

This can be expressed as follows:

\[
GA(Z) = 2(MN_1) \sqrt{(N_1)(M+N_z)} / (N_1 + M+N_z) + 2(N_1N_2) \sqrt{(M+N_2)(N_1 + N_3)} / (M+N_2 + N_1 + N_3)
\]

\[+ 2 \sum_{i=2}^{r-2} N_iN_{i+1} \sqrt{((N_{i-1} + N_{i+1})(N_i + N_{i+2}))/((N_{i-1} + N_{i+1} + N_i + N_{i+2}))}
\]

\[+ 2(N_{r-2}N_{r-1}) \sqrt{(N_{r-3} + N_{r-1})(N_{r-2} + N_r)} / (N_{r-3} + N_{r-1} + N_{r-2} + N_r) + 2(N_rN) \sqrt{(N_{r-1} + N)(N_r)} / (N_{r-1} + N + N_r)
\]

(iii) \( SCI(Z) = \sum_{uv \in E} (1 / \sqrt{d_u + d_v}) = \sum_{uv \in E(N_i, M+N_z)} (1 / \sqrt{d_u + d_v}) + \sum_{uv \in E(M+N_i, N_z)} (1 / \sqrt{d_u + d_v}) + \sum_{uv \in E(N_z, N_z, M+N_z)} (1 / \sqrt{d_u + d_v}) + \ldots + \sum_{uv \in E(N_i, N_z, N_i, N_z)} (1 / \sqrt{d_u + d_v}) + \sum_{uv \in E((N_i, M+N_z), N_z, N_z, M+N_z)} (1 / \sqrt{d_u + d_v}) + \sum_{uv \in E(N_i, N_i, M+N_z)} (1 / \sqrt{d_u + d_v})

\[
\sum_{uv \in E(N_i, M+N_z)} (1 / \sqrt{d_u + d_v}) + \sum_{uv \in E(M+N_i, N_z)} (1 / \sqrt{d_u + d_v}) + \sum_{uv \in E(N_z, N_z, M+N_z)} (1 / \sqrt{d_u + d_v}) + \ldots + \sum_{uv \in E(N_i, N_z, N_i, N_z)} (1 / \sqrt{d_u + d_v}) + \sum_{uv \in E((N_i, M+N_z), N_z, N_z, M+N_z)} (1 / \sqrt{d_u + d_v}) + \sum_{uv \in E(N_i, N_i, M+N_z)} (1 / \sqrt{d_u + d_v})
\]
Using Table 1, we get

\[
SCI(Z) = \frac{(MN_1)}{\sqrt{(N_1) + (M + N_2)}} + \frac{(N_1N_2)}{\sqrt{(M + N_2) + (N_1 + N_3)}} + \frac{(N_2N_3)}{\sqrt{(N_1 + N_3) + (N_2 + N_4)}} + \ldots + \frac{(N_{r-2}N_{r-1})}{\sqrt{(N_{r-3} + N_{r-1}) + (N_{r-2} + N_r)}} + \frac{(N_{r-1}N_r)}{\sqrt{(N_{r-2} + N_r)(N_{r-1} + N)}} + \frac{(N_2)}{\sqrt{(N_{r-1} + N)}} (32)
\]

This can be abbreviated as follows:

\[
SCI(Z) = \frac{(MN_1)}{\sqrt{(N_1) + (M + N_2)}} + \frac{(N_1N_2)}{\sqrt{(M + N_2) + (N_1 + N_3)}} + \frac{(N_2N_3)}{\sqrt{(N_1 + N_3) + (N_2 + N_4)}} + \ldots + \frac{(N_{r-2}N_{r-1})}{\sqrt{(N_{r-3} + N_{r-1}) + (N_{r-2} + N_r)}} + \frac{(N_{r-1}N_r)}{\sqrt{(N_{r-2} + N_r)(N_{r-1} + N)}} + \frac{(N_2)}{\sqrt{(N_{r-1} + N)}} . (33)
\]

(iv) \( AZI(Z) = \sum_{\text{atom}} E \left( d_u \times d_v / d_u + d_v + d_x \right)^3 = \sum_{\text{atom}} E(N_1, M + N_2) \left( d_u \times d_v / d_u + d_v + d_x \right)^3 + \sum_{\text{atom}} E(M + N_2, N_1 + N_3) \left( d_u \times d_v / d_u + d_v + d_x \right)^3 + \sum_{\text{atom}} E(N_1 + N_3, N_2 + N_4) \left( d_u \times d_v / d_u + d_v + d_x \right)^3 + \ldots + \sum_{\text{atom}} E(N_{r-2} + N_{r-1}, N_{r-1} + N) \left( d_u \times d_v / d_u + d_v + d_x \right)^3 + \sum_{\text{atom}} E(N_{r-1} + N, N_r) \left( d_u \times d_v / d_u + d_v + d_x \right)^3 \]

Substituting values from Table 1, we get

\[
AZI(Z) = (MN_1) \left( \frac{(N_1) (M + N_2)}{N_1 + M + N_2} \right)^3 + (N_1N_2) \left( \frac{(M + N_2)(N_1 + N_3)}{M + N_2 + N_1 + N_3} \right)^3 + (N_2N_3) \left( \frac{(N_1 + N_3)(N_2 + N_4)}{N_1 + N_3 + N_2 + N_4} \right)^3 + \ldots + (N_{r-2}N_{r-1}) \left( \frac{(N_{r-3} + N_{r-1})(N_{r-2} + N_r - 2)}{N_{r-3} + N_{r-1} + N_{r-2} + N_r} \right)^3 + (N_{r-1}N_r) \left( \frac{(N_{r-2} + N_r)(N_{r-1} + N - 2)}{N_{r-2} + N_r + N_{r-1} + N} \right)^3 + (N_rN) \left( \frac{(N_{r-1} + N)(N_r - 2)}{N_{r-1} + N + N_r} \right)^3 . (34)
\]

This can be abbreviated as follows:

\[
AZI(Z) = (MN_1) \left( \frac{(N_1) (M + N_2)}{N_1 + M + N_2} \right)^3 + (N_1N_2) \left( \frac{(M + N_2)(N_1 + N_3)}{M + N_2 + N_1 + N_3} \right) + \sum_{i=2}^{r-2} N_iN_{i+1} \left( \frac{(N_{i-1} + N_i)(N_i + N_{i+2})}{N_{i-1} + N_i + N_1 + N_{i+2}} \right)^3 + (N_{r-1}N_r) \left( \frac{(N_{r-2} + N_r)(N_{r-1} + N - 2)}{N_{r-2} + N_r + N_{r-1} + N} \right)^3 + (N_rN) \left( \frac{(N_{r-1} + N)(N_r - 2)}{N_{r-1} + N + N_r} \right)^3 . (35)
\]

4. Conclusions

The deep neural network is helpful in modeling compounds with desirable physical and chemical properties employing the structure of compounds. This paper gives computational insight into the degree-dependent topological indices, which include the Randic index, Zagreb index, multiplicative Zagreb indices, harmonic index, ABC index, GA index, and sum-connectivity index of a general DNN with r-hidden layers. These indices correlate the structure with the properties such as boiling point, molar refractivity (MR), molar volume (MV), polar surface area, surface tension, enthalpy of vaporization, flash point, and many others. The results
computed in the above theorems give generally closed formulas that can be exploited to compute the topological indices of neural networks under study by giving specific values to the input parameters. The values of the computed indices grow with the growth of hidden layers and also depend on the number of nodes in each layer.

A deep neural network is an important tool used in experimental design, data reduction, fault diagnosis, and process control. The QSAR studies must be integrated with the neural network approach in order to achieve a more physical understanding of the system. The use of DNN provides an alternative way of predicting physical properties and its linkage with topological indices can further enhance theoretical achievements.

This study can be extended further by analyzing the distance-based topological indices such as the Wiener index, Harary index, and PI index. Computation of spectral invariants of deep neural networks such as energy, Estrada energy, and Kirchhoff index is also open for further research in this area.

Data Availability
No data were used to support the findings of this study.

Conflicts of Interest
The authors declare that they have no conflicts of interest regarding the publication of this paper.

Acknowledgments
The study was supported by the Science & Technology Bureau of Chengdu 2020-YF09-0005-SN and Sichuan Science and by the Technology program 2021YFH0107 Erasmus + SHYFTE Project 598649-EPP-1-2018-1-FR-EPPKA2-CBHE-JP and by the National Key Research and Development Program under Grant 2018YFB0904205.

References
[1] J. Cao and R. Li, “Fixed-time synchronization of delayed memristor-based recurrent neural networks,” Science China Information Sciences, vol. 60, no. 3, pp. 032201–032215, 2017.
[2] T. P. Tran, T. T. S. Nguyen, P. Tsai, and X. Kong, “BSPNN: boosted subspace probabilistic neural network for email security,” Artificial Intelligence Review, vol. 35, no. 4, pp. 369–382, 2011.
[3] T. P. Tran, L. Cao, D. Tran, and C. D. Nguyen, “Novel intrusion detection using probabilistic neural network and adaptive boosting,” International Journal of Computer Science and Information Security, vol. 6, no. 1, pp. 83–91, 2009.
[4] M. Yang and H. Wei, “Application of a neural network for the prediction of crystallization kinetics,” Industrial & Engineering Chemistry Research, vol. 45, no. 1, pp. 70–75, 2006.
[5] O. S. Kharitonova, V. V. Bronskaya, T. V. Ignashina, A. A. Al-Muntaser, and L. E. Khairrullina, “Modeling of adsorption process using neural networks,” IOP Conference Series: Earth and Environmental Science, vol. 315, no. 3, pp. 032025-032026, 2019.
[6] A. Velásco-Mejía, V. Vallejo-Becerra, A. U. Chávez-Ramírez, J. Torres-González, Y. Reyes-Vidal, and F. Castañeda-Zaldivar, “Modeling and optimization of a pharmaceutical crystallization process by using neural networks and genetic algorithms,” Powder Technology, vol. 292, pp. 122–128, 2016.
[7] M. Azzam, N. A. K. Aramouni, M. N. Ahmad, M. Awad, W. Kwapiszki, and J. Zeaiter, “Dynamic optimization of dry reformer under catalyst sintering using neural networks,” Energy Conversion and Management, vol. 157, pp. 146–156, 2018.
[8] M. Bagheri, A. Akbari, and S. A. Mirbagheri, “Advanced control of membrane fouling in filtration systems using artificial intelligence and machine learning techniques: a critical review,” Process Safety and Environmental Protection, vol. 123, pp. 229–252, 2019.
[9] M. Randić, “Characterization of molecular branching,” Journal of the American Chemical Society, vol. 97, no. 23, pp. 6609–6615, 1975.
[10] B. Bollobas and P. Erdos, “Graphs of extremal weights,” Ars Combinatoria, vol. 50, pp. 225–233, 1998.
[11] I. Gutman and N. Trinajstić, “Graph theory and molecular orbitals. Total $\phi$-electron energy of alternant hydrocarbons,” Chemical Physics Letters, vol. 17, no. 4, pp. 535–538, 1972.
[12] M. Ghorbani and M. Hosseinzadeh, “A new version of Zagreb indices,” Filomat, vol. 26, no. 1, pp. 93–100, 2012.
[13] G. H. Shirdel, H. Rezapour, and A. M. Sayadi, “The hyperzagreb index of graph operations,” Iranian Journal of Mathematical Chemistry, vol. 4, pp. 213–220, 2013.
[14] M. Estrada, L. Torres, L. Rodriguez, and I. Gutman, “An atombond connectivitiy index: modelling the enthalpy of formation of alkanes,” Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry, vol. 37, pp. 849–855, 1998.
[15] B. Zhou and N. Trinajstić, “On general sum-connectivity index,” Journal of Mathematical Chemistry, vol. 47, no. 1, pp. 210–218, 2010.
[16] D. Vukičević and B. Furtula, “Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges,” Journal of Mathematical Chemistry, vol. 46, no. 4, pp. 1369–1376, 2009.
[17] M. Javidi and J. Cao, “Computing topological indices of probabilistic neural network,” Neural Computing & Applications, vol. 30, no. 12, pp. 3869–3876, 2018.
[18] S. Mondal, N. De, and A. Pal, “Molecular descriptors of neural networks with chemical significance,” Revue Roumaine de Chimie, vol. 65, no. 11, pp. 1031–1044, 2021.
[19] J. B. Liu, Z. Raza, and M. Javidi, “Zagreb connection numbers for cellular neural networks,” Discrete Dynamics in Nature and Society, vol. 2020, Article ID 803804, 8 pages, 2020.
[20] M. Javidi, M. Abbas, J. B. Liu, W. C. Teh, and J. Cao, “Topological properties of four-layered neural networks,” Journal of Artificial Intelligence and Soft Computing Research, vol. 9, no. 2, pp. 111–122, 2019.
[21] J. B. Liu, J. Zhao, S. Wang, M. Javidi, and J. Cao, “On the topological properties of the certain neural networks,” Journal of Artificial Intelligence and Soft Computing Research, vol. 8, no. 4, pp. 257–268, 2018.
[22] C. Wang, J. B. Liu, and S. Wang, “Sharp upper bounds for multiplicative Zagreb indices of bipartite graphs with given diameter,” Discrete Applied Mathematics, vol. 227, pp. 156–165, 2017.
[23] R. Khalid, N. Idrees, and M. Jawwad Saif, “Topological characterization of Book graph and stacked Book graph,”
[24] W. Gao, W. Wang, and M. R. Farahani, “Topological indices study of molecular structure in anticancer drugs,” Journal of Chemistry, vol. 2016, Article ID 3216327, 8 pages, 2016.

[25] N. Idrees, M. Jawwad Saif, A. Sadiq, A. Rauf, and F. Hussain, “Topological indices of H-naphtalenic nanosheet,” Open Chemistry, vol. 16, no. 1, pp. 1184–1188, 2018.

[26] N. Idrees, M. J. Saif, A. Rauf, and S. Mustafa, “First and second Zagreb eccentricity indices of thorny graphs,” Symmetry, vol. 9, no. 1, p. 7, 2017.

[27] J. B. Liu, Y. Bao, W. T. Zheng, and S. Hayat, “Network coherence analysis on a family of nested weighted n-polygon networks,” Fractals, vol. 29, no. 08, pp. 2150260–2150276, 2021.

[28] J. B. Liu, T. Zhang, Y. Wang, and W. Lin, “The Kirchhoff index and spanning trees of Möbius/cylinder octagonal chain,” Discrete Applied Mathematics, vol. 307, pp. 22–31, 2022.

[29] S. Afridi, M. Yasin Khan, and G. Ali, “On generalized topological indices for some special graphs,” Journal of Mathematics, vol. 2022, p. 21, 2022.