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Some Computational Aspects of Boron Triangular Nanotubes

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Abstract: The recent discovery of boron triangular nanotubes competes with carbon in many respects. The closed form of M-polynomial of nanotubes produces closed forms of many degree-based topological indices which are numerical parameters of the structure and, in combination, determine properties of the concerned nanotubes. In this report, we give M-polynomials of boron triangular nanotubes and recover many important topological degree-based indices of these nanotubes. We also plot surfaces associated with these nanotubes that show the dependence of each topological index on the parameters of the structure.

Keywords: M-polynomial; degree-based index; boron nanotubes

1. Introduction

Nanotechnology is creating new structures between 1 and 100 nm. It creates many new materials and devices with a wide range of applications in medicine, electronics, and computers. Nanotechnology is expected to revolutionize the 21st century. Amongst the nanomaterials, nanocrystals, nanowires, and nanotubes constitute three major categories, the last two being one-dimensional. Since the discovery of carbon nanotubes in 1991, interests in one-dimensional nanomaterials has remarkably grown, and a phenomenal number of research articles are being published on nanotubes as well as on nanowires. Nanotubes are 3-D structures formed out of a 2-D lattice. The most significant nanotubes are carbon nanotubes and boron triangular nanotubes (Figure 1).

Boron nanotubes are becoming increasingly interesting because of their remarkable properties, such as their structural stability, work function, transport properties, and electronic structure [1]. A boron triangular sheet is obtained from a carbon hexagonal sheet by adding an extra atom to the center of each hexagon (Figure 2). Scientists believe that boron triangular nanotubes are a better conductor than carbon hexagonal nanotubes.

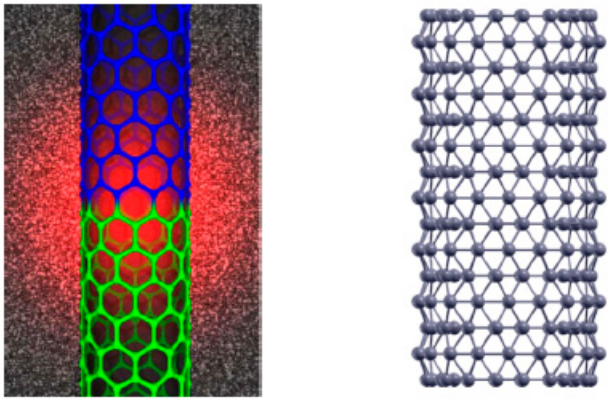

Figure 1. Carbon hexagonal nanotube (**a**) and boron triangular nanotube (**b**).

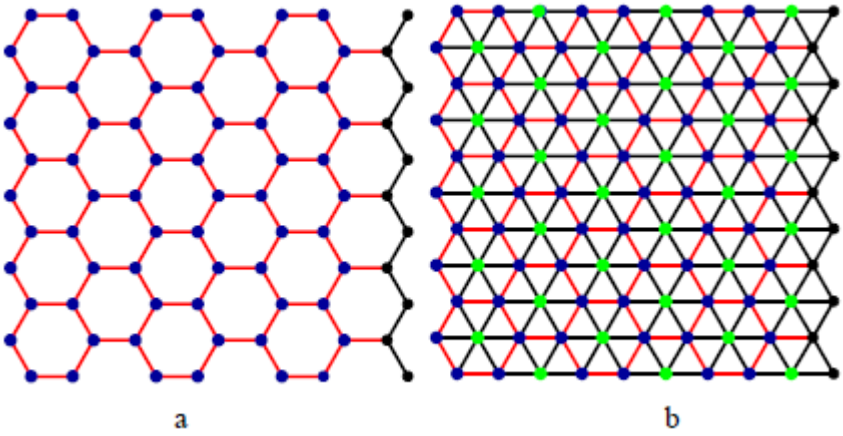

Figure 2. 2D lattice of carbon hexagonal nanotube (**a**) and boron triangular nanotube (**b**).

In chemical graph theory, a molecular graph is a simple graph (having no loops and multiple edges) in which atoms and chemical bonds between them are represented by vertices and edges, respectively. A graph $G(V, E)$ with vertex set $V(G)$ and edge set $E(G)$ is connected if there is a connection between any pair of vertices in G. A network is simply a connected graph having no multiple edges and loops. The degree of a vertex is the number of vertices which are connected to that fixed vertex by the edges. In a chemical graph, the degree of any vertex is at most 4. The distance between two vertices u and v is denoted as $d(u, v) = d_G(u, v)$ and is the length of shortest path between u and v in graph G. The number of vertices of G, adjacent to a given vertex v, is the "degree" of this vertex, and will be denoted by $d_v(G)$ or, if misunderstanding is not possible, simply by d_v. The concept of degree is somewhat closely related to the concept of valence in chemistry. For details on the basics of graph theory, any standard text such as [2] can be of great help.

Cheminformatics is another emerging field in which quantitative structure-activity (QSAR) and structure-property (QSPR) relationships predict the biological activities and properties of the nanomaterial. In these studies, some physico-chemical properties and topological indices are used to predict bioactivity of the chemical compounds [3–7]. Algebraic polynomials have also useful applications in chemistry, such as Hosoya polynomial (also called Wiener polynomial) [8], which plays a vital role in determining distance-based topological indices. Among other algebraic polynomials, the M-polynomial [9], introduced in 2015, plays the same role in determining the closed form of many degree-based topological indices [10–14]. The main advantage of M-polynomial is the wealth of information that it contains about degree-based graph invariants.

In this article, we compute a closed form of some degree-based topological indices of boron triangular nanotubes by using an M-polynomial.

Definition 1. *[9] The M-polynomial of G is defined as*

$$M(G,x,y) = \sum_{\delta \le i \le j \le \Delta} m_{ij}(G) x^i y^j, \tag{1}$$

where $\delta = Min\{d_v : v \in V(G)\}$, $\Delta = Max\{d_v : v \in V(G)\}$, and $m_{ij}(G)$ is the edge $vu \in E(G)$ such that $\{d_v, d_u\} = \{i, j\}$.

Weiner, in 1947 approximated the boiling point of alkanes as $\alpha W(G) + \beta P_3 + \gamma$, where α, β, and γ are empirical constants, $W(G)$ is the Weiner index, and P_3 is the number of paths of length 3 in G [15]. Thus, Weiner laid the foundation of Topological index, which is also known as the connectivity index. Many chemical experiments require the determination of the chemical properties of emerging nanotubes and nanomaterials. Chemical-based experiments reveal that, out of more than 140 topological indices, no single index in strong enough to determine many physico-chemical properties, although, in combination, these topological indices can do this to some extent. The Wiener index is originally the first and most studied topological index (for details, [16,17]). The Randić index, [18] denoted by $R_{-\frac{1}{2}}(G)$ and introduced by Milan Randić in 1975, is also one of the oldest topological indexes. The Randić index is defined as

$$R_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}. \tag{2}$$

In 1998, working independently, Bollobas and Erdos [19] and Amic et al. [20] proposed the generalized Randić index and has been studied extensively by both chemists and mathematicians [21], and many mathematical properties of this index have been discussed in [22]. For a detailed survey, refer to [23].

The general Randić index is defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{(d_u d_v)^\alpha}, \tag{3}$$

and the inverse Randić index is defined as $RR_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$.

Obviously, $R_{\frac{-1}{2}}(G)$ is the particular case of $R_\alpha(G)$ when $\alpha = -\frac{1}{2}$.

The Randić index is also the most popular, the most often applied, and the most studied among all other topological indices. Many papers and books such as [24,25] are written on this topological index. Randić himself wrote two reviews on his Randić index [26,27], and there are three other reviews [28–30]. The suitability of the Randić index for drug design was immediately recognized; eventually, the index was used for this purpose, and now has been used on countless occasions. The physical reason for the success of such a simple graph invariant is still an enigma, although several more-or-less plausible explanations were offered.

Gutman and Trinajstić introduced first Zagreb index and second Zagreb index, which are defined as $M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$ and $M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v)$, respectively. For detail about these indices, we refer the reader to [31–35].

Both the first Zagreb index and the second Zagreb index give greater weights to the inner vertices and edges, and smaller weights to the outer vertices and edges, which opposes intuitive reasoning. Hence, they were amended as follows [36]: for a simple connected graph G, the second modified Zagreb index is defined as

$$^{m}M_2(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}. \quad (4)$$

The symmetric division index [SDD] is one of the 148 discrete Adriatic indices and is a good predictor of the total surface area for polychlorobiphenyls [37]. The symmetric division index of a connected graph G is defined as

$$\mathrm{SDD(G)} = \sum_{uv \in E(G)} \left\{ \frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)} \right\}. \quad (5)$$

Another variant of the Randić index is the harmonic index, defined as

$$H(G) = \sum_{vu \in E(G)} \frac{2}{d_u + d_v}. \quad (6)$$

As far as we know, this index first appeared in [38]. Favaron et al. [39] considered the relation between the harmonic index and the eigenvalues of graphs.

The inverse sum-index is the descriptor that was selected in [40] as a significant predictor of the total surface area of octane isomers and for which the extremal graphs obtained with the help of MathChem have a particularly simple and elegant structure. The inverse sum-index is defined as

$$I(G) = \sum_{vu \in E(G)} \frac{d_u d_v}{d_u + d_v}. \quad (7)$$

The augmented Zagreb index of G proposed by Furtula et al. [41] is defined as

$$A(G) = \sum_{vu \in E(G)} \left\{ \frac{d_u d_v}{d_u + d_v - 2} \right\}^3. \quad (8)$$

This graph invariant has proven to be a valuable predictive index in the study of the heat of formation in octanes and heptanes [41], whose prediction power is better than the atom-bond connectivity index (please refer to [42–44] for its research background). Moreover, the tight upper and lower bounds for the augmented Zagreb index of chemical trees, and the trees with minimal augmented Zagreb index, were obtained in [41].

The following Table 1 relates some well-known degree-based topological indices with M-polynomials [9].

Table 1. Derivation of some degree-based topological indices from M-polynomials.

Topological Index	Derivation from $M(G;x,y)$
First Zagreb index	$(D_x + D_y)(M(G;x,y))_{x=y=1}$
Second Zagreb index	$(D_x D_y)(M(G;x,y))_{x=y=1}$
Modified Second Zagreb index	$(S_x S_y)(M(G;x,y))_{x=y=1}$
Randić index	$\left(D_x^{\alpha} D_y^{\alpha}\right)(M(G;x,y))_{x=y=1}$
Inverse Randić index	$\left(S_x^{\alpha} S_y^{\alpha}\right)(M(G;x,y))_{x=y=1}$
Symmetric Division Index	$(D_x S_y + S_x D_y)(M(G;x,y))_{x=y=1}$
Harmonic Index	$2S_x J(M(G;x,y))_{x=1}$
Inverse sum Index	$S_x J D_x D_y (M(G;x,y))_{x=1}$
Augmented Zagreb Index	$S_x{}^3 Q_{-2} J D_x{}^3 D_y{}^3 (M(G;x,y))_{x=1}$

where

$$D_x = x\frac{\partial(f(x,y)}{\partial x},\ D_y = y\frac{\partial(f(x,y)}{\partial y},\ S_x = \int_0^x \frac{f(t,y)}{t}dt, S_y = \int_0^y \frac{f(x,t)}{t}dt\ ,\ J(f(x,y)) = f(x,x),$$
$$Q_\alpha(f(x,y)) = x^\alpha f(x,y).$$

2. Results

In this section, we provide our computational results.

2.1. M-Polynomials

In Figure 3, we represent a boron triangular nanotube, by a planar graph, $BNT_t[m,n]$ of order n × m, where m and n represent the number of items in each row and each column, respectively. There are $\frac{3nm}{2}$ vertices and $\frac{3m(3n-2)}{2}$ edges in the 2D lattice graph of boron triangular nanotubes.

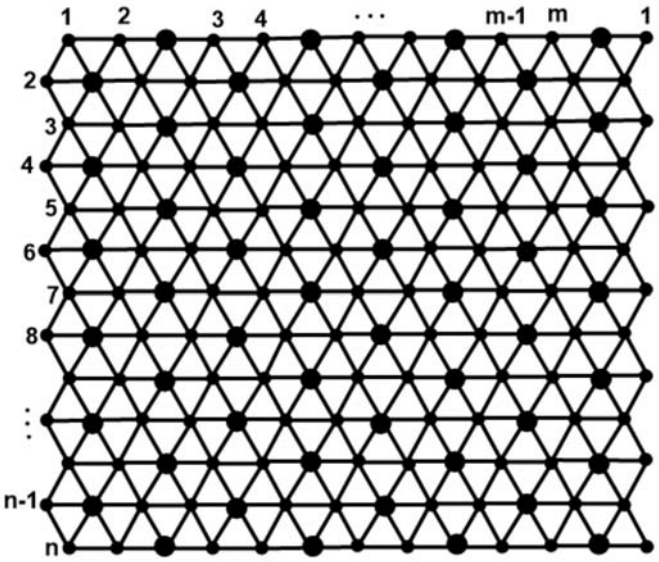

Figure 3. 2D lattice of the boron triangular nanotube.

There are two types of vertices with respect to degree, i.e., $V_{\{2\}} = \{v \in V(BNT_t[m,n]) : d_v = 4\}$ and $V_{\{6\}} = \{\{v \in V(BNT_t[m,n]) : d_v = 6\}$. The partition of the edge set of $BNT_t[m,n]$ is given in Table 2.

Table 2. Edge partition of edge set of $BNT_t[m,n]$.

$(d_u,\ d_v)$	(4, 4)	(4, 6)	(6, 6)
Number of edges	$3m$	$6m$	$\frac{m}{2}(9n-24)$

Theorem 1. *Let $BNT_t[m,n]$ be boron triangular nanotubes. Then,*

$$M(BNT_t[m,n];x,y) = 3mx^4y^4 + 6mx^4y^6 + \frac{m}{2}m(9n-24)x^6y^6. \tag{9}$$

Proof. From Table 2, we have following edge partition:

$$E_{\{4,4\}} = \{e = uv \in E(BNT_t[m,n]) : d_u = 4, d_v = 4\}, \tag{10}$$

$$E_{\{4,6\}} = \{e = uv \in E(BNT_t[m,n]) : d_u = 4, d_v = 6\}, \tag{11}$$

$$\text{and } E_{\{6,6\}} = \{e = uv \in E(BNT_t[m,n]) : d_u = 6, d_v = 6\}, \tag{12}$$

such that $\left|E_{\{4,4\}}\right| = 3m$, $\left|E_{\{4,6\}}\right| = 6m$, $\left|E_{\{6,6\}}\right| = \frac{m}{2}(9n-24)$. Thus, by definition, the M-polynomial of $BNT_t[m,n]$ is

$$\begin{aligned} M(BNT_t[m,n];\, x\,, y) &= \sum_{i\leq j} m_{ij}(BNT_t[m,n])x^i y^j \\ &= \sum_{4\leq 4} m_{44}(BNT_t[m,n])x^4y^4 + \sum_{4\leq 6} m_{46}(BNT_t[m,n])x^4y^6 + \sum_{6\leq 6} m_{66}(BNT_t[m,n])x^6y^6 \\ &= \sum_{uv\in E_{\{4,4\}}} m_{44}(BNT_t[m,n])x^4y^4 + \sum_{uv\in E_{\{4,6\}}} m_{46}(BNT_t[m,n])x^4y^6 + \sum_{uv\in E_{\{6,6\}}} m_{66}(BNT_t[m,n])x^6y^6 \\ &= \left|E_{\{4,4\}}\right|x^2y^4 + \left|E_{\{4,6\}}\right|x^4y^6 + \left|E_{\{6,6\}}\right|x^6y^6 \\ &= 3mx^4y^4 + 6mx^4y^6 + \tfrac{m}{2}(9n-24)x^6y^6. \end{aligned}$$

Figure 4 presents the Maple 13 plot of the M-polynomial of the boron triangular nanotubes. Clearly, the values drastically decrease, as $X \to \pm 1$, $Y \to \pm 2$. For most of $[-1,1] \times [-2,2]$, values remain stable.

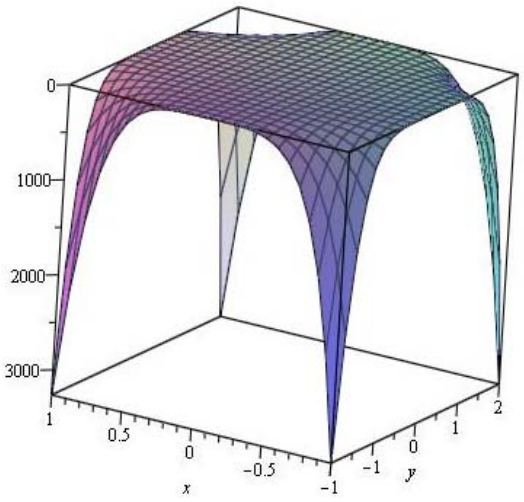

Figure 4. 3D plot of the M-polynomial of $BNT_t[m,n]$.

2.2. Topological Indices

Proposition 1. *Let $BNT_t[m,n]$ be the boron triangular nanotube. Then,*

1. $M_1(BNT_t[m,n]) = 54mn - 60m$.
2. $M_2(BNT_t[m,n]) = 162mn - 240m$.
3. ${}^{m}M_2(BNT_t[m,n]) = \frac{5}{48}m + \frac{1}{8}mn$.
4. $R_a(BNT_t[m,n]) = \frac{3}{2}m\left(3n(36)^{\alpha} + 2(16)^{\alpha} + 4(24)^{\alpha} - 8(36)^{\alpha}\right)$.
5. $RR_a(BNT_t[m,n]) = \frac{3m}{(16)^{\alpha}} + \frac{m}{6^{\alpha-1}4^{\alpha}} + \frac{3m(3n-8)}{(36)^{\alpha}}$.
6. $SDD(BNT_t[m,n]) = 9mn - 5m$.

Proof. Let

$$f(x,y) = M(BNT_t[m,n];x\,,y) = 3mx^4y^4 + 6mx^4y^6 + \frac{m}{2}(9n-24)x^6y^6, \tag{13}$$

$$\text{then} D_x(f(x,y)) = 12mx^4y^4 + 24mx^4y^6 + 3m(9n-24)x^6y^6, \tag{14}$$

$$D_y(f(x,y)) = 12mx^4y^4 + 36mx^4y^6 + 3m(9n-24)x^6y^6, \tag{15}$$

$$D_xD_y(f(x,y)) = 48mx^4y^4 + 144mx^4y^6 + 18m(9n-24)x^6y^6, \tag{16}$$

$$S_x(f(x,y)) = \frac{3}{4}mx^4y^4 + \frac{3}{2}mx^4y^6 + \frac{m}{12}(9n-24)x^6y^6, \tag{17}$$

$$S_yS_x(f(x,y)) = \frac{3}{16}mx^4y^4 + \frac{1}{4}mx^4y^6 + \frac{m}{72}(9n-24)x^6y^6, \tag{18}$$

$$D_x{}^{\alpha}D_y{}^{\alpha}(f(x,y)) = 3\times 4^{2\alpha}mx^4y^4 + 6^{\alpha+1}\times 4^{\alpha}mx^4y^6 + \frac{6^{2\alpha}m}{2}(9n-24)x^6y^6, \tag{19}$$

$$S_x{}^{\alpha}S_y{}^{\alpha}(f(x,y)) = \frac{3}{4^{2\alpha}}mx^4y^4 + \frac{1}{4^{\alpha}6^{\alpha-1}}mx^4y^6 + \frac{m}{2\times 6^{2\alpha}}(9n-24)x^6y^6, \tag{20}$$

$$S_yD_x(f(x,y)) = 3mx^4y^4 + 4mx^4y^6 + \frac{1}{2}m(9n-24)x^6y^6, \tag{21}$$

$$S_xD_y(f(x,y)) = 3mx^4y^4 + 9mx^4y^6 + \frac{1}{2}m(9n-24)x^6y^6. \tag{22}$$

Now, from Table 1,

1. $M_1(BNT_t[m,n]) = (D_x+D_y)(M(G;x,y))\big|_{x=y=1} = 54mn-60m.$
2. $M_2(BNT_t[m,n]) = D_xD_y(M(G;x,y))\big|_{x=y=1} = 162mn-240m.$
3. ${}^{m}M_2(BNT_t[m,n]) = S_xS_y(M(G;x,y))\big|_{x=y=1} = \frac{5}{48}m+\frac{1}{8}mn.$
4. $R_a(BNT_t[m,n]) = D_x^{\alpha}D_y^{\alpha}(M(G;x,y))\Big|_{x=y=1} = \frac{3}{2}m\big(3n(36)^{\alpha}+2(16)^{\alpha}+4(24)^{\alpha}-8(36)^{\alpha}\big).$
5. $RR_a(BNT_t[m,n]) = S_x^{\alpha}S_y^{\alpha}(M(G;x,y))\Big|_{x=y=1} = \frac{3m}{(16)^{\alpha}}+\frac{m}{6^{\alpha-1}4^{\alpha}}+\frac{3m(3n-8)}{(36)^{\alpha}}.$
6. $SDD(BNT_t[m,n]) = \big(D_xS_y+S_xD_y\big)(M(G;x,y))\big|_{x=y=1} = 9mn-5m.$

Proposition 2. *Let $BNT_t[m,n]$ be the boron triangular nanotube. Then,*

1. $H(BNT_t\,[m,n]\,) = -\frac{1}{20}m+\frac{3}{4}mn.$
2. $I(BNT_t[m,n]) = -\frac{78}{5}m+\frac{27}{2}mn.$
3. $A(BNT_t[m,n]) = -\frac{383606}{1125}m+\frac{26244}{125}mn.$

Proof. Let

$$f(x,y) = M(BNT_t[m,n];x\,,y) = 3mx^4y^4 + 6mx^4y^6 + \frac{m}{2}(9n-24)x^6y^6, \tag{23}$$

$$\text{then } S_xJ(f(x,y)) = \frac{3}{8}mx^8 + \frac{3}{5}mx^{10} + \frac{m}{24}(9n-24)x^{12}, \tag{24}$$

$$S_xJD_xD_y(f(x,y)) = 6mx^8 + \frac{72}{5}mx^{10} + \frac{3}{2}m(9n-24)x^{12}, \tag{25}$$

$$S_x{}^3Q_{-2}JD_x{}^3D_y{}^3(f(x,y)) = \frac{3\times 4^6}{6^3}mx^6 + \frac{6^4\times 4^3}{8^3}mx^8 + \frac{6^6m}{2\times 10^3}(9n-24)x^{10}. \tag{26}$$

Now, from Table 1,

1. $H(BNT_t[m,n]\,) = 2S_xJ(M(G;x,y))|_{x=1} = -\frac{1}{20}m+\frac{3}{4}mn.$
2. $I(BNT_t[m,n]) = S_xJD_xD_y(M(G;x,y))\big|_{x=1} = -\frac{78}{5}m+\frac{27}{2}mn.$
3. $A(BNT_t[m,n]) = S_x{}^3Q_{-2}JD_x{}^3D_y{}^3(M(G;x,y))\Big|_{x=1} = -\frac{383606}{1125}m+\frac{26244}{125}mn.$

3. Conclusions and Discussion

In this article, we computed the closed form of M-polynomial for boron triangular nanotubes. Then, we derived many degree-based topological indices for boron triangular nanotubes. These indices can help us to understand its physical features, chemical reactivity, and biological activities, such as the boiling point, the heat of formation, the fracture toughness, the strength, the conductivity, and the hardness. From this point of view, a topological index can be regarded as a score function that maps each molecular structure to a real number and is used as a descriptor of the molecule under testing. These results can also play a vital part in the determination of the significance of boron triangular nanotubes in electronics and industry. Because of its hardness, it can be used in the preparation of armor. We also want to remark that similar techniques can be used to determine M-polynomials and topological indices about α-boron nanotubes. Now, we provide the computer-based analysis of each topological index with involved parameters. Although graphs are similar, but have different gradients; see Figure 5.

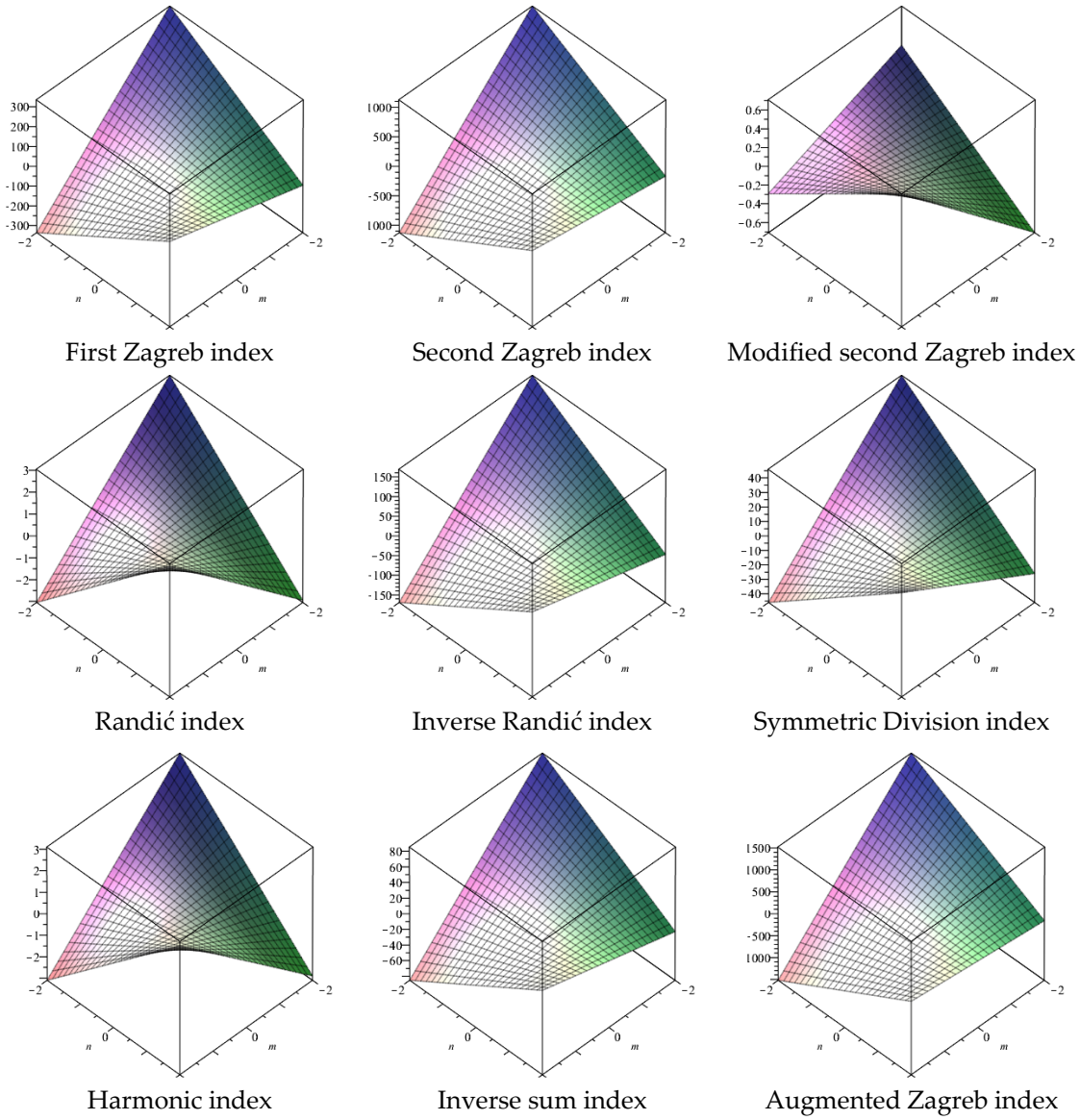

Figure 5. 3D plots of topological indices.

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