Research Article

On Degree-Based Topological Indices for Strong Double Graphs

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A topological index is a characteristic value which represents some structural properties of a chemical graph. We study strong double graphs and their generalization to compute Zagreb indices and Zagreb coindices. We provide their explicit computing formulas along with an algorithm to generate and verify the results. We also find the relation between these indices. A 3D graphical representation and graphs are also presented to understand the dynamics of the aforementioned topological indices.

1. Introduction

Chemical graph theory is an important topological field of mathematical chemistry that deals with mathematical modelling of chemical compound structures. A molecular structure of a compound consists of many atoms. Specially, hydrocarbons are chemical compounds which consist of carbon and hydrogen atoms. A graph consisting of hydrocarbons is known as a molecular graph which represents the carbon structure of a molecule [1].

We consider a simple molecular graph, say G , which consists of nonhydrogen atoms and covalent bonds. In graph theory, the nonhydrogen atoms are represented by a set of vertices $V = V(G)$ and the covalent bonds with the set of edges $E = E(G)$. The number of atoms and bonds in a structure is represented by $n = |V|$ and $m = |E|$, respectively. The valency of an atom is represented by $\mathfrak{R}_G(v)$, and it is known as the degree of vertex $v \in V(G)$, which also represents the number of adjacent (or neighboring) vertices of V . A set consisting of neighboring vertices of v is known as open neighborhood and denoted as $N(v) = \{w \in V(G) : vw \in E(G)\}$. If the vertex v is included in open neighborhood, then the set of vertices is called closed neighborhood, and it is denoted as $N[v] = N(v) \cup \{v\}$.

A double graph $D(G)$ is generated by taking two copies of a graph G and connecting every vertex v_i in one copy with the opened neighborhood $N(v_i)$ of the corresponding vertex

with its second copy. For details, see Figure 1 in which a path graph P_4 and its double graph are presented. A strong double graph $S D(G)$ is generated by taking two copies of a graph G and connecting every vertex v_i in one copy with closed neighborhood $N[v_i] = N(v_i) \cup \{v_i\}$ of the corresponding vertex with its second copy. For details, see Figure 2 in which a strong double graph of P_4 and its k -iterated strong double graph are presented.

A complement $\bar{G}$ of a graph G consists of the same set of vertices, where two vertices v and w are adjacent by an edge vw if and only if they are not adjacent in G . Hence, $vw \in E(\bar{G}) \Leftrightarrow vw \notin E(G)$. A complement of a graph consists of a number of edges and the degree of vertex v which are represented as $\bar{m} = \binom{n}{2} - m$ and $d_{\bar{G}}(v) = n - 1 - \mathfrak{R}_G(v)$, respectively.

A molecular descriptor is known as the topological index provides specific information about the structure of molecules. In graph theory, the molecular structure is considered as a graph G . The topological index is also known as the connectivity index [2, 3]. Topological indices are largely applied in chemistry to develop the quantitative structure-activity relationship (QSAR) in which the characteristics of molecules can be correlated with their chemical structures [4]. The physicochemical properties of a molecule can also be explained through topological indices. The first index of a

FIGURE 1: The graph P_4 and its double graph. (a) P_4 . (b) $D(P_4)$. FIGURE 2: The strong double graph of P_4 and its generalization. (a) $SD^*(P_4)$. (b) $SD^{*2}(P_4)$.

chemical graph was introduced by Harold Wiener [5] in 1947 as an aid to determining the boiling point of the paraffin compound. This index is known as the Wiener index and defined as $W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v)$, where the notation $d(u, v)$ represents the distance between u and v .

A topological index is defined as a function $T: \psi \rightarrow \mathbb{R}$, where ψ is the set of finite simple graphs and $\mathbb{R}$ is a set of real numbers which satisfy the relation $T(G) = T(H)$ if G is isomorphic to H . Recently published work [6, 7] motivated us to further investigate the Zagreb indices and coindices of strong double graphs.

The first Zagreb index $M_1(G)$ and second Zagreb index $M_2(G)$ were introduced by Gutman and Trinajstić in 1972 [8] and elaborated by Nikolić et al. after 30 years in 2003 [9]. $M_1(G)$ and $M_2(G)$ are defined as

$$\begin{aligned} M_1(G) &= \sum_{uv \in E(G)} [\mathfrak{R}_G(u) + \mathfrak{R}_G(v)], \\ M_2(G) &= \sum_{uv \in E(G)} [\mathfrak{R}_G(u)\mathfrak{R}_G(v)]. \end{aligned} \quad (1)$$

The first Zagreb index is also written as $\sum_{v \in V(G)} [\mathfrak{R}_G(v)]^2$.

Recently, some useful versions of Zagreb indices have been discovered, such as multiplicative Zagreb indices [3, 7, 10], multiplicative sum Zagreb indices [11, 12], Zagreb coindices [6], and multiplicative Zagreb coindices [13].

The important variants of the Zagreb index are the first and second Zagreb coindices, which are defined as follows, respectively:

$$\begin{aligned} \overline{M}_1(G) &= \sum_{u \neq v; uv \notin E(G)} [\mathfrak{R}_G(u) + \mathfrak{R}_G(v)], \\ \overline{M}_2(G) &= \sum_{u \neq v; uv \notin E(G)} [\mathfrak{R}_G(u)\mathfrak{R}_G(v)]. \end{aligned} \quad (2)$$

Doslic [14] introduced $\overline{M}_1(G)$ and $\overline{M}_2(G)$ in 2008. In 2009, Ashrafi et al. [15] determined the extremal values of these new invariants for some special graphs. They [6] also explored their fundamental properties and provided some explicit formulas for these versions under different graph operations.

2. Main Results

In this section, we study Zagreb indices and Zagreb coindices of strong double graphs. We also study these indices for generalized k -iterated strong double graphs. We use the concept of edge partition to reduce computation complexity and obtain computing formulas for these indices.

For the sake of simplicity, we consider $SD(G) = G^{1*} = G^*$ and $G^{k*} = (G^{(k-1)*})^*$ for $k \geq 2$. Assume that $G^{0*} = G$ for the sake of consistency.

In the following theorem, we study the first and second Zagreb indices of the strong double graph.

Theorem 1. Let G be a simple connected graph of order n and size m ; then,

- (i) $M_1(G^*) = 8M_1(G) + 16m + 2n$
- (ii) $M_2(G^*) = 16M_2(G) + 12M_1(G) + 12m + n$

Proof. For the sake of convenience, we label all vertices in G as $\{v_1, v_2, \dots, v_n\}$. Suppose that x_i and y_i are the corresponding clone vertices, in strong double graph G^* , of v_i for each $i = 1, \dots, n$.

For any given vertex v_i in G and its clone vertices x_i and y_i , there exists $d_{G^*}(x_i) = d_{G^*}(y_i) = 2\mathfrak{R}_G(v_i) + 1$ by the definition of the strong double graph.

For $v_i, v_j \in V(G)$, if $v_i v_j \in E(G)$, then $x_i x_j \in E(G^*)$, $y_i y_j \in E(G^*)$, $x_i y_j \in E(G^*)$, and $y_i x_j \in E(G^*)$.

So, we only need to consider the total contribution of the following three types of adjacent vertex pairs both to $M_1(G^*)$ and to $M_2(G^*)$.

Type 1: the adjacent vertex pairs $\{x_i, x_j\}$ and $\{y_i, y_j\}$, where $v_i v_j \in E(G)$

Type 2: the adjacent vertex pairs $\{x_i, y_i\}$ for each $i = 1, \dots, n$

Type 3: the adjacent vertex pairs $\{x_i, y_j\}$ and $\{y_i, x_j\}$, where $v_i v_j \in E(G)$

The total contribution of adjacent vertex pairs of type 1 in $M_1(G^*)$ is given by

$$\begin{aligned} \sum_{x_i x_j \in E(G^*)} [d_{G^*}(x_i) + d_{G^*}(x_j)] &= \sum_{y_i y_j \in E(G^*)} [d_{G^*}(y_i) + d_{G^*}(y_j)] \\ &= \sum_{v_i v_j \in E(G)} [(2\Re_G(v_i) + 1) + (2\Re_G(v_j) + 1)] \\ &= 2 \sum_{v_i v_j \in E(G)} [\Re_G(v_i) + \Re_G(v_j)] + 2|E(G)|_{v_i v_j \in E(G)} \\ &= 2M_1 + 2m, \end{aligned} \quad (3)$$

and $M_2(G^*)$ is given by

$$\begin{aligned} \sum_{x_i x_j \in E(G^*)} [d_{G^*}(x_i) \cdot d_{G^*}(x_j)] &= \sum_{y_i y_j \in E(G^*)} [d_{G^*}(y_i) \cdot d_{G^*}(y_j)] \\ &= \sum_{v_i v_j \in E(G)} [(2\Re_G(v_i) + 1) \cdot (2\Re_G(v_j) + 1)] \\ &= 4 \sum_{v_i v_j \in E(G)} [\Re_G(v_i) \cdot \Re_G(v_j)] + 2 \sum_{v_i v_j \in E(G)} [\Re_G(v_i) + \Re_G(v_j)] + |E(G)|_{v_i v_j \in E(G)} \\ &= 4M_2 + 2M_1 + m. \end{aligned} \quad (4)$$

The total contribution of adjacent vertex pairs of type 2 in $M_1(G^*)$ is given by

$$\begin{aligned} \sum_{x_i y_i \in E(G^*)} [d_{G^*}(x_i) + d_{G^*}(y_i)] &= \sum_{v_i \in V(G)} [(2\Re_G(v_i) + 1) + (2\Re_G(v_i) + 1)] \\ &= 4 \sum_{v_i \in V(G)} \Re_G(v_i) + 2|V(G)|_{v_i \in V(G)} \\ &= 8m + 2n, \end{aligned} \quad (5)$$

and $M_2(G^*)$ is given by

$$\begin{aligned} \sum_{x_i y_i \in E(G^*)} [d_{G^*}(x_i) + d_{G^*}(y_i)] &= \sum_{v_i \in V(G)} [(2\Re_G(v_i) + 1) \cdot (2\Re_G(v_i) + 1)] \\ &= 4 \sum_{v_i \in V(G)} [\Re_G(v_i)]^2 + 4 \sum_{v_i \in V(G)} \Re_G(v_i) + |V(G)|_{v_i \in V(G)} \\ &= 4M_1(G) + 8m + n. \end{aligned} \quad (6)$$

The total contribution of adjacent vertex pairs of type 3 in $M_1(G^*)$ is given by

$$\begin{aligned} \sum_{x_i y_i \in E(G^*)} [d_{G^*}(x_i) + d_{G^*}(y_i)] &= \sum_{y_i x_j \in E(G^*)} [d_{G^*}(y_i) + d_{G^*}(x_i)] \\ &= \sum_{v_i v_j \in E(G)} [(2\Re_G(v_i) + 1) + (2\Re_G(v_j) + 1)] \\ &= 2 \sum_{v_i v_j \in E(G)} [\Re_G(v_i) + \Re_G(v_j)] + |E(G)|_{v_i v_j \in E(G)} \\ &= 2M_1(G) + 2m, \end{aligned} \quad (7)$$

and $M_2(G^*)$ is given by

$$\begin{aligned}
 \sum_{x_i y_j \in E(G^*)} [d_{G^*}(x_i) \cdot d_{G^*}(y_j)] &= \sum_{y_i x_j \in E(G^*)} [d_{G^*}(y_i) \cdot d_{G^*}(x_j)] \\
 &= \sum_{v_i v_j \in E(G)} [(2\mathfrak{R}_G(v_i) + 1) \cdot (2\mathfrak{R}_G(v_j) + 1)] \\
 &= 4 \sum_{v_i v_j \in E(G)} [\mathfrak{R}_G(v_i) \cdot \mathfrak{R}_G(v_j)] + 2 \sum_{v_i v_j \in E(G)} [\mathfrak{R}_G(v_i) + \mathfrak{R}_G(v_j)] + |E(G)|_{v_i v_j \in E(G)} \\
 &= 4M_2(G) + 2M_1(G) + m.
 \end{aligned} \tag{8}$$

Therefore, by using equations (3), (5) and (7), we have

$$\begin{aligned}
 M_1(G^*) &= \sum_{x_i x_j \in E(G^*)} [d_{G^*}(x_i) + d_{G^*}(x_j)] + \sum_{y_i y_j \in E(G^*)} [d_{G^*}(y_i) + d_{G^*}(y_j)] \\
 &\quad + \sum_{x_i y_i \in E(G^*)} [d_{G^*}(x_i) + d_{G^*}(y_i)] + \sum_{x_i y_j \in E(G^*)} [d_{G^*}(x_i) + d_{G^*}(y_j)] + \sum_{y_i x_j \in E(G^*)} [d_{G^*}(y_i) + d_{G^*}(x_j)] \\
 &= (2M_1(G) + 2m) + (2M_1(G) + 2m) + (8m + 2n) + (2M_1(G) + 2m) + (2M_1(G) + 2m) \\
 &= 8M_1(G) + 16m + 2n.
 \end{aligned} \tag{9}$$

By using (4), (6) and (8), we also have

$$\begin{aligned}
 M_2(G^*) &= \sum_{x_i x_j \in E(G^*)} [d_{G^*}(x_i) \cdot d_{G^*}(x_j)] + \sum_{y_i y_j \in E(G^*)} [d_{G^*}(y_i) \cdot d_{G^*}(y_j)] \\
 &\quad + \sum_{x_i y_i \in E(G^*)} [d_{G^*}(x_i) \cdot d_{G^*}(y_i)] + \sum_{x_i y_j \in E(G^*)} [d_{G^*}(x_i) \cdot d_{G^*}(y_j)] + \sum_{y_i x_j \in E(G^*)} [d_{G^*}(y_i) \cdot d_{G^*}(x_j)] \\
 &= (4M_2(G) + 2M_1(G) + m) + (4M_2(G) + 2M_1(G) + m) \\
 &\quad + (4M_1(G) + 8m + n) + (4M_2(G) + 2M_1(G) + m) + (4M_2(G) + 2M_1(G) + m) \\
 &= 16M_2(G) + 12M_1(G) + 12m + n.
 \end{aligned} \tag{10}$$

In this theorem, we study the first and second Zagreb coindices of the strong double graph. $\square$

Theorem 2. Let G be a simple connected graph of order n and size m ; then,

- (i) $\overline{M}_1(G^*) = 8\overline{M}_1(G) + 4n^2 - 4n - 8m$
- (ii) $\overline{M}_2(G^*) = 16\overline{M}_2(G) + 8\overline{M}_1(G) + 2n^2 - 2n - 4m$

Proof. For the sake of convenience, we label all vertices in G as $\{v_1, v_2, \dots, v_n\}$. Suppose that x_i and y_i are the corresponding clone vertices, in strong double graph G^* , of v_i for each $i = 1, \dots, n$.

For any given vertex v_i in G and its clone vertices x_i and y_i , there exists $d_{G^*}(x_i) = d_{G^*}(y_i) = 2\mathfrak{R}_G(v_i) + 1$ by the definition of the strong double graph.

For $v_i, v_j \in V(G)$, if $v_i v_j \notin E(G)$, then $x_i x_j \notin E(G)$, $y_i y_j \notin E(G)$, $x_i y_j \notin E(G)$, and $y_i x_j \notin E(G)$.

So, we only need to consider the total contribution of the following two types of nonadjacent vertex pairs both to $\overline{M}_1(G^*)$ and to $\overline{M}_2(G^*)$.

Type 1: the nonadjacent vertex pairs $\{x_i, x_j\}$ and $\{y_i, y_j\}$, where $v_i v_j \notin E(G)$

Type 2: the nonadjacent vertex pairs $\{x_i, y_j\}$ and $\{y_i, x_j\}$, where $v_i v_j \notin E(G)$

The total contribution of nonadjacent vertex pairs of type 1 in $\overline{M}_1(G^*)$ is given by

$$\begin{aligned}
\sum_{x_i, x_j \notin E(G^*)} [d_{G^*}(x_i) + d_{G^*}(x_j)] &= \sum_{y_i, y_j \notin E(G^*)} [d_{G^*}(y_i) + d_{G^*}(y_j)] \\
&= \sum_{v_i, v_j \notin E(G)} [(2\Re_G(v_i) + 1) + (2\Re_G(v_j) + 1)] \\
&= 2 \sum_{v_i, v_j \notin E(G)} [\Re_G(v_i) + \Re_G(v_j)] + 2|E(\overline{G})| \\
&= 2M_1(G) - 2m + n^2 - n,
\end{aligned} \tag{11}$$

and $\overline{M}_2(G^*)$ is given by

$$\begin{aligned}
\sum_{x_i, x_j \notin E(G^*)} [d_{G^*}(x_i) \cdot d_{G^*}(x_j)] &= \sum_{y_i, y_j \notin E(G^*)} [d_{G^*}(y_i) \cdot d_{G^*}(y_j)] \\
&= \sum_{v_i, v_j \notin E(G)} [(2\Re_G(v_i) + 1) \cdot (2\Re_G(v_j) + 1)] \\
&= 4 \sum_{v_i, v_j \notin E(G)} [\Re_G(v_i) \cdot \Re_G(v_j)] + 2 \sum_{v_i, v_j \notin E(G)} [\Re_G(v_i) + \Re_G(v_j)] + |E(\overline{G})| \\
&= 4M_2(G) + 2M_1(G) + \frac{1}{2}(n^2 - n - 2m).
\end{aligned} \tag{12}$$

The total contribution of nonadjacent vertex pairs of type 2 in $\overline{M}_1(G^*)$ is given by

$$\begin{aligned}
\sum_{x_i, y_j \notin E(G^*)} [d_{G^*}(x_i) + d_{G^*}(y_j)] &= \sum_{y_i, x_j \notin E(G^*)} [d_{G^*}(y_i) + d_{G^*}(x_j)] \\
&= \sum_{v_i, v_j \notin E(G)} [(2\Re_G(v_i) + 1) + (2\Re_G(v_j) + 1)] \\
&= 2 \sum_{v_i, v_j \notin E(G)} [\Re_G(v_i) + \Re_G(v_j)] + 2|E(\overline{G})| \\
&= 2M_1(G) - 2m + n^2 - n,
\end{aligned} \tag{13}$$

and $\overline{M}_2(G^*)$ is given by

$$\begin{aligned}
\sum_{x_i, y_j \notin E(G^*)} [d_{G^*}(x_i) \cdot d_{G^*}(y_j)] &= \sum_{y_i, x_j \notin E(G^*)} [d_{G^*}(x_i) \cdot d_{G^*}(y_j)] \\
&= \sum_{v_i, v_j \notin E(G)} [(2\Re_G(v_i) + 1) \cdot (2\Re_G(v_j) + 1)] \\
&= 4 \sum_{v_i, v_j \notin E(G)} [\Re_G(v_i) \cdot \Re_G(v_j)] + 2 \sum_{v_i, v_j \notin E(G)} [\Re_G(v_i) + \Re_G(v_j)] + |E(\overline{G})| \\
&= 4M_2(G) + 2M_1(G) + \frac{1}{2}(n^2 - n - 2m).
\end{aligned} \tag{14}$$

Therefore, by using equations (11) and (13), we have

$$\begin{aligned}
 \overline{M}_1(G^*) &= \sum_{x_i, x_j \notin E(G^*)} [d_{G^*}(x_i) + d_{G^*}(x_j)] = \sum_{y_i, y_j \notin E(G^*)} [d_{G^*}(y_i) + d_{G^*}(y_j)] \\
 &+ \sum_{x_i, y_j \notin E(G^*)} [d_{G^*}(x_i) + d_{G^*}(y_j)] + \sum_{y_i, x_j \notin E(G^*)} d_{G^*}(y_i) + d_{G^*}(x_j) \\
 &= (2M_1(G) - 2m + n^2 - n) + (2M_1(G) - 2m + n^2 - n) \\
 &+ (2M_1(G) - 2m + n^2 - n) + (2M_1(G) - 2m + n^2 - n) \\
 &= 8M_1(G) - 8m + 4n^2 - 4n.
 \end{aligned} \tag{15}$$

By using equations (12) and (14), we also have

$$\begin{aligned}
 \overline{M}_2(G^*) &= \sum_{x_i, x_j \notin E(G^*)} [d_{G^*}(x_i) \cdot d_{G^*}(x_j)] = \sum_{y_i, y_j \notin E(G^*)} [d_{G^*}(y_i) \cdot d_{G^*}(y_j)] \\
 &+ \sum_{x_i, y_j \notin E(G^*)} [d_{G^*}(x_i) \cdot d_{G^*}(y_j)] + \sum_{y_i, x_j \notin E(G^*)} d_{G^*}(y_i) \cdot d_{G^*}(x_j) \\
 &= \left(4M_2(G) + 2M_1(G) + \frac{1}{2}(n^2 - n - 2m)\right) + \left(4M_2(G) + 2M_1(G) + \frac{1}{2}(n^2 - n - 2m)\right) \\
 &+ \left(4M_2(G) + 2M_1(G) + \frac{1}{2}(n^2 - n - 2m)\right) + \left(4M_2(G) + 2M_1(G) + \frac{1}{2}(n^2 - n - 2m)\right) \\
 &= 16M_2(G) + 8M_1(G) + 2(n^2 - n - 2m).
 \end{aligned} \tag{16}$$

Now, we present the first and second indices and coindices of k -iterated strong double graphs. $\square$

Theorem 3. Let G be a nontrivial graph of order n and size m , and let G^{k*} be its k -iterated strong double graph. Then,

- (i) $M_1(G^{k*}) = 8^k M_1(G) + 2^{2(k+1)}(2^k - 1)m + 2^k(2^k - 1)^2 n$
- (ii) $M_2(G^{k*}) = 3 \cdot 2^{3k-1} \cdot (2^k - 1)M_1(G) + 4^{2k}M_2(G) + 3 \cdot 2^{2k} \cdot (2^k - 1)^2 m + 2^{k-1}(2^k - 1)^3 n$
- (iii) $\overline{M}_1(G^{k*}) = 8^k \overline{M}_1(G) + (2^k - 1)4^k(n^2 - n - 2m)$
- (iv) $\overline{M}_2(G^{k*}) = 2^{4k} \overline{M}_2(G) + 2^{3k} \cdot (2^k - 1) \overline{M}_1(G) + 2^{2k-1} \cdot (2^k - 1)^2(n^2 - n - 2m)$

Proof. For any nontrivial graph G with n vertices and m edges, the number of vertices in G^* is $2n$ and the number of edges in G^* is $2m$ plus those edges between the sets $\{x_1, x_2, \dots, x_n\}$ and $\{y_1, y_2, \dots, y_n\}$, that is, $4^k m + n$.

Now, we deduce that G^{k*} has $2^k m$ vertices and $4^k m + (2^{2k-1} - 2^{k-1})n$ edges.

- (i) $M_1(G^{k*}) = 8^k M_1(G) + 2^{2(k+1)}(2^k - 1)m + 2^k(2^k - 1)^2 n$.

As we know,

$$M_1(G^*) = 8M_1(G) + 16m + 2n. \tag{17}$$

Using the size of strong double graph $m = 4^k m + (2^{2k-1} - 2^{k-1})n$, we have

$$\begin{aligned}
 M_1(G^*) &= 8M_1(G) + 16\{4^k m + (2^{2k-1} - 2^{k-1})n\} + 2n, \\
 M_1(G^{k*}) &= 8M_1(G^{(k-1)*}) + 4 \cdot 2^{2k} m + (2^{2k-1} - 2^{k-1} + 2)n.
 \end{aligned} \tag{18}$$

By Theorem 1 and the definition of the k -iterated strong double graph, for $k \geq 1$, we have

$$\begin{aligned}
M_1(G^{k*}) &= 8M_1(G^{(k-1)*}) + 4 \cdot 2^{2k}m + (8 \cdot 2^{2k-2} - 8 \cdot 2^{k-1} + 2^k)n \\
M_1(G^{k*}) &= 8\{8M_1(G^{(k-2)*}) + 4 \cdot 2^{2k-2}m + (8 \cdot 2^{2k-4} - 8 \cdot 2^{k-2} + 2^{k-1})n\} \\
&\quad + 4 \cdot 2^{2k}m + (8 \cdot 2^{2k-2} - 8 \cdot 2^{k-1} + 2^k)n \\
&= 8^2M_1(G^{(k-2)*}) + 12 \cdot 2^{2k}m + 2^{2k-1}(6 \cdot 2^{2k} - 15 \cdot 2^k)n \\
&= 8^2\{8M_1(G^{(k-3)*}) + 4 \cdot 2^{2k-4}m + (8 \cdot 2^{2k-6} - 8 \cdot 2^{k-3} + 2^{k-2})n\} \\
&\quad + 12 \cdot 2^{2k}m + 2^{2k-1}(6 \cdot 2^{2k} - 15 \cdot 2^k)n \\
&= 8^3M_1(G^{(k-3)*}) + 28 \cdot 2^{2k}m + (14 \cdot 2^{2k} - 63 \cdot 2^k)n \\
M_1(G^{k*}) &= 8^k M_1(G) + 2^{2(k+1)}(2^k - 1)m + 2^k(2^k - 1)^2 n.
\end{aligned} \tag{19}$$

$$(ii) \quad M_2(G^{k*}) = 3 \cdot 2^{3k-1} \cdot (2^k - 1)M_1(G) + 4^{2k}M_2(G) + 3 \cdot 2^{2k} \cdot (2^k - 1)^2 m + 2^{k-1}(2^k - 1)^3 n.$$

As we know,

$$M_2(G^*) = 16M_2(G) + 12M_1(G) + 12m + n. \tag{20}$$

Using $M_1(G^*) = 8M_1(G) + 4 \cdot 2^{2k}m + (2^{2k-1} - 2^{k-1} + 2)n$ and the number of edges of strong double graph $m = 4^k m + (2^{2k-1} - 2^{k-1})n$, we have

$$\begin{aligned}
M_2(G^*) &= 16M_2(G) + 12\{8M_1(G) + 4 \cdot 2^{2k}m + (2^{2k-1} - 2^{k-1} + 2)n\} + 12\{4^k m + (2^{2k-1} - 2^{k-1})n\} + n, \\
M_2(G^*) &= 16M_2(G) + 96M_1(G) + (192 + 12 \cdot 2^{2k})m + (6 \cdot 2^{2k} - 6 \cdot 2^k + 25)n.
\end{aligned} \tag{21}$$

By Theorem 1 and the definition of the k -iterated strong double graph, for $k \geq 1$, we have

$$\begin{aligned}
M_2(G^*) &= 16M_2(G^{(k-1)*}) + 12 \cdot 2^{3(k-1)}M_1(G) + (6 \cdot 2^{3(k-1)} + 6 \cdot 2^{5(k-1)})m + (6 \cdot 4^{k-1} - 6 \cdot 2^{k-1} + 5^{2(k-1)})n \\
&= 16\{16M_2(G^{(k-2)*}) + 12 \cdot 2^{3(k-2)}M_1(G) + (6 \cdot 2^{3(k-2)} + 6 \cdot 2^{5(k-2)})m\} \\
&\quad + 16 \cdot (6 \cdot 4^{k-2} - 6 \cdot 2^{k-2} + 5^{2(k-2)})n + 12 \cdot 2^{3(k-1)}M_1(G) \\
&\quad + (6 \cdot 2^{3(k-1)} + 6 \cdot 2^{5(k-1)})m + (6 \cdot 4^{k-1} - 6 \cdot 2^{k-1} + 5^{2(k-1)})n \\
&= 16^2M_2(G^{(k-1)*}) + \frac{9 \cdot 2^{3(k)}}{2}M_1(G) + \left(\frac{9 \cdot 2^{3k}}{4} + \frac{9 \cdot 2^{5k}}{32}\right)m + \left(\frac{15 \cdot 2^{2k}}{2} - \frac{41 \cdot 5^{2k}}{625} + 27 \cdot 2^k + 1\right)n, \\
M_2(G^{k*}) &= 16^2\{16M_2(G^{(k-3)*}) + 12 \cdot 2^{3(k-3)}M_1(G) + (6 \cdot 2^{3(k-3)} + 6 \cdot 2^{5(k-3)})m\} \\
&\quad + 16^2 \cdot (6 \cdot 4^{k-3} - 6 \cdot 2^{k-3} + 5^{2(k-3)})n + \frac{9 \cdot 2^{3(k)}}{2}M_1(G) \\
&\quad + \left(\frac{9 \cdot 2^{3k}}{4} + \frac{9 \cdot 2^{5k}}{32}\right)m + \left(\frac{15 \cdot 2^{2k}}{2} - \frac{41 \cdot 5^{2k}}{625} + 27 \cdot 2^k + 1\right)n, \\
M_2(G^*) &= 16^3M_2(G^{(k-3)*}) + \frac{21 \cdot 2^{3k}}{2}M_1(G) + \left(\frac{21 \cdot 2^{3k}}{4} + \frac{21 \cdot 2^{5k}}{64}\right)m + \left(\frac{63 \cdot 2^{2k}}{2} + \frac{1281 \cdot 5^{2k}}{15625} + 219 \cdot 2^k + 1\right)n, \\
&\vdots \\
M_2(G^{k*}) &= 3 \cdot 2^{3k-1} \cdot (2^k - 1)M_1(G) + 4^{2k}M_2(G) + 3 \cdot 2^{2k} \cdot (2^k - 1)^2 m + 2^{k-1}(2^k - 1)^3 n.
\end{aligned} \tag{22}$$

$$\begin{aligned} \text{(iii)} \quad \overline{M}_1(G^{*k}) &= 8^k \overline{M}_1(G) + (2^k - 1)4^k(n^2 - n - 2m). \\ M_1(G^*) &= 8\overline{M}_1(G^*) - 8m + 4n^2 + 4n. \end{aligned} \quad (23)$$

By Theorem 1 and the definition of the k -iterated strong double graph, for $k \geq 1$, we have

$$\begin{aligned} M_1(G^{k*}) &= 8\overline{M}_1(G^{(k-1)*}) - 2^{2k+1}m + 2^{2k}n^2 + 2^{2k}n \\ M_1(G^{k*}) &= 8\{8\overline{M}_1(G^{(k-2)*}) - 2^{2(k-1)+1}m + 2^{2(k-1)}n^2 + 2^{2(k-1)}n\} \\ &\quad - 2^{2k+1}m + 2^{2k}n^2 + 2^{2k}n \\ &= 8^2 M_1(G^{(k-2)*}) - 6 \cdot 2^{2k}m + 3 \cdot 2^{2k}n^2 + 3 \cdot 2^{2k}n \\ &= 8^2 \{8\overline{M}_1(G^{(k-3)*}) - 2^{2(k-2)+1}m + 2^{2(k-2)}n^2 + 2^{2(k-2)}n\} - 6 \cdot 2^{2k}m \\ &\quad + 3 \cdot 2^{2k}n^2 + 3 \cdot 2^{2k}n \\ &= 8^3 \overline{M}_1(G^{(k-3)*}) - 14 \cdot 2^{2k}m + 7 \cdot 2^{2k}n^2 + 7 \cdot 2^{2k}n \\ &\quad \vdots \\ M_1(G^{k*}) &= 8^k \overline{M}_1(G) + (2^k - 1)4^k(n^2 - n - 2m). \end{aligned} \quad (24)$$

$$\text{(iv)} \quad \overline{M}_2(G^{*k}) = 2^{4k} \overline{M}_2(G) + 2^{3k} \cdot (2^k - 1) \overline{M}_1(G) + 2^{2k-1} \cdot (2^k - 1)^2 (n^2 - n - 2m).$$

$$\overline{M}_2(G^{k*}) = 16\overline{M}_2(G^{(k-1)*}) + 8\overline{M}_1(G^{(k-1)*}) + 2(n^2 - n - 2m), \quad (26)$$

and using $\overline{M}_1(G^*) = 8\overline{M}_1(G) - 8m + 4n^2 + 4n$, we have

$$\overline{M}_2(G^*) = 16\overline{M}_2(G) + 8\overline{M}_1(G) + 2(n^2 - n - 2m). \quad (25)$$

By Theorem 1 and the definition of the k -iterated strong double graph, for $k \geq 1$, we have

$$\begin{aligned} \overline{M}_2(G^{k*}) &= 16\overline{M}_2(G^{(k-1)*}) + 8\{8\overline{M}_1(G) - 8m + 4n^2 + 4n\} + 2(n^2 - n - 2m) \\ &= 16\overline{M}_2(G^{(k-1)*}) + 64\overline{M}_1(G) + 32(n^2 - n - 2m) + 2(n^2 - n - 2m). \end{aligned} \quad (27)$$

By rearranging the terms, we have

$$\begin{aligned}
\overline{M}_2(G^{k*}) &= 16\overline{M}_2(G^{(k-1)*}) + 8 \cdot 8^{(k-1)}\overline{M}_1(G) + 32^{(k-1)}(n^2 - n - 2m) \\
&\quad + 2^{(3k-3)}(n^2 - n - 2m) \\
&= 16\{16\overline{M}_2(G^{(k-2)*}) + 8 \cdot 8^{(k-2)}\overline{M}_1(G) + 32^{(k-2)}(n^2 - n - 2m)\} \\
&\quad + 16 \cdot 2^{(3k-6)}(n^2 - n - 2m) + 8 \cdot 8^{(k-1)}\overline{M}_1(G) \\
&\quad + 32^{(k-1)}(n^2 - n - 2m) + 2^{(3k-3)}(n^2 - n - 2m) \\
&= 16^2\overline{M}_2(G^{(k-2)*}) + 3 \cdot 2^{(3k)}\overline{M}_1(G) + \frac{3 \cdot 2^{(5k)}}{64}(n^2 - n - 2m) \\
&\quad + \frac{3 \cdot 2^{(3k)}}{8}(n^2 - n - 2m) \\
&= 16^2\{16\overline{M}_2(G^{(k-3)*}) + 8 \cdot 8^{(k-3)}\overline{M}_1(G) + 32^{(k-3)}(n^2 - n - 2m)\} \\
&\quad + 16^2 \cdot 2^{(3k-9)}(n^2 - n - 2m) + 3 \cdot 2^{(3k)}\overline{M}_1(G) \\
&\quad + \frac{3 \cdot 2^{(5k)}}{64}(n^2 - n - 2m) + \frac{3 \cdot 2^{(3k)}}{8}(n^2 - n - 2m) \\
&= 16^3\overline{M}_2(G^{(k-3)*}) + 7 \cdot 2^{(3k)}\overline{M}_1(G) + \frac{7 \cdot 2^{(5k)}}{128}(n^2 - n - 2m) \\
&\quad + \frac{7 \cdot 2^{(3k)}}{8}(n^2 - n - 2m) \\
&\vdots \\
\overline{M}_2(G^{k*}) &= 2^{4k}\overline{M}_2(G) + 2^{3k} \cdot (2^k - 1)\overline{M}_1(G) + 2^{2k-1} \cdot (2^k - 1)^2(n^2 - n - 2m).
\end{aligned} \tag{28}$$

Here, we present an algorithm to generate and verify the first and second Zagreb indices and coindices of any finite simple connected graph G . This algorithm is based on the adjacency matrix of G (Algorithm 1). $\square$

Example 1. Let A , B , and C be the matrices of path graph P_4 and strong double graphs $SD^{1*}(P_4)$ and $SD^{2*}(P_4)$, respectively. These matrices are square and symmetric, and

choose value 1 (one) at the i th row and j th column if v_i and v_j are adjacent vertices in a graph; otherwise, it is 0. The suggested algorithm is applied on these matrices to compute the first Zagreb index IM_1 , second Zagreb index IM_2 , first Zagreb coindex CM_1 , and second Zagreb coindex CM_2 . These adjacency matrices have been obtained by drawing the respective graphs in “GraphTea” software; this software is easily available, and it is free of cost.

Input: A is an adjacency matrix of a finite simple connected graph
 Output: IM_1, IM_2, CM_1, CM_2
 Variables used: nr = number of rows in A , nc = number of columns in A ,
 (1) $IM_1 := 0, IM_2 := 0, CM_1 := 0, CM_2 := 0$
 (2) for $i = 1$ to nr
 (3) for $j = i$ to nc
 (4) $s_i :=$ sum of i th row of A ,
 (5) $s_j :=$ sum of j th column of A .
 (6) if $A(i, j) = 1$
 (7) $IM_1 := IM_1 + (S_i + S_j)$
 (8) $IM_2 := IM_2 + (S_i * S_j)$
 (9) end if
 (10) if $A(i, j) = 0$ and $i \neq j$
 (11) $CM_1 := CM_1 + (S_i + S_j)$
 (12) $CM_2 := CM_2 + (S_i * S_j)$
 (13) end if
 (14) end for j
 (15) end for i

ALGORITHM 1: Computing the first Zagreb index IM_1 , second Zagreb index IM_2 , first Zagreb coindex CM_1 , and second Zagreb coindex CM_2 .

$$\begin{aligned}
 A &= \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \\
 B &= \begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \end{bmatrix}, \\
 C &= \left\{ \begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \end{bmatrix} \right\}.
 \end{aligned} \tag{29}$$

FIGURE 3: 3D surface plot of Zagreb indices and coindices of $SD(P_n)$. FIGURE 4: 3D curve plot of Zagreb indices and coindices of $SD(P_n)$.

The result of the algorithm is given as follows:

Graph	Matrix	AM_1	AM_2	CM_1	CM_2
P_4	A	10	8	8	5
$SD^{1*}(P_4)$	B	136	288	88	156
$SD^{2*}(P_4)$	C	756	2652	864	2802

(30)

Now, we provide graphs of Zagreb indices and coindices. Such type of graphical representation will be more helpful to study the dynamics of topological descriptors of the molecular graphs. Here, we present the strong double graph of the path graph, $SD(P_n)$, where $2 \leq n \leq 21$ and $m = n - 1$. In Figure 3, the behaviour of the first Zagreb index M_1 and second Zagreb index M_2 is linear as the straight plane, and the behaviour of the first Zagreb coindex CM_1 and second Zagreb coindex CM_2 is nonlinear as the curved form. In

Figure 4, we have drawn the curves of these indices and coindices for $SD(P_n)$ to understand their dynamics. This figure shows the relation between Zagreb indices and coindices as $M_1 \leq M_2 \leq CM_1 \leq CM_2$.

3. Conclusion

We have presented generalized explicit formulas to calculate the first Zagreb index $M_1(G)$, second Zagreb index $M_2(G)$, first Zagreb coindex $\overline{M}_1(G)$, and second Zagreb coindex $\overline{M}_2(G)$ of the strong double graph $SD(G)$ and k -iterated strong double graph $SD^{k*}(G)$. The relation between these indices and coindices is also presented as $M_1 \leq M_2 \leq CM_1 \leq CM_2$. We have also presented an algorithm with a given adjacency matrix to verify these indices and coindices by programming and numerically. Computer-generated graphs are also given to understand the dynamics of these indices and coindices.

This family of graphs can be considered for other degree-based and distance-related topological indices for further studies.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that there are no conflicts of interest.

Authors' Contributions

All authors contributed equally to this work.

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