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The Zagreb-coindex of Four Operations on Graphs

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ABSTRACT

In 1972, within a study of the structure-dependency of total π-electron energy (E), it was shown that E depends on the sum of squares of the vertex degrees of the molecular graph (later named first Zagreb index), and thus provides a measure of the branching of the carbon-atom skeleton. Topological indices are found to be very useful in chemistry, biochemistry and nanotechnology in isomer discrimination, structure–property relationship, structure-activity relationship and pharmaceutical drug design. In chemical graph theory, a topological index is a number related to a graph which is structurally invariant. One of the oldest most popular and extremely studied topological indices are well–known Zagreb indices. In a (molecular) graph G, the Zagreb topological index is equal to the sum of squares of the degrees of vertices of G and the Zagreb-coindex is defined as the sum of a graph's vertex degrees which is not adjacent. In this paper, we obtain the Zagreb-coindex of four operations on graphs.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For a graph G, we let $d_G(v)$ be the degree of a vertex v in G.

Topological index is a type of a Molecular descriptor that is calculated based on the Molecular graph of a chemical compound [10]. Topological indices are numerical parameters of a graph which characterize its topology and usually graph invariant. Topological indices play an important role in Mathematical chemistry, especially in the QSPR and QSAR modeling.

The Zagreb indices are two topological indices among the oldest and most studied topological indices. These two indices first appeared in [8] and were elaborated in [7]. For a Molecular graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are respectively defined as follows:

$$M_1(G) = \sum_{v\in V(G)} d_G^2(v) \text{ and, } M_2(G) = \sum_{uv\in E(G)} d_G(u)\, d_G(v)\,.$$

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The complement of a graph G is denoted by $\bar{G}$ and is the simple graph with the same vertex set $V(G)$ in which two vertices are adjacent in $\bar{G}$ if and only if they are not adjacent in G. Doslic in [4], defined the Zagreb-coindex of a graph G as follows:

$$\bar{Z}(G) = \sum_{uv \notin E(G)} [d_G(u) + d_G(v)].$$

Some topological indices and topological coindices were recently studied in [1, 3, 9].
The sum of two connected graphs G_1 and G_2, which is denoted by $G_1 + G_2$ is a graph such that the set of vertices is $V(G_1) \times V(G_2)$ and two vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ of $G_1 + G_2$ are adjacent if and only if $[u_1 = v_1$ and $(u_2, v_2) \in E(G_2)]$ or $[u_2 = v_2$ and $(u_1, v_1) \in E(G_1)]$ where $E(G)$ is the set of edges of a graph G. For a connected graph G, there are four related graphs as follows :
$S(G)$ is obtained by inserting an additional vertex in each edge of G.
$R(G)$ is obtained from G by adding a new vertex corresponding to each edge of G, then joining each new vertex to the end vertices of the corresponding edge.
$Q(G)$ is obtained from G by inserting a new vertex into each edge of G, then joining with edges those pairs of new vertices on adjacent edge of G.
$T(G)$ has as its vertices the edges and vertices of G. Adjacency in $T(G)$ is defined as adjacency or incidence for the corresponding elements of G.

Suppose that G_1 and G_2 be two connected graphs. Based on above four new graphs defined in (a), (b), (c) and (d), Eliasi and Taeri in [5] introduced four new operations on these graphs in the following:
Let f be one of the symbols S, R, Q or T. The f-sum $G_1 +_f G_2$ is a graph with the set of vertices $V(G_1 +_f G_2) = (V(G_1) \cup E(G_1)) \times V(G_2))$ and two vertices (u_1, u_2) and (v_1, v_2) of $G_1 +_f G_2$ are adjacent if and only if $[u_1 = v_1 \in V(G_1)$ and $(u_2, v_2) \in E(G_2)]$ or $[u_2 = v_2 \in V(G_2)$ and $(u_1, v_1) \in E(f(G_1))]$.
In this paper, we determine first and second Zagreb-coindex for $G_1 +_f G_2$ and $\overline{G_1 +_f G_2}$ where G_1 and G_2 are simple graphs and, f is one of the symbols S, R, Q or T.

2. Zagreb-coindex for $G_1 +_f G_2$ and $\overline{G_1 +_f G_2}$

Let G_1 and G_2 be two graph of order n_1 and n_2 with $|G_1| = m_1$ and $|G_2| = m_2$.
Observation 1.
The number of vertices for $G_1 +_f G_2$ where $f = S, R, Q$ and T is $n_1 n_2 + m_1 n_2$
The number of edges for $G_1 +_S G_2$ is $2m_1 n_2 + n_1 m_2$.
The number of edges for $G_1 +_R G_2$ is $3m_1 n_2 + n_1 m_2$.
The number of edges for $G_1 +_Q G_2$ is $n_1 m_2 + n_2 \left(m_1 + \frac{1}{2} M_1(G_1)\right)$.
The number of edges for $G_1 +_T G_2$ is $n_1 m_2 + n_2 \left(2m_1 + \frac{1}{2} M_1(G_1)\right)$.

In the following theorems, n are the number of vertices and edges $G_1 +_f G_2$ respectively, according to observation 1, and also the theorems are proved based on the results obtained from sources [2, 6].

Theorem1. $\overline{M_1}(G_1 +_f G_2) = 2m(n-1) - M_1(G_1 +_f G_2)$.

Proof. We prove the theorem for $f = S$. For $f = R, Q$ and T the proof is analogous.
We know that,

$$\sum_{(u_1,v_1) \in v(G_1 +_s G_2)} \sum_{(u_2,v_2) \in v(G_1 +_s G_2)} [d_{G_1} +_s G_2(u_1, v_1) + d_{G_1} +_s G_2(u_2, v_2)] = 4mn \qquad (1)$$

The left side of relation 1 can also be written as follows:

$$\sum_{(u_1,v_1)\in V(G_1 +_S G_2)} \sum_{(u_2,v_2)\in V(G_1 +_S G_2)} \left[d_{G_1 +_S G_2}(u_1,v_1) + d_{G_1 +_S G_2}(u_2,v_2)\right] =$$

$$2 \sum_{(u_1,v_1)(u_2,v_2)\in E(G_1 +_S G_2)} \left[d_{G_1 +_S G_2}(u_1,v_1) + d_{G_1 +_S G_2}(u_2,v_2)\right]$$

$$+ 2 \sum_{(u_1,v_1)(u_2,v_2)\notin E(G_1 +_S G_2)} \left[d_{G_1 +_S G_2}(u_1,v_1) + d_{G_1 +_S G_2}(u_2,v_2)\right]$$

$$+ 2 \sum_{(u_1,v_1)=(u_2,v_2)\in V(G_1 +_S G_2)} \left[d_{G_1 +_S G_2}(u_1,v_1) + d_{G_1 +_S G_2}(u_2,v_2)\right]$$

$$= 2\, M_1(G_1 +_S G_2) + 2\overline{M_1}(G_1 +_S G_2) + 4m$$

By comparing the relations (1) and (2) and according to observation 1, the desired result is obtained.

Theorem 2. $\overline{M_2}\left(G_1 +_f G_2\right) = 2m^2 - \frac{1}{2} M_1\left(G_1 +_f G_2\right) - M_2\left(G_1 +_f G_2\right)$.

Proof. Suppose that m and n are selected from observation 1. We prove the theorem for $f = S$. For $f = R, Q\ and\ T$ the proof is analogous.

We know that,

$$\sum_{(u_1,v_1)\in v(G_1+_S G_2)} \sum_{(u_2,v_2)\in v(G_1+_S G_2)} [\boldsymbol{d}_{G_1+_S G_2}(u_1,v_1).\, d_{G_1+_S G_2}(u_2,v_2) = 4m^2 \qquad (2)$$

The left side of relation (1) can also be written as follows:

$$\sum_{(u_1,v_1)\in V(G_1 +_S G_2)} \sum_{(u_2,v_2)\in V(G_1 +_S G_2)} \left[d_{G_1 +_S G_2}(u_1,v_1).\, d_{G_1 +_S G_2}(u_2,v_2)\right] =$$

$$2 \sum_{(u_1,v_1)(u_2,v_2)\in E(G_1 +_S G_2)} \left[d_{G_1 +_S G_2}(u_1,v_1).\, d_{G_1 +_S G_2}(u_2,v_2)\right]$$

$$+ 2 \sum_{(u_1,v_1)(u_2,v_2)\notin E(G_1 +_S G_2)} \left[d_{G_1 +_S G_2}(u_1,v_1)\, .\, d_{G_1 +_S G_2}(u_2,v_2)\right]$$

$$+ \sum_{(u_1,v_1)=(u_2,v_2)\in V(G_1 +_S G_2)} \left[d_{G_1 +_S G_2}(u_1,v_1)\, .\, d_{G_1 +_S G_2}(u_2,v_2)\right]$$

$$= 2\, M_2(G_1 +_S G_2) + 2\, \overline{M_2}(G_1 +_S G_2) + M_1(G_1 +_S G_2) \qquad (3)$$

By comparing the relations (2) and (3) and according to observation 1, the proof is completed.☐

Theorem 3. $M_1\left(\overline{G_1 +_f G_2}\right) = n(n-1)^2 - 4m(n-1) + M_1\left(G_1 +_f G_2\right)$.

Proof. We prove the theorem for $f = S$. For $f = R, Q\ and\ T$ the proof is analogous. It is easy to see that for any vertex $(u, v) \in \overline{G_1 +_S G_2}$ we have,

$$d_{\overline{G_1 +_S G_2}}(u,v) = (n-1) - d_{G_1 +_S G_2}(u,v) \quad (4)$$

Since

$$M_1(G_1 +_S G_2) = \sum_{(u_1,v_1)(u_2,v_2)\in E(G_1 +_S G_2)} \left[d_{G_1 +_S G_2}(u_1,v_1) + d_{G_1 +_S G_2}(u_2,v_2)\right]$$

Then,

$$\begin{aligned} M_1\left(\overline{G_1 +_S G_2}\right) &= \sum_{(u_1,v_1)(u_2,v_2)\in E(\overline{G_1 +_S G_2})} \left[d_{\overline{G_1 +_S G_2}}(u_1,v_1) + d_{\overline{G_1 +_S G_2}}(u_2,v_2)\right] \\ &= \sum_{(u_1,v_1)(u_2,v_2)\in E(\overline{G_1 +_S G_2})} \left[(n-1) - d_{G_1 +_S G_2}(u_1,v_1) + (n-1) - d_{G_1 +_S G_2}(u_2,v_2)\right] \\ &= \sum_{(u_1,v_1)(u_2,v_2)\in E(\overline{G_1 +_S G_2})} 2(n-1) + \sum_{(u_1,v_1)(u_2,v_2)\in E(\overline{G_1 +_S G_2})} \left[d_{G_1 +_S G_2}(u_1,v_1) + d_{G_1 +_S G_2}(u_2,v_2)\right] \end{aligned}$$

The number of edges of $\overline{G_1 +_S G_2}$ is $\binom{n}{2} - m$ and $(u_1,v_1)(u_2,v_2) \in E(\overline{G_1 +_S G_2})$ means that, $(u_1,v_1)(u_2,v_2) \notin E(G_1 +_S G_2)$.

Therefore

$M_1\left(\overline{G_1 +_S G_2}\right) = 2(n-1)\left[\binom{n}{2} - m\right] + \overline{M_1}(G_1 +_S G_2)$. Using Theorem 5 and simplifying the expression, the proof of the theorem is completed.☐

Similar to the method mentioned above, the following theorem can be proved and we omit the proof.

Theorem 4. $M_2\left(\overline{G_1 +_f G_2}\right) = (n-1)^2\left[\binom{n}{2} - m\right] - (n-1)\overline{M_1}\left(G_1 +_f G_2\right) + \overline{M_2}\left(G_1 +_f G_2\right)$.

3. Conclusions

In a (molecular) graph G, the Zagreb topological index is equal to the sum of squares of the degrees of vertices of G and the Zagreb-coindex is defined as the sum of a graph's vertex degrees which is not adjacent. In this paper, we calculated Zagreb topological coindex for connected graphs obtained by new operation (introduced by Eliasi and Taeri [5]) between two graphs.

Conflict of interest: The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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