First Zagreb Coindex of Transformation Graphs

Rathnamma. K. V[1]

[1] *Department of Mathematics*
Government College for Women
Chintamani, Chikkaballapura, Karnataka, India
Email:rathnakv01@gmail.com

Abstract

The first Zagreb coindex is the sum of the degrees of pair of nonadjacent vertices in a graph G. In this paper, we obtain first Zagreb coindex of eight kinds of transformation graphs, which are generalization of total graphs.

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1 Introduction

Let $G = (V, E)$ be a graph. The number of vertices of G we denote by n and the number of edges we denote by m, thus $|V(G)| = n$ and $|E(G)| = m$. The complement of G, denoted by $\bar{G}$, is a graph which has the same vertices as G, and in which two vertices are adjacent if and only if they are not adjacent in G. By the open neighborhood of a vertex v of G we mean the set $N_G(v) = \{u \in V(G) \colon uv \in E(G)\}$. By the closed neighborhood of a vertex v of G we mean the set $N_G[v] = N_G(v) \cup \{v\}$. The degree of a vertex v, denoted by $d_G(v)$, is the cardinality of its open neighborhood. A vertex is called isolated if it has no neighbors, while it is called universal if it is adjacent to all other vertices. Let S be a subset of the set of vertices of G, and let $u \in S$. The distance between two vertices of a graph is the number of edges in a shortest path connecting them. The eccentricity of a vertex is the greatest distance between it and any other vertex.

Many real world situations are conveniently be described by means of a diagram. A mathematical abstraction of situations of this type gives rise to the concept of a graph. During the last decade, there has been an upsurge of interest in research in the applications of graph theory in chemistry. Numerous Mathematicians and Chemists interest lie in this area. Molecular structures are represented by a graph where atoms are vertices and covalent chemical bonds are termed as molecular topology. A Topological index is a non empirical numerical invariant of a chemical graph that quantifies the structure and the branching pattern of the molecule. Topological indices are used in the development of Quantitative Structure Activity Relationship in which the biological activity or other properties of molecules are correlated with their chemical structure.

A graph invariant is any function on a graph that does not depend on a labeling of its vertices. Such quantities are also called topological indices. Hundreds of different invariants have been employed to date (with unequal success) in QSAR/QSPR studies. Among more useful of them appear two that are known under various names, but mostly as Zagreb indices. Due to their chemical relevance they have been subject of numerous papers in chemical literature [7, 8, 9, 11]. There are two invariants called the first Zagreb index and second Zagreb index [2, 3, 6, 10, 15, 17], defined as

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

In fact, one can rewrite the first Zagreb index as $M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))$.

Noticing that contribution of nonadjacent vertex pairs should be taken into account when computing the weighted Winer polynomials of certain composite graphs (see [2] defined first Zagreb coindex and second Zagreb coindex as

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} (d_G(u) + d_G(v)) \text{ and } \overline{M_2}(G) = \sum_{uv \notin E(G)} d_G(u)d_G(v), \text{ respectively.}$$

2 Transformation Graphs and Total Transformation Graphs

Transformation graphs takes information from the original graph and converts source information into a new structure. If it is possible to figure out the given graph from the transformed graph in polynomial time, such operation may be used to survey miscellaneous structural properties of the original graph considering the transformation graphs. Therefore it fosters to study the research of transformation graphs and their structural properties [19].

Sampathkumar [18] introduced the concepts of semitotal-point graph and semitotal-line graph which are stated as follows:

Let $G = (V, E)$ be a graph. The *semitotal-line graph* $T_1(G)$ is a graph with $V(T_1(G)) = V(G) \cup E(G)$ and any two vertices $u, v \in T_1(G)$ are adjacent if and only if (1) u and v are adjacent edges in G and (2) one is a vertex of G and other is an edge of G incident with it. Note that the definition of semitotal-line graph and Middle graphs [1] are same. These two concepts have been introduced in the same year.

The *semitotal-point graph* $T_2(G)$ is a graph with $V(T_1(G)) = V(G) \cup E(G)$ and any two vertices $u, v \in T_2(G)$ are adjacent if and only if (1) u and v are adjacent vertices in G and (2) one is a vertex of G and other is an edge of G incident with it.

Let $G = (V, E)$ be a graph and x, y, z be three variables taking values + or −. The total transformation graph G^{xyz} is a graph having $V(G) \cup E(G)$ as a vertex set, and for $\alpha, \beta \in V(G) \cup E(G)$, α and β are adjacent in G^{xyz} if and only if

1. $\alpha, \beta \in V(G)$, α, β are adjacent in G if $x = +$ and α and β are not adjacent in G if $x = -$.
2. $\alpha, \beta \in E(G)$, α, β are adjacent in G if $y = +$ and α and β are not adjacent in G if $y = -$.
3. $\alpha \in V(G)$ and $\beta \in E(G)$, α, β are incident in G if $z = +$ and α and β are not incident in G if $z = -$.

Note 1. Since there are eight distinct 3-permutations of $\{+, -\}$, we obtain eight graphical transformations of G. It is interesting to see that G^{+++} is exactly the total graph $T(G)$

of G and G^{---} is the complement of $T(G)$. Also for a given graph G, G^{++-} and G^{--+}, G^{+-+} and G^{-+-}, G^{-++} and G^{+--} are the other three pairs of complementary graphs. In this paper, we obtained some new properties of Zagreb coindices. We mainly give explicit formulae for the first Zagreb coindex of Semitotal-point graph, semitotal-line graph and eight total transformation graphs.

3 Results

We begin with the following straightforward observations.

Observation 1. *Every vertex $u \in V(G)$ contributes exactly $(n - d_G(u) - 1)d_G(u)$ to the sum of $\overline{M_1}(G)$. Hence $\overline{M_1}(G) = \sum_{u\in V(G)} (n - d_G(u) - 1)d_G(u)$.*

Observation 2. *For a positive integer k, we have $\xi_k(G) = \sum_{v\in V(G)} (d_G(v))^k$. One can see that $\xi_1(G)$ is just the number of edges in G, and $\xi_2(G)$ is just first Zagreb index of $M_1(G)$.*

Observation 3. *For any nonempty graph G, it holds*

$$\sum_{uv\in E(G)} [(d_G(u))^2 + (d_G(v))^2] = \sum_{w\in V(G)} (d_G(w))^3 = \xi_3(G).$$

Theorem 3.1. *Let G be a nontrivial graph of order n and size m. Then*

$$\overline{M_1}(T_1(G)) = 2m(m + n - 1) + (m + n - 2)M_1(G) - 2M_2(G) - \xi_3(G).$$

Proof. Suppose $e_i = u_iv_i (i = 1, 2, \cdots, m)$ is a vertex in $T_1(G)$. It can be easily seen that $d_{T_1(G)}(e_i) = d_G(u_i) + d_G(v_i)$ and if $u \in V(T_1(G)) \cap V(G)$, then $d_{T_1(G)}(u) = d_G(G)$. Therefore by the means of Observation 1,

$$\overline{M_1}(T_1(G)) = \sum u \in V(T_1(G))(n - d_{T_1(G)}(u) - 1)d_{T_1(G)}(u)$$

$$\overline{M_1}(T_1(G)) = \sum_{u\in V(T_1(G))} (m+n-(d_G(u)+d_G(v))-1)(d_G(u)+d_G(v)) + \sum_{u\in V(T_1(G)\cap V(G))} (m+n-d_G(u)-1)d_G(u)$$

$$\begin{aligned}
&= (m + n - 1)M_1(G) - \sum_{u,v\in E(G)} (d_G(u) + d_G(v))^2 + 2m^2 + 2mn - M_1(G) - 2m \\
&= (m + n - 2)M_1(G) + 2m(m + n - 1) - \left\{ \sum_{u,v\in E(G)} [(d_G(u))^2 + (d_G(v))^2] + 2 \sum_{u,v\in E(G)} (d_G(u)d_G(v)) \right\} \\
&= 2m(m + n - 1) + (m + n - 2)M_1(G) - 2M_2(G) - \xi_3(G),
\end{aligned}$$

as desired. □

Theorem 3.2. *Let G be a nontrivial graph of order n and size m. Then*

$$\overline{M_1}(T_2(G)) = (3m+3n-5)2m - 4M_1(G).$$

Proof. Since $T_2(G)$ has $m+n$ vertices. Therefore, by means of Observation 1,

$$\begin{aligned}\overline{M_1}(T_1(G)) &= \sum_{u\in V(T_2(G))} (n - d_{T_2(G)}(u) - 1) d_{T_2(G)}(u) \\ &= \sum_{u\in V(T_2(G))\cap V(G)} (n - d_{_{T_2(G)}}(u) - 1)(d_{_{T_2(G)}}(u)) + \sum_{u\in V(T_2(G)\cap E(G))} (n - d_{_{T_2(G)}}(u) - 1) d_{_{T_2(G)}}(u)\end{aligned}$$

Note that for $u \in V(T_2(G)) \cap V(G)$, $d_{_{T_2(G)}}(u) = 2d_G(u)$ and for $u \in V(T_2(G) \cap E(G)$, $d_{_{T_2(G)}}(u) = 2$. Therefore ,

$$\begin{aligned}\overline{M_1}(T_1(G)) &= \sum_{u\in V(T_2(G))\cap V(G)} (m+n-2d_{_{(G)}}(u) - 1)(2d_{_{(G)}}) + \sum_{u\in V(T_2(G)\cap E(G))} (m+n-2-1)2 \\ &= 4m^2 + 4mn - 4M_1(G) - 4m + 2(m+n-3)m \\ &= 6m^2 + 6mn - 10m - 4M_1(G) \\ &= (3m+3n-5)2m - 4M_1(G).\end{aligned}$$

as desired. □

We need the following theorems for our further results.

Theorem 3.3. *[17] Let G be a nontrivial graph of order n and size m. Then*

$$\overline{M_1}(T(G)) = 4m(n+m-1) + (n+m-5)M_1(G) - 2M_2(G) - \xi_3(G).$$

Theorem 3.4. *[2] Let G be a simple graph. Then $\overline{M_1}(G) = \overline{M_1}(\overline{G})$.*

Theorem 3.5. *Let G be a nontrivial graph of order n and size m. Then*

$$\overline{M_1}(G^{+++}) = 4m(n+m-1) + (n+m-5)M_1(G) - 2M_2(G) - \xi_3(G).$$

Proof. Follows from Theorem 6 due to the fact that $T(G) = G^{+++}$. □

Theorem 3.6. *Let G be a nontrivial graph of order n and size m. Then*

$$\overline{M_1}(G^{---}) = 4m(n+m-1) + (n+m-5)M_1(G) - 2M_2(G) - \xi_3(G).$$

Proof. Follows from Theorem 8 and Theorem 7 due to the fact that $\overline{G^{+++}} = G^{---}$. □

Theorem 3.7. *Let G be a nontrivial graph of order n and size m. Then*

$$\overline{M_1}(G^{++-}) = m[n(n-1) + (n-4)(m+3)] + (m-n+7)M_1(G) - 2M_2(G) - \xi_3(G).$$

Proof. Note that G^{++-} has $(m+n)$ vertices and for $u \in V(G^{++-}) \cap V(G)$, $d_{G^{++-}}(u) = m$ and for $u \in V(G^{++-}) \cap E(G)$, $d_{G^{++-}}(u) = d_G(u) + d_G(v) + n - 4$. Therefore by the means of Observation 1,

$$\overline{M_1}(G^{++-}) = \sum_{u \in V(G^{++-})} (n - d_{G^{++-}}(u) - 1) d_{G^{++-}}(u)$$

$$\overline{M_1}(G^{++-} = \sum_{u \in V(G^{++-})} (m + n - m - 1)m + \sum_{u \in V(G^{++-})} (m + n - (d_G(u) + d_G(v) + n - 4) - 1)(d_G(u) + d_G(v) + n - 4)$$

$$= mn(n-1) + (m - n + 7)M_1(G) + m(n-4)(m+3) - \sum_{u,v \in E(G)} (d_G(u) + d_G(v))^2$$

$$= m[n(n-1) + (n-4)(m+3)] + (m - n + 7)M_1(G) - \left\{ \sum_{u,v \in E(G)} [(d_G(u))^2 + (d_G(v))^2] + 2M_2(G) \right\}$$

$$= m[n(n-1) + (n-4)(m+3)] + (m - n + 7)M_1(G) - 2M_2(G) - \xi_3(G).$$

This completes the proof. □

Theorem 3.8. *Let G be a nontrivial graph of order n and size m. Then*

$$\overline{M_1}(G^{--+}) = m[n(n-1) + (n-4)(m+3)] + (m - n + 7)M_1(G) - 2M_2(G) - \xi_3(G).$$

Proof. Follows from Theorem 10 and Theorem 7 due to the fact that $\overline{G^{++-}} = G^{--+}$. □

Theorem 3.9. *Let G be a nontrivial graph of order n and size m. Then*

$$\overline{M_1}(G^{+-+}) = m[(n-4)(m+3) + 4(n+m-1)] + (m - n + 3)M_1(G) - 2M_2(G) - \xi_3(G).$$

Proof. Note that G^{+-+} has $(m+n)$ vertices. By the means of Observation 1, we have

$$\overline{M_1}(G^{+-+}) = \sum_{u \in V(G^{+-+})} (n - d_{G^{++-}}(u) - 1) d_{G^{+-+}}(u)$$

$$\overline{M_1}(G^{+-+}) = \sum_{u \in V(G^{+-+}) \cap V(G)} (n - d_{G^{+-+}}(u) - 1)(d_{G^{+-+}}(u)) + \sum_{u \in V(G^{+-+}) \cap E(G))} (n - d_{G^{+-+}}(u) - 1) d_{G^{+-+}}(u)$$

Note that for $u \in V(G^{+-+}) \cap V(G)$, $d_{G^{+-+}}(u) = 2d_G(u)$ and for $u \in V(G^{+-+}) \cap E(G)$, $d_{G^{+-+}}(u) = m + 3 - (d_G(u) + d_G(v)$. Hence, by the means of Observation 1, we have,

$$\overline{M_1}(G^{+-+}) = \sum_{u\in V(G^{+-+})\cap V(G)} (m+n-2d_G(u)-1)2d_G(u) + \sum_{u\in V(G^{+-+})\cap E(G))} (m+n-(m+3-(d_G(u)+d_G(v)))-1)(m+3-(d_G(u)+d_G(v))$$

$$= (m-n+3)M_1(G)+m[(m+3)(n-4)+4(n+m-1)] - \sum_{u,v\in E(G)} [(d_G(u))^2+(d_G(v))^2] - 2M_2(G)$$
$$= (m-n+3)M_1(G)+m[(m+3)(n-4)+4(n+m-1)] - 2M_2(G) - \xi_3(G)$$
$$= m[(n-4)(m+3)+4(n+m-1)] + (m-n+3)M_1(G) - 2M_2(G) - \xi_3(G).$$

This completes the proof. □

Theorem 3.10. *Let G be a nontrivial graph of order n and size m. Then*

$$\overline{M_1}(G^{-+-}) = m[(n-4)(m+3)+4(n+m-1)] + (m-n+3)M_1(G) - 2M_2(G) - \xi_3(G).$$

Proof. Follows from Theorem 12 and Theorem 7 due to the fact that $\overline{G^{+-+}} = G^{-+-}$. □

Theorem 3.11. *Let G be a nontrivial graph of order n and size m. Then*

$$\overline{M_1}(G^{-++}) = mn(n-1) + (m+n-1)M_1(G) - 2M_2(G) - \xi_3(G).$$

Proof. Note that G^{-++} has $(m+n)$ vertices and for $u \in V(G^{-++})\cap V(G)$, $d_{G^{+-+}}(u) = n-1$ and for $u \in V(G^{+-+}) \cap E(G)$, $d_{G^{+-+}}(u) = d_G(u) + d_G(v)$. Therefore by the means of Observation 1, we have,

$$\overline{M_1}(G^{-++}) = \sum_{u\in V(G^{-++})} (n-d_{G^{-++}}(u)-1)d_{G^{-++}}(u)$$

$$\overline{M_1}(G^{-++}) = \sum_{u\in V(G^{-++})\cap V(G)} (n-d_{G^{-++}}(u)-1)(d_{G^{-++}}(u)) + \sum_{u\in V(G^{-++})\cap E(G))} (n-d_{G^{-++}}(u)-1)d_{G^{-++}}(u)$$

$$\overline{M_1}(G^{-++}) = \sum_{u\in V(G^{-++})\cap V(G)} (m+n-(n-1)-1)(n-1) + \sum_{u\in V(G^{-++})\cap E(G))} (m+n-(d_G(u)+d_G(v))-1)(d_G(u)+d_G(v))$$

$$= mn(n-1)+(m+n-1)M_1(G) - \left\{\sum_{u,v\in E(G)} (d_G(u)+d_G(v))^2\right\}$$
$$= mn(n-1)+(m+n-1)M_1(G) - \left\{\sum_{u,v\in E(G)} (d_G(u))^2+(d_G(v))^2 - 2M_2(G)\right\}$$
$$= mn(n-1)+(m+n-1)M_1(G) - 2M_2(G) - \xi_3(G).$$

, as desired. □

Theorem 3.12. *Let G be a nontrivial graph of order n and size m. Then*

$$\overline{M_1}(G^{+--}) = mn(n-1) + (m+n-1)M_1(G) - 2M_2(G) - \xi_3(G).$$

Proof. Follows from Theorem 14 and Theorem 7 due to the fact that $\overline{G^{-++}} = G^{+--}$. □

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