Modified Zagreb Index of Some Chemical Structure Trees

Research Article

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Abstract: In this work, first and second modified Zagreb index of Bethe trees, Dendrimer trees, Fascia graph and special type of trees, namely, Polytree are computed.

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1. Introduction

In this article, we are concerned with simple graphs, that is finite and undirected graphs without loops or multiple edges. Let G be such a graph and $V(G)$ and $E(G)$ be its vertex set and edge set, respectively. An edge of G, connecting the vertices u and v will be denoted by uv. The degree $d(v)$ of a vertex $v \in V(G)$ is the number of vertices of G adjacent to v. The most elementary constituents of a (molecular) graph are vertices, edges, vertex-degrees, walks and paths [11]. They are the basis of many graph-theoretical invariants referred to as topological index, which have found considerable use in Zagreb index. The vertex-degree-based graph invariants $M_1(G) = \sum\limits_{v \in V(G)} d(v)^2$ and $M_2(G) = \sum\limits_{uv \in E(G)} d(u)d(v)$ are known under the name first and second Zagreb index, respectively. These have been conceived in the 1970s and found considerable applications in chemistry [4, 7, 8]. The Zagreb indices were subject to a large number of mathematical studies, of which we mention only a few nearest [5, 6].

1.1. Preliminaries

Definition 1.1. *Let G be a graph. The degree of a vertex v of G is denoted by $d(v)$. If $d(v) = 1$, then v is said to be a pendant vertex in G and the edge incident with v is referred to as pendant edge.*

Definition 1.2. *The set of neighbours of v is denoted by $N_G(v)$. As usual, P_n and S_n denote the path and the star on n vertices respectively.*

Definition 1.3. *The first and the second modified Zagreb index were defined as ${}^m M_1(G) = \sum\limits_{v \in V(G)} \dfrac{1}{d(v)^2}$ and ${}^m M_2(G) = \sum\limits_{uv \in E(G)} \dfrac{1}{d(u)d(v)}$, where $d(v)$ is the degree of the vertex v in G.*

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Assuming that the graph G has more than one cut-vertex, Balakrishnan *et al.* obtained an expression for Wiener Index of the graph G in terms of the blocks of G and other quantities [3]. Similar to this, we obtain an expression for the modified Zagreb index of a graph with a cut-vertex and with more than one cut-vertex. As an application, this topological index is computed for Bethe trees and dendrimer trees. Also, the modified Zagreb index of Fasciagraph and a special type of trees, namely, polytree are computed. We conclude this section with some notation and terminology. For other notations in graph theory, may be consulted [2].

2.   Modified Zagreb Indices of Graphs with more than One Cut-Vertex

In this section, we compute the second Zagreb indices of a graph with a cut-vertex and with more than one cut-vertex.

Theorem 2.1. *Let G be a simple connected graph with a cut-vertex u. Let H_i, $1 \leq i \leq r$, be the components of $G - u$. Let $G_i = G\left[V\left(H_i\right) \bigcup \{u\}\right]$. Then*

$$
{}^{m}M_2(G) = \sum_{i=1}^{r} {}^{m}M_2\left(G_i\right) - \sum_{i=1}^{r} \sum_{w \in N_{G_i}(u)} \left\{ \frac{k - k_i}{(k)\left(k_i\right)\left(d\left(w\right)\right)^2} \right\} \tag{1}
$$

where $d_G\left(u\right) = k$ and $d_{G_i}\left(u\right) = k_i$.

Proof.

$$
{}^{m}M_2(G) = \sum_{i=1}^{r} {}^{m}M_2\left(G_i\right) - \sum_{i=1}^{r} \sum_{w \in N_{G_i}(u)} \frac{1}{k_i d(w)} + \sum_{i=1}^{r} \sum_{w \in N_{G_i}(u)} \frac{1}{k d(w)}
$$

$$
= \sum_{i=1}^{r} {}^{m}M_2\left(G_i\right) - \sum_{i=1}^{r} \sum_{w \in N_{G_i}(u)} \left\{ \frac{k - k_i}{(k)\left(k_i\right)\left(d\left(w\right)\right)^2} \right\}
$$

$\square$

Theorem 2.2. *Let $\mathscr{C} = \{v_1, v_2, \ldots, v_l\}$ be the set of all cut-vertices and $\mathscr{B} = \{B_1, B_2, \ldots, B_k\}$ be the set of all blocks of a simple connected graph G. Then*

$$
{}^{m}M_2(G) = \sum_{i=1}^{k} {}^{m}M_2(B_i) - \sum_{i=1}^{l} \sum_{B \in B_i'} \sum_{\substack{x \in N_B(v_i) \\ x \notin \mathscr{C}}} \left\{ \frac{1}{d_B(v_i) d_B(x)} - \frac{1}{d_G(v_i) d_G(x)} \right\}
$$
$$
- \sum_{i=1}^{l} \sum_{B \in B_i'} \sum_{\substack{x \in N_B(v_i) \\ x \in \mathscr{C}}} \left\{ \frac{1}{d_B(v_i) d_B(x)} - \frac{1}{d_G(v_i) d_G(x)} \right\} \tag{2}
$$

where $B_i' = \{B \in \mathscr{B} | v_i \in B\}, \quad 1 \leq i \leq l.$

Proof.   Clearly $d_G(v_i) = \sum\limits_{B \in B_i'} d_B(v_i)$, for $1 \leq i \leq l$ and $E(G) = \bigcup\limits_{i=1}^{k} E(B_i)$. Let $e = uv \in E(G)$. Obviously $e \in B_i$ for some i. If $u, v \notin \mathscr{C}$, then the weight of e in G is the same as the weight of e in B_i. Let us consider the case that either u or $v \in \mathscr{C}$. Without loss of generality, assume that $u \in \mathscr{C}$. The weight of e in B_i is less by $\left\{ \frac{1}{d_{B_i}(u) d_{B_i}(v)} - \frac{1}{d_G(u) d_G(v)} \right\}$ from the weight of e in G. Similarly if $u, v \in \mathscr{C}$ then the weight of e in B_i is less by $\left\{ \frac{1}{d_{B_i}(u) d_{B_i}(v)} - \frac{1}{d_G(u) d_G(v)} \right\}$ from the weight of e in G. Hence

$$
{}^{m}M_2(G) = \sum_{i=1}^{k} {}^{m}M_2(B_i) - \sum_{i=1}^{l} \sum_{B \in B_i'} \sum_{\substack{x \in N_B(v_i) \\ x \notin \mathscr{C}}} \left\{ \frac{1}{d_B(v_i) d_B(x)} - \frac{1}{d_G(v_i) d_G(x)} \right\}
$$

$$
- \sum_{i=1}^{l} \sum_{B \in B_i'} \sum_{\substack{x \in N_B(v_i) \\ x \in \mathscr{C}}} \left\{ \frac{1}{d_B(v_i) d_B(x)} - \frac{1}{d_G(v_i) d_G(x)} \right\}
$$

□

Using the above theorem we can calculate the modified Zagreb index of a graph with a cut-edge as follows.

Corollary 2.3. *Let $uv \in E(G)$ be a cut-edge of G and let G_1 and G_2 be the two components of $G - uv$. Then*

$$^m M_2(G) =^m M_2(G_1) +^m M_2(G_2) - \left\{ \sum_{w \in N(u)-\{v\}} \frac{1}{d(u)(d(u)-1)(d(w))^2} \right.$$
$$\left. + \sum_{w \in N(v)-\{u\}} \frac{1}{d(w)(d(w)-1)(d(v))^2} - \frac{1}{d(u)d(v)} \right\}$$

3. Modified Zagreb Indices of Generalized Bethe Trees

In a tree, any vertex can be chosen as the root vertex. The level of a vertex on a tree is one more than its distance from the root vertex. Suppose T is an unweighted rooted tree such that its vertices at the same level have equal degrees. The root vertex is at level 1 and T has k levels. In [1], Rojo and Robbiano, called such a tree as generalized Bethe tree. They denoted the class of generalized Bethe tree of k levels by B_k.
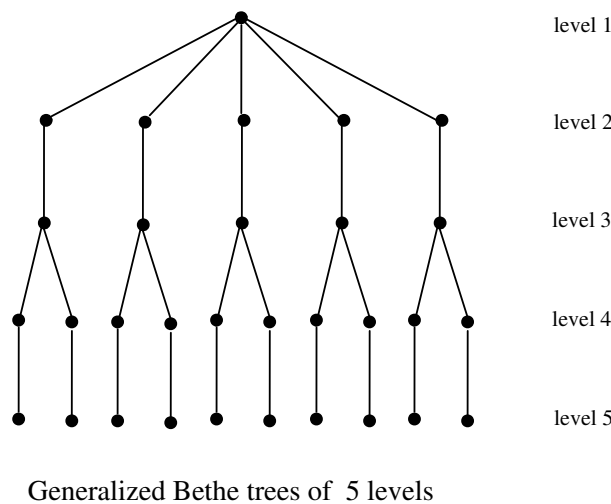

Generalized Bethe trees of 5 levels

Figure 1:

Theorem 3.1. *Let B_k be a generalized Bethe tree of k levels. If d_1 denotes the degree of rooted vertex, d_i denotes degree of the vertices on the ith level of B_k for $1 \leq i \leq k$ and n_i denotes the number of vertices on the ith level of B_k for $1 \leq i \leq k$, then the first and second modified zagreb index of B_k is computed as follows.* $^m M_1(B_k) = \frac{n_i}{d_i^2}$ *and* $^m M_2(B_k) = \frac{1}{d_2} + \sum_{i=2}^{k-1} \frac{n_i(d_i-1)}{d_i d_{i+1}}$

Proof. The first modified Zagreb index of Bethe tree is obvious. $|V(B_k)| = 1 + \sum_{i=1}^{k} \prod_{j=1}^{i} d_j$ and each block of B_k is K_2, nothing but the edges of B_k. In B_k the rooted vertex belongs to d_1 blocks and the vertices in i^{th} level of B_k belongs to d_i blocks, $2 \leq i \leq k$. Therefore $^m M_2(B_k) = \frac{n_1 d_1}{d_1 d_2} + \sum_{i=2}^{k-1} \frac{n_i(d_i-1)}{d_i d_{i+1}} = \frac{1}{d_2} + \sum_{i=2}^{k-1} \frac{n_i(d_i-1)}{d_i d_{i+1}}$ (since $n_1 = 1$).

□

A dendrimer tree $T_{k,d}$ is a rooted tree such that degree of whose non-pendant vertices is equal to d and distance between the rooted vertex and pendant vertices is equal to k. So $T_{k,d}$ can be considered as a generalized Bethe tree with k levels such that non-pendant vertices have equal degree. We can compute the modified Zagreb indices of dendrimer tree as follows.
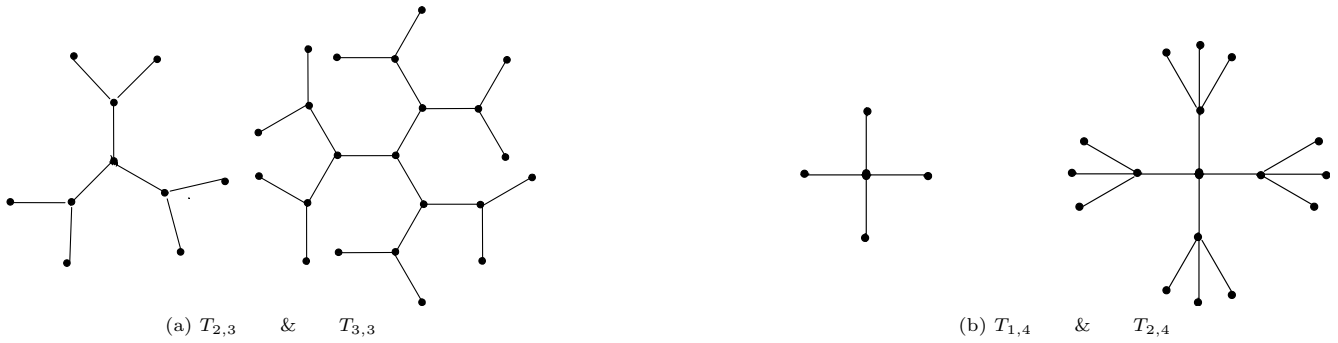
(a) $T_{2,3}$ & $T_{3,3}$ (b) $T_{1,4}$ & $T_{2,4}$

Figure 2:

Corollary 3.2. *Let $T_{k,d}$ be a dendrimer tree of k levels whose degree of the non-pendant vertices is equal to d, d_i denotes degree of the vertices on the ith level of B_k for $1 \le i \le k$ and n_i denotes the number of vertices on the ith level of B_k for $1 \le i \le k$. Then $^m M_1(T_{k,d}) = \dfrac{n_i}{d_i^2}$ and $^m M_2(T_{k,d}) = \dfrac{d_1}{d_1 d_2} + \sum\limits_{i=2}^{k-1} \dfrac{d(d_i - 1)}{d_i d_{i+1}}$*

Remark 3.3. *If $d = 2, 3$ in $T_{k,d}$, then*

$$^m M_1(T_{2,3}) = 58/9, ^m M_1(T_{3,3}) = 118/9 \ \text{ and}$$

$$^m M_2(T_{2,3}) = {}^m M_2(T_{3,3}) = 5$$

4. First and Second Modified Zagreb Indices of Fasciagraph and Polytree

In this section we give the exact formula of First and second modified Zagreb indices for growing graphs namely fasciagraph and growing tree namely polytree.

Theorem 4.1. *Let G be a simple connected graph and $u, v \in V(G)$ such that u and v are non adjacent. Let G_k be a graph obtained from k copies of G such that the vertex u of one copy of G is adjacent to the vertex v of the next copy of G except the terminals. Then*

$$^m M_1(G_k) = k^m M_1(G) - (k-1) \left\{ \sum_{i=1}^{k-1} \frac{1}{d(v_i)^2} - \frac{1}{(d(v_i)+1)^2} - \sum_{i=1}^{k-1} \frac{1}{d(v_i)^2} - \frac{1}{(d(v_i)+1)^2} \right\} \tag{3}$$

and where $d(v_i)$ denotes the degree of the vertex v in the ith copy , $1 \le i < k$ and $d(u_i)$ denotes the degree of the vertex u in the ith copy , $1 < i \le k$

$$^m M_2(G_k) = k^m M_2(G) - (k-1) \left\{ \sum_{w \in N_G(u)} \frac{1}{d(u)(d(u)+1)(d(w))^2} \right.$$
$$\left. + \sum_{w \in N_G(v)} \frac{1}{d(w)(d(w)+1)(d(v))^2} - \frac{1}{(d(u)+1)(d(v)+1)} \right\} \tag{4}$$

Proof.

$$^m M_1(G_k) = k^m M_1(G) - (k-1) \left\{ \sum_{i=1}^{k-1} \frac{1}{d(v_i)^2} - \frac{1}{(d(v_i)+1)^2} \right\} - (k-1) \left\{ \sum_{i=1}^{k-1} \frac{1}{d(v_i)^2} - \frac{1}{(d(v_i)+1)^2} \right\} \tag{5}$$

Hence

$$^m M_1(G_k) = k^m M_1(G) - (k-1) \left\{ \sum_{i=1}^{k-1} \frac{1}{d(v_i)^2} - \frac{1}{(d(v_i)+1)^2} - \sum_{i=1}^{k-1} \frac{1}{d(v_i)^2} - \frac{1}{(d(v_i)+1)^2} \right\} \tag{6}$$

We can prove this by the method of induction on k. Let $k = 2$. Then

$$^m M_2(G_2) = 2\,^m M_2(G) - \sum_{w \in N(u)} \frac{1}{d(u)d(w)} - \sum_{w \in N(v)} \frac{1}{d(v)d(w)}$$

$$+ \sum_{w \in N(u)} \frac{1}{(d(u)+1)d(w)} + \sum_{w \in N(v)} \frac{1}{(d(v)+1)d(w)} + \frac{1}{(d(u)+1)(d(v)+1)}$$

$$= 2\,^m M_2(G) - \left\{ \sum_{w \in N(u)} \frac{1}{[d(u)d(w)][d(u)d(w)+1]} \right.$$

$$\left. + \sum_{w \in N(v)} \frac{1}{[d(v)d(w)][(d(v)+1)d(w)]} - \frac{1}{(d(u)+1)(d(v)+1)} \right\}$$

Assume the result for G_{k-1} . Let u and v be the vertices corresponding to $(k-1)^{th}$ and k^{th} copies of G_k respectively. Then

$$^m M_2(G_k) =\,^m M_2(G_{k-1}) +\,^m M_2(G) - \sum_{w \in N(u)} \frac{1}{d(u)d(w)} - \sum_{w \in N(v)} \frac{1}{d(v)d(w)}$$

$$+ \sum_{w \in N(u)} \frac{1}{(d(u)+1)d(w)} + \sum_{w \in N(v)} \frac{1}{(d(v)+1)d(w)} + \frac{1}{(d(u)+1)(d(v)+1)}$$

$$=\,^m M_2(G_{k-1}) +\,^m M_2(G) - \left\{ \sum_{w \in N(u)} \frac{1}{[d(u)d(w)][(d(u)+1)d(w)]} \right.$$

$$\left. + \sum_{w \in N(v)} \frac{1}{[d(v)d(w)][(d(v)+1)d(w)]} - \frac{1}{(d(u)+1)(d(v)+1)} \right\}$$

$$= (k-1)\,^m M_2(G) - (k-2) \left\{ \sum_{w \in N_G(u)} \frac{1}{[d(u)d(w)][(d(u)+1)d(w)]} \right.$$

$$\left. + \sum_{w \in N_G(v)} \frac{1}{[d(v)d(w)][(d(v)+1)d(w)]} - \frac{1}{(d(u)+1)(d(v)+1)} \right\}$$

$$+\,^m M_2(G) - \left\{ \sum_{w \in N(u)} \frac{1}{[d(u)d(w)][(d(u)+1)d(w)]} \right.$$

$$\left. + \sum_{w \in N(v)} \frac{1}{[d(v)+d(w)][d(v)+d(w)+1]} - \frac{1}{d(u)+d(v)+2} \right\}$$

$$= k\,^m M_2(G) - (k-1) \left\{ \sum_{w \in N_G(u)} \frac{1}{d(u)(d(u)+1)(d(w))^2} \right.$$

$$\left. + \sum_{w \in N_G(v)} \frac{1}{d(w)(d(w)+1)(d(v))^2} - \frac{1}{(d(u)+1)(d(v)+1)} \right\}$$

$\square$

Fasciagraph is a class of polygraph. The structure of the simplest fasciagraph F is uniquely specified by the structure of the monomer unit G and the number of monomer units. Every unit of F is adjacent with two units except the terminal units. A fasciagraph is a polygraph with k copies of a fixed graph G such that the vertex u in the ith copy is adjacent to the vertex v in the $(i+1)^{th}$ copy of G, $i = 1, 2, \ldots, k-1$.
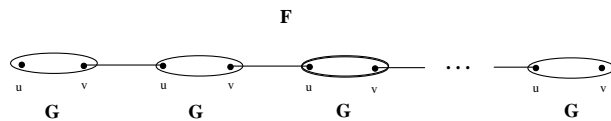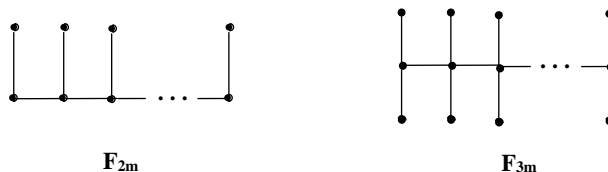

Figure 3: G_k

Corollary 4.2. *Let F be a fasciagraph composed of k copies of a graph G. Then*

$$^m M_2(F) = k\,^m M_2(G) - (k-1) \left\{ \sum_{w \in N_G(u)} \frac{1}{d(u)(d(u)+1)(d(w))^2} + \sum_{w \in N_G(v)} \frac{1}{d(v)(d(v)+1)(d(w))^2} - \frac{1}{d(u)+1)(d(v)+1)} \right\}$$

Consider a chemical polytree F_{nk} consisting of k copies of the star S_n such that u is the centre vertex of S_n. Using the above theorem we have modified Zagreb indices of polytree in terms of order of the star.

F$_{2m}$　　　　　　**F$_{3m}$**

Corollary 4.3. *Let F_{nk} be a chemical polytree consisting of k copies of the star S_n such that u is the centre vertex of S_n.*
Then $^mM_1(F_{nk}) = k(n-1) + \dfrac{2}{n^2} + \dfrac{k-2}{(n+1)^2}$ *and* $^mM_2(F_{nk}) = \dfrac{2(n-1)}{n} + \dfrac{(k-2)(n-1)}{n+1} + \dfrac{2}{n(n+1)} + \dfrac{k-3}{(n+1)^2}$

Proof.　　Since u is the centre vertex of S_n,　$d(u) = n-1$ and $d(w) = 1$, we get the result.　　　　□

Remark 4.4. *Chemically relevant fasciagraphs F_{nk} correspond to the cases $n = 2$ and $n = 3$.*

$$^mM_1(F_{2k}) = \frac{40k+10}{36} \quad and$$
$$^mM_2(F_{2k}) = \frac{4k+3}{9}$$
$$^mM_1(F_{3k}) = \frac{153k+14}{144} \quad and$$
$$^mM_2(F_{3k}) = \frac{35k-1}{48}$$

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