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Computing Multiplicative Zagreb Indices with respect to Chromatic and Clique Numbers

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ABSTRACT. In the present study we compute some bounds of multiplicative Zagreb indices and then we study these topological indices by using concept of chromatic number and clique number.

Keywords: Multiplicative Zagreb index, clique number, independence number, chromatic number.

1. INTRODUCTION

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. If e is an edge of G, connecting the vertices u and v, then we write $e = uv$ and say "u and v are adjacent". A connected graph is a graph such that there is a path between all pairs of vertices.

The ***chromatic number*** of a graph G, denoted by $\chi(G)$, is the minimum number of colors such that G can be colored with these colors in such a way that no two adjacent vertices have the same color. An ***independent set*** in a graph is a set of vertices no two of which are adjacent. An independent set in a graph is maximum if the graph contains no larger independent set and maximal if the set cannot be extended to a larger independent set; a maximum independent set is necessarily maximal, but not conversely. The cardinality of any maximum independent set in a graph G is called the independent number of G and is denoted by $\alpha(G)$. A ***clique*** in a graph is a set of mutually adjacent vertices. The maximum size of a clique in a graph G is called the clique number of G and denoted by $\omega(G)$. Clearly, a set of vertices S is a clique of a simple graph G if and only if it is a stable set of its complement $\overline{G}$. In particular, $\alpha(G) = \omega(\overline{G})$. For any two nonadjacent vertices x and y in

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graph G, we use $G + xy$ to denote the graph obtained from adding a new edge xy to graph G. Similarly, for $e = xy$ in $E(G)$, $G - xy$ represents a new graph obtained from graph G by deleting the edge $e = xy$.

Let $X_{n,k}$ and $W_{n,k}$ be the set of connected graphs of order n with chromatic number k and the set of connected graphs of order n with clique number k, respectively.

A k–partite graph is a graph whose vertices can be divided into k disjoint sets U_1, U_2, …, U_k such that every edge connects a vertex in U_i to one in U_j, $(i, j = 1, 2, \ldots, n)$ that is, U_i's are independent sets. A complete bipartite graph is a bipartite graph such that every pair of graph vertices in different sets are adjacent.

The ***Turán graph*** $T_n(k)$ is a complete k-partite graph whose partition sets differ in size by at most 1. Denote by $K_k((n-k)^1)$ the graph obtained by identifying one vertex of K_k with a pendent vertex of path P_{n-k+1}. In this paper we compute some bounds of multiplicative Zagreb indices.

2. DEFINITIONS AND PRELIMINARIES

Let $\mathfrak{G}$ be the class of finite graphs. A ***topological index*** is a function $\mu\colon \mathfrak{G} \to \mathbb{R}^+$ with this property that $\mu(G) = \mu(H)$ if G and H are isomorphic. Obviously, the number of vertices and the number of edges are topological index. The ***Wiener number*** [1] is the first reported distance based topological index and is defined as half sum of the distances between all the pairs of vertices in a molecular graph. If $x, y \in V(G)$ then the distance $d_G(x,y)$ between x and y is defined as the length of any shortest path in G connecting x and y.

The ***Zagreb indices*** have been introduced more than thirty years ago by Gutman and Trinajstić [2]. They are defined as:

$$M_1(G) = \sum_{v\in V(G)} \left(\mathrm{d}(v)\right)^2 \text{ and } M_2(G) = \sum_{uv\in E(G)} \mathrm{d}(u)\cdot \mathrm{d}(v),$$

where degree of vertex u is denoted by $d(u)$.

Recently, some new versions of Zagreb indices are considered by mathematicians. For example, in [3] Gutman introduced the multiplicative version of the Zagreb indices as follows:

$$PM_1(G) = \prod_{u\in V(G)} (d(u))^2 \text{ and } PM_2(G) = \prod_{uv\in E(G)} d(u)\cdot d(v).$$

In [3,4] Gutman *et al.* determined the extremal trees among all trees with $n \geq 5$ vertices with respect to the multiplicative Zagreb indices. Also in [4] authors studied some properties of Narumi–Katayama index defined as follows [5]:

$$NK(G) = \prod_{u\in V(G)} d(u).$$

Finally, the modified Narumi–Katayama index is defined by Ghorbani *et al.* as follows:

$$NK^{*}(G)=\prod_{u\in V(G)} d(u)^{d(u)}.$$

It is clear that the second multiplicative Zagreb index and the modified Narumi–Katayama index are the same. In [6] the extremal graphs are characterized with respect to modified Narumi–Katayama index. We encourage readers to references [7–12] for more details about the multiplicative topological indices. Here our notations are standard and mainly taken from [13–16].

3. MAIN RESULTS

In the following by using definitions of both the first and the second multiplicative Zagreb indices of graphs, the proof of two lemmas are obvious but we use of them in the proof of Theorem 9.

Lemma 1. Let G be a graph with two non–adjacent vertices $u,v\in V(G)$. Then we have $PM_i(G+uv)>PM_i(G)$, for $i=1, 2$.

Lemma 2. Let G be a graph with $e\in E(G)$. Then we have $PM_i(G-e)<PM_i(G)$, $i=1, 2$.

In the following let $n_1+n_2+\cdots+n_k=n$ and the complete k–partite graph of order n whose partition sets are of size $n_1, n_2, \ldots, n_k$ is denoted by $K_{n_1,n_2,\ldots,n_k}$.

Lemma 3.

$$PM_1\left(K_{n_1,n_2,\ldots,n_k}\right)=\prod_{i=1}^{k}\left(n-n_i\right)^{2n_i},$$
$$PM_2\left(K_{n_1,n_2,\ldots,n_k}\right)=\prod_{i=1}^{k}\prod_{j=i+1}^{k}\left(\left(n-n_i\right)\left(n-n_j\right)\right)^{n_in_j}.$$

Proof. For $j\in\{1,2,\ldots,k\}$, in a partition set of size n_j in $K_{n_1,n_2,\ldots,n_k}$, each vertex is of degree $n-n_j$. This completes the proof.

In the following suppose that $1<k<n$ and $n=kq+r$ where $0\le r<k$, *i.e.*, $q=\lfloor n/k\rfloor$. We obtain the maximal multiplicative Zagreb indices of $\chi_{n,k}$.

Lemma 4. Let $G_i\in\chi_{n,k}$ be a graph with the maximal multiplicative Zagreb index PM_i for $i\in\{1,2\}$. Then G_i must be of the form $K_{n_1,n_2,\ldots,n_k}$ where $i\in\{1,2\}$.

Proof. Using Lemma 2 and the definition of the set $\chi_{n,k}$, this lemma follows immediately.

Lemma 5. Let $G \in \chi_{n,k}$. Then

$$PM_1\left(T_n(k)\right) = \left(n - \lceil n/k \rceil\right)^{2r\lceil n/k \rceil}\left(n - \lfloor n/k \rfloor\right)^{2(k-r)\lfloor n/k \rfloor},$$

$$PM_2\left(T_n(k)\right) = \left(n - \lceil n/k \rceil\right)^{2\binom{r}{2}\lceil n/k \rceil^2}\left(n - \lfloor n/k \rfloor\right)^{2\binom{k-r}{2}\lfloor n/k \rfloor^2} \times\left(\left(n - \lceil n/k \rceil\right)\left(n - \lfloor n/k \rfloor\right)\right)^{r(r-k)\lceil n/k \rceil\lfloor n/k \rfloor}.$$

Proof. From the definition of chromatic number, any graph G belong to $X_{n,k}$ has k color classes each of which is an independent set. Suppose that the k classes have order $n_1, n_2, . . . ,n_k$ respectively. From Lemma 4, we can verify that a graph which serves the maximal Zagreb index PM_i for $i \in \{1,2\}$ will be a complete k-partite graph $K_{n_1,n_2,\ldots,n_k}$. Suppose that a graph $G_i \in \chi_{n,k}$ has the maximal multiplicative Zagreb index PM_i for i = 1, 2. Now we claim that G_i must be $T_n(k)$:

Case 1. For the first multiplicative Zagreb index PM_1. Otherwise, without loss of generality, we assume that the orders of two classes, say n_1 and n_2, satisfy $n_2 - n_1 \geq 2$. When $k = 2$, note that $n_1 + n_2 = n$. By Lemma 3, we have:

$$PM_1\left(K_{n_1,n_2}\right) = {n_1}^{2n_2}{n_2}^{2n_1} \text{ and } PM_2\left(K_{n_1+1,n_2-1}\right) = \left(n_1+1\right)^{2(n_2-1)}\left(n_2-1\right)^{2(n_1+1)}.$$

Let $A = \dfrac{PM_2\left(K_{n_1+1,n_2-1}\right)}{PM_1\left(K_{n_1,n_2}\right)}$, then

$$A = \frac{\left(n_1+1\right)^{2(n_2-1)}\left(n_2-1\right)^{2(n_1+1)}}{{n_1}^{2n_2}{n_2}^{2n_1}} = \frac{\left(n_1+1\right)^{2n_2}\left(n_2-1\right)^{2n_1}\left(n_2-1\right)^2}{{n_1}^{2n_2}{n_2}^{2n_1}\left(n_1+1\right)^2}$$

$$= \left(\frac{\left(n_1+1\right)\left(n_2-1\right)}{n_1 n_2}\right)^{2n_1}\left(\frac{n_1+1}{n_1}\right)^{2(n_2-n_1)}\left(\frac{n_2-1}{n_1+1}\right)^2 > 1.$$

This is a contradiction to the choice of G_1. In generally for $k \geq 3$, we have:

$$PM_1\left(K_{n_1,n_2,\ldots,n_k}\right) = \left(n-n_1\right)^{2n_1}\left(n-n_2\right)^{2n_2}\prod_{i=3}^{k}\left(n-n_i\right)^{2n_i},$$

$$PM_2\left(K_{n_1+1,n_2-1,\ldots,n_k}\right) = \left(n-n_1-1\right)^{2(n_1+1)}\left(n-n_2+1\right)^{2(n_2-1)}\prod_{i=3}^{k}\left(n-n_i\right)^{2n_i}$$

and

$$A=\frac{\left(n-n_1-1\right)^{2(n_1+1)}\left(n-n_2+1\right)^{2(n_2-1)}}{\left(n-n_1\right)^{2n_1}\left(n-n_2\right)^{2n_2}}$$
$$=\frac{\left(n-n_1-1\right)^{2n_1}\left(n-n_2+1\right)^{2n_2}\left(n-n_1-1\right)^{2}}{\left(n-n_1\right)^{2n_1}\left(n-n_2\right)^{2n_2}\left(n-n_2+1\right)^{2}}$$
$$=\left(\frac{\left(n-n_1-1\right)\left(n-n_2+1\right)}{\left(n-n_1\right)\left(n-n_2\right)}\right)^{2n_1}\left(\frac{n-n_2+1}{n-n_2}\right)^{2(n_2-n_1)}\left(\frac{n-n_1-1}{n-n_2+1}\right)^{2}>1.$$

This is a contradiction to the choice of G_1.

Case 2. For the second multiplicative Zagreb index PM_2. Without loss of generality, we assume that the orders of two classes, say n_p and n_q with $1\leq p<q\leq k$, satisfy $n_q-n_p\geq 2$. For convenience, let $\sum_i^j n_i=0$ if $j<i$. Set

$$B_1=\prod_{i=1}^{p-1}\prod_{\substack{j=i+1\\ j\neq p,q}}^{k}\left(\left(n-n_i\right)\left(n-n_j\right)\right)^{n_in_j},\qquad B_2=\prod_{i=p+1}^{q-1}\prod_{\substack{j=i+1\\ j\neq p,q}}^{k}\left(\left(n-n_i\right)\left(n-n_j\right)\right)^{n_in_j},$$
$$B_3=\prod_{i=q+1}^{k}\prod_{\substack{j=i+1\\ j\neq p,q}}^{k}\left(\left(n-n_i\right)\left(n-n_j\right)\right)^{n_in_j}.$$

Suppose also $B=B_1.B_2.B_3$, by Lemma 3, we have

$$PM_2\left(K_{n_1,n_2,\ldots,n_p,\ldots,n_q,\ldots,n_k}\right)=B\left(\prod_{\substack{i=1\\ j\neq p,q}}^{k}\left(n-n_p\right)\left(n-n_i\right)\right)^{n_in_p}\prod_{\substack{i=1\\ j\neq p,q}}^{k}\left(\left(n-n_q\right)\left(n-n_i\right)\right)^{n_in_q}$$
$$\times\left(\left(n-n_p\right)\left(n-n_q\right)\right)^{n_pn_q},$$
$$PM_2\left(K_{n_1,\ldots,n_{P+1},\ldots,n_{q-1},\ldots,n_k}\right)=B\left(\prod_{\substack{i=1\\ j\neq p,q}}^{k}\left(\left(n-n_p-1\right)\left(n-n_i\right)\right)^{n_i\left(n_p+1\right)}\prod_{\substack{i=1\\ j\neq p,q}}^{k}\left(\left(n-n_q-1\right)\left(n-n_i\right)\right)^{n_i\left(n_q-1\right)}\right)$$
$$\times\left(\left(n-n_p-1\right)\left(n-n_q+1\right)\right)^{\left(\left(n_p+1\right)\right)\left(n_q-1\right)}.$$

$$A=\frac{PM_2\left(K_{n_1,\ldots,n_{P+1},\ldots,n_{q-1},\ldots,n_k}\right)}{PM_2\left(K_{n_1,n_2,\ldots,n_p,\ldots,n_q,\ldots,n_k}\right)}=\left(\prod_{\substack{i=1\\ j\neq p,q}}^{k}\frac{\left(\left(n-n_p-1\right)\left(n-n_i\right)\right)^{n_i\left(n_p+1\right)}\left(\left(n-n_q+1\right)\left(n-n_i\right)\right)^{n_i\left(n_q-1\right)}}{\left(\left(n-n_p\right)\left(n-n_i\right)\right)^{n_in_p}\left(\left(n-n_p\right)\left(n-n_i\right)\right)^{n_in_q}}\right)$$
$$\times\left(\frac{\left(\left(n-n_p\right)\left(n-n_q\right)\right)^{\left(n_p+1\right)\left(n_q-1\right)}}{\left(\left(n-n_p\right)\left(n-n_q\right)\right)^{n_pn_q}}\right)$$
$$\geq\prod_{\substack{i=1\\ j\neq p,q}}^{k}\frac{\left(\left(n-n_p-1\right)\left(n-n_i\right)\right)^{n_i\left(n_p+1\right)}\left(\left(n-n_q-1\right)\left(n-n_i\right)\right)^{n_i\left(n_q-1\right)}}{\left(\left(n-n_p\right)\left(n-n_i\right)\right)^{n_in_p}\left(\left(n-n_p\right)\left(n-n_i\right)\right)^{n_in_q}}$$

$$= \prod_{\substack{i=1\\ j\neq p,q}}^{k} \frac{\left(\left(n-n_p-1\right)\left(n-n_i\right)\right)^{n_in_p}\left(\left(n-n_q+1\right)\left(n-n_i\right)\right)^{n_in_q}\left(\left(n-n_p-1\right)\left(n-n_i\right)\right)^{n_i}}{\left(\left(n-n_p\right)\left(n-n_i\right)\right)^{n_in_p}\left(\left(n-n_q\right)\left(n-n_i\right)\right)^{n_in_q}\left(\left(n-n_q-1\right)\left(n-n_i\right)\right)^{n_i}}$$

$$= \prod_{\substack{i=1\\ j\neq p,q}}^{k} \frac{\left(n-n_p-1\right)^{n_in_p}\left(n-n_q-1\right)^{n_in_q}\left(n-n_p-1\right)^{n_i}}{\left(n-n_p\right)^{n_in_p}\left(n-n_q\right)^{n_in_q}\left(n-n_q-1\right)^{n_i}}$$

$$= \prod_{\substack{i=1\\ j\neq p,q}}^{k} \left(\frac{\left(n-n_p-1\right)^{n_p}\left(n-n_q-1\right)^{n_q}}{\left(n-n_p\right)^{n_p}\left(n-n_q\right)^{n_q}}\right)^{n_i}\left(\frac{n-n_p-1}{n-n_q-1}\right)^{n_i}$$

$$\geq \prod_{\substack{i=1\\ j\neq p,q}}^{k} \left(\left(\frac{\left(n-n_p-1\right)\left(n-n_q+1\right)}{\left(n-n_p\right)\left(n-n_q\right)}\right)^{n_p}\left(\frac{n-n_q+1}{n-n_q}\right)^{n_q-n_p}\right)^{n_i} > 1.$$

Lemma 6 [17]. Suppose $G = (V, E)$ be a graph with clique number less or equal than k. Hence there is a graph $H = (V, F)$ in which for any vertex such as v, $d_H(v) \leq d_G(v)$.

Corollary 7. Let $G \in W_{n,k}$. Then

$$PM_1\left(T_n(k)\right) = \left(n-\left\lceil\frac{n}{k}\right\rceil\right)^{2r\left\lceil\frac{n}{k}\right\rceil}\left(n-\left\lfloor\frac{n}{k}\right\rfloor\right)^{2(k-r)\left\lfloor\frac{n}{k}\right\rfloor},$$

$$PM_2\left(T_n(k)\right) = \left(n-\left\lceil\frac{n}{k}\right\rceil\right)^{2\binom{r}{2}\left\lceil\frac{n}{k}\right\rceil^2}\left(n-\left\lfloor\frac{n}{k}\right\rfloor\right)^{2\binom{k-r}{2}\left\lfloor\frac{n}{k}\right\rfloor^2}\left(\left(n-\left\lceil\frac{n}{k}\right\rceil\right)\left(n-\left\lfloor\frac{n}{k}\right\rfloor\right)\right)^{r(r-k)\left\lceil\frac{n}{k}\right\rceil\left\lfloor\frac{n}{k}\right\rfloor}.$$

Proof. It follows by Lemma 5 and Corollary 6.

In the following denoted by $G_{u,v}(p, q)$ means a graph obtained from G by attaching paths of lengths p and q to vertices u and v, respectively.

Lemma 8 [18]. Suppose a and b are two positive integers and x and y be two vertices in graph G, such that $deg_G(x) \geq deg_G(y) > 1$. Then $PM_i(G_{x,y}(a,b)) > PM_i(G_x(a+b))$, for $i = 1, 2$.

In the following theorem we obtain some bounds for every graph belong to $W_{n,k}$ respect to the graph $G_{u,v}(p, q)$.

Theorem 9. Let $G \in W_{n,k}$. Then we have:

$$PM_1(G) \geq PM_1\left(K_k(n-k)^1\right) \text{ and } PM_2(G) \geq PM_2\left(K_k(n-k)^1\right).$$

Proof. Let $G \in W_{n,k}$ has the smallest first multiplicative Zagreb index. By using definition of $W_{n,k}$, G is containing a complete subgraph K_k. Without loss of generality, let $V(K_k) = \{v_1, v_2, \dots v_k\}$. By Lemma 1, G is a graph obtained from complete graph K_k, by attaching some trees to the some vertices of K_k. Suppose $W = \{v_1, v_2, \dots, v_t\}$, $t \le k$, $\deg_G(v_i) > k-1\}$. One can see easily that all trees attached to the vertices of K_k should be paths and so all vertices of W have degree k. Suppose W has at least two vertices such as u and v. By using Lemma 1, $G \cong G_{u,v}(p,q)$ can be transformed to $G_u(p + q)$ or $G_v(p + q)$ with smaller first multiplicative Zagreb index and this is a contradiction. This implies, $|W| = 1$ and so,

$$PM_1(G) \ge PM_1\left(K_k(n-k)^1\right) = \left((k-1)^{(k-1)}.k.2^{n-k-1}\right)^2$$
$$= k^2(k-1)^{2(k-1)}4^{(n-k-1)}.$$

This completes the first claim. For the second one can easily see that

$$PM_2(G) \ge PM_2\left(K_k(n-k)^1\right) = \frac{(k-1)^{2\binom{k}{2}}}{(k-1)^{2(k-1)}}\left(k(k-1)\right)^{k-1}.2k.4^{(n-k-2)}.2$$

$$= \frac{(k-1)^{2\frac{k(k-1)}{2}}}{(k-1)^{2(k-1)}}k^{k-1}(k-1)^{(k-1)}.2k.2^{2n-2k-4}.2$$

$$= (k-1)^{k(k-1)-(k-1)}k^{(k-1)}.2k.2^{2n-2k-4}.2$$

$$= (k-1)^{(k-1)^2}.k^k.2^{2(n-k-1)}.$$

4. CONCLUSION

The Zagreb index is a graphic invariant much used recently in QSAR/QSPR studies. Its mathematical properties have been intensively researched. In this paper, we study the product version of Zagreb indices and we computed the relation between these topological indices and other graph invariants.

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