Some Bounds on Forgotten Topological Index

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Abstract: *The forgotten index F(G) is defined as the sum of cubes of the degrees of the vertices of the graph G. In this paper we establish some new upper bounds for the Forgotten Topological index involving the number of vertices, the number of edges and the maximum and minimum vertex degree.*

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1. INTRODUCTION

In 1972, Gutman and Trinajsti'c [2,3] made the study on total π -electron energy of the molecular structure and introduced two vertex degree-based graph variants. These variants are defined as

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

In Chemical literature M_1 and M_2 are named as first and second Zagreb indices [6]. The Zagreb indices are used by various researchers in the studies of quantitative structure property relationships (QSPR) and quantitative structure activity relationship (QSAR). These indices are also viewed as a molecular structure-descriptors [6,7]. Various results on its chemical applications and mathematical properties are identified in [8,9,11,12]. These papers contain also a review of the usage of Zagreb indices as well as a survey of literature over these indices.

In 2015, Furtula and Gutman [5] reinvestigated this index and they showed that the predictive ability of this index is almost similar to that of first Zagreb index and for the entropy and acentric factor, both of them yield correlation coefficients greater than 0.95. They named this index as *forgotten topological index* or *F-index*, denoted by F(G).

$$F(G) = \sum_{v \in V(G)} d(v)^3.$$

Some bounds for the forgotten topological index are seen in [4,5] and the extremal values of *F-index* for trees are seen in [1].

2. PRELIMINARIES

All graphs under discussion are finite, undirected and simple. Let G=(V,E) be a simple graph with n vertices and m edges. Denote by uv the edge of G, connecting the vertices u and v. A line graph L(G) obtained from G in which $V(L(G)) = E(G)$, where two vertices of L(G) are adjacent if and only if they are adjacent edges of G. As usual $\Delta = \Delta(G)$ and $\delta = \delta(G)$ are the maximum and minimum degree of G, respectively. The symbols P_n, $K_{1,n-1}$, C_n also denote the path, star, and cycle graphs on n vertices. A Bigreed graph is a graph in which each vertex is of degree either δ or Δ .

3. MAIN RESULTS

In 2010, Bo Zhou and Trinajsti'c [13] have used the equivalent index for F(G) and presented the following relation

$$F(G) = \sum_{uv \in E(G)} \left[d(u)^2 + d(v)^2 \right] = \sum_{u \in V(G)} \sum_{v \in N(u)} d(u)^2.$$

The same authors gave the relation between F(G) and M_2(G), the identity for the forgotten topological index.

$$F(G) = \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in N(u)}\left[d(u) - d(v)\right]^2 + \sum_{u\in V(G)}\sum_{v\in N(u)} d(u)d(v),$$

which is equivalent to

$$F(G) = \sum_{uv\in E(G)}\left[d(u) - d(v)\right]^2 + 2M_2(G),$$

which is mentioned as equation (7) in [5].

Proposition 3.1. Let G be a graph with m edges. Then

$$F(G) = M_1^2(L(G)) + 4M_1(G) - 2M_2(G) - 4m$$

Proposition 3.2. Let G be a graph on n vertices and $m \geq 1$ edges. Then 3.1

$$M_1^3(G) \leq 2M_2^1(G) + nM_1^2(G) - 4m^2$$

Later in 2012, Illi'c and Bo Zhou [10] proposed a new lower bound for $M_1^3(G)$.

Proposition 3.3. If G is a connected graph, then

$$M_1^3(G) \leq \frac{2m - (\Delta^2 - \delta^2)}{n} M_1^2(G) + \frac{2m(n-1)(\Delta^2 - \delta^2)}{n}.$$

In 2009, Bo Zhou, Trinajsti'c [19] obtained the bounds for the general sum-connectivity index.

Proposition 3.4. Let G be a tree with $n \geq 4$ vertices. Then

$$18 + 16(n-3) - 2M_2(G) \leq F(G) \leq n^2(n-1) - 2M_2(G)$$

with left (right, respectively) equality if and only if G = P_n (G = S_n, respectively).

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Proposition 3.5. Let G be a triangle-free graph with n vertices and edges. Then

$$F(G) \leq mn^2 - 2M_2(G)$$

with equality if and only if G is a complete bipartite graph.

Theorem 3.6. Let G be a simple graph of with n vertices and m edges. Then

$$F(G) \leq \frac{\alpha(n)(\Delta^2 - \delta^2)(\Delta - \delta) + 2mM_1(G)}{n}$$

Where $\alpha(n) = n\left[\frac{n}{2}\right]\left(1 - \frac{1}{n}\left[\frac{n}{2}\right]\right)$, where [x] denotes integer part of a real number x and equality holds if and only if G is regular.

Proof: Let $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$ be real numbers for which there exist real constants a, b, A and B, so that for each i, i = 1,2, ..., n, $a \leq a_i \leq A$ and $b \leq b_i \leq B$.

Then the following inequality is valid [17]

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq \alpha(n)(A - a)(B - b),$$

Where $\alpha(n) = n\left[\frac{n}{2}\right]\left(1 - \frac{1}{n}\left[\frac{n}{2}\right]\right)$ and equality holds if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$. By setting $a_i = d(v)^2, b_i = d(v)$, we have $A = \Delta^2, a = \delta^2$, which completes our claim.

For $\alpha \in \mathbf{R}$ and G be a simple graph. Then

(3.3) $$F(G) \leq \frac{(\Delta+\delta)^2 M_1(G)^2}{8\Delta\delta m},$$

equality holds if and only if G is regular.

Proof: In order to obtain (3.3), we use Cassel's inequality [18]. Let $a_1, a_2, \cdots a_n$ and $b_1, b_2, \cdots b_n$ be sequences of positive real numbers and $w_1, w_2, \cdots w_n$ a sequence of non negative real numbers. Suppose that

$$m = \min_{i=1,n}\left\{\frac{a_i}{b_i}\right\} \text{ and } M = \max_{i=1,n}\left\{\frac{a_i}{b_i}\right\}$$

Then one has the inequality

$$\sum_{i=1}^{n} w_i a_i^2 \sum_{i=1}^{n} w_i b_i^2 \leq \frac{(m+M)^2}{4mM}\left(\sum_{i=1}^{n} w_i a_i b_i\right)^2.$$

The equality holds when $w_1 = \frac{1}{a_1 b_1}, w_n = \frac{1}{a_n b_n}, w_2 = \cdots = w_{n-1} = 0, m = \frac{a_n}{b_1}$.

By setting the values $a_i = d(v_i), b_i = 1$ and the weight $w_i = d(v_i)$, we have

$$\sum_{i=1}^{n} d(v)^3 \sum_{i=1}^{n} d(v) \leq \frac{(m+M)^2}{4mM}\left(\sum_{i=1}^{n} d(v)^2\right)^2.$$

Put $m = \delta$ and $M = \Delta$ completes the proof. The equality holds for regular graphs.

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