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A note on the first reformulated Zagreb index

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ABSTRACT

Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be a simple graph with n vertices and m edges. Denote by $d(e_i)$ $(i = 1, 2, \dots, m)$ an edge degree, and by $EM_1 = \sum_{i=1}^{m} d(e_i)^2$ first reformulated Zagreb index of graph G. Upper and lower bounds of graph invariant EM_1 are obtained.

1. Introduction

Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be a simple graph, with the sequence of vertex degrees $d_1 \ge d_2 \ge \cdots \ge d_n > 0$, $d_i = d(i)$ $(i = 1, 2, \dots, n)$. If ith and jth vertices of graph G are adjacent, we denote it as $i \sim j$. The edge connecting vertices i and j will be denoted by $e = \{i, j\}$. The degree of edge $e = \{i, j\}$ is defined as $d(e) = d_i + d_j - 2$.

A single number that can be used to characterize some property of the graph is called a *topological index* for that graph. Obviously, the number of vertices and the number of edges are topological indices.

Two vertex-degree based topological indices, the first and the second Zagreb index, M_1 and M_2, are defined as (see [7])

$$M_1 = \sum_{i=1}^{n} d_i^2 \quad \text{and} \quad M_2 = \sum_{i \sim j} d_i d_j .$$

The Zagreb indices belong among the oldest and most studied molecular structure descriptors and found significant applications in chemistry. Nowadays, there exist hundreds of papers on Zagreb indices and related matter. For the recent results on Zagreb indices, the interested reader can refer to [1,8,10,14,17,24,25]. Let us note that the Zagreb indices are special cases of Randić index (see for example [15,16,22]). Details on other vertex–based topological indices can be found in [9,21].

In [18], an edge-degree graph topological index, named reformulated Zagreb index, EM_1, is defined as

$$EM_1 = \sum_{i=1}^{m} d(e_i)^2 .$$

Reformulated Zagreb index, particularly its upper/lower bounds has attracted recently the attention of many mathematicians and computer scientists (see for example [4,6,11,12,18,23,26]). In this paper we state some new inequalities that set upper and lower bounds of the invariant EM_1. Some of the obtained inequalities are generalization of the results published in the literature.

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2. Preliminaries

In what follows, we outline a few results of spectral graph theory and state a few analytical inequalities that will be needed in the subsequent considerations.

Equality that establishes relation between graph invariants EM_1, M_1, M_2 and $F_1 = \sum_{i=1}^{n} d_i^3$, known as forgotten topological index, was proved in [13,26]. It has been shown that

Lemma 1 ([26]). *let G be a simple graph with n vertices and m edges. Then*

$$EM_1 = F_1 + 4m + 2M_2 - 4M_1. \tag{1}$$

In the same paper the following was proved

Lemma 2 ([26]). *Let G be a graph with order n and size m ($m \geq 1$). Then*

$$EM_1 \leq (n-4)M_1 + 4M_2 - 4m^2 + 4m, \tag{2}$$

with equality if and only if any two non-adjacent vertices have equal degree.

Based on (1) in [12] the following inequality that establishes lower bound of EM_1 in terms of m, M_1 and M_2 was proved.

Lemma 3 ([12]). *Let G be a simple graph with n vertices and m edges. Then*

$$EM_1 \geq \frac{2m}{n}M_1 + 4m + 2M_2 - 4M_1, \tag{3}$$

with equality if and only if G is regular.

In [4] the following result that determines lower bound of EM_1 in terms of m and M_1 was proved.

Lemma 4 ([4]). *Let G be a simple graph with n vertices and m edges. Then*

$$EM_1 \geq \frac{(M_1 - 2m)^2}{m}, \tag{4}$$

with equality if and only if G is regular.

In [2] the following result was proven.

Lemma 5 ([2]). *Let $p_1, p_2, \ldots, p_n$ be non-negative real numbers, and $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ real numbers with the properties*

$$0 < r_1 \leq a_i \leq R_1 < +\infty \quad \text{and} \quad 0 < r_2 \leq b_i \leq R_2 < +\infty,$$

for each $i = 1, 2, \ldots, n$. Furthermore, let S be a subset of $I_n = \{1, 2, \ldots, n\}$ which minimizes the expression

$$\left| \sum_{i \in S} p_i - \frac{1}{2}\sum_{i=1}^{n} p_i \right|. \tag{5}$$

Then

$$\left| \sum_{i=1}^{n} p_i \sum_{i=1}^{n} p_i a_i b_i - \sum_{i=1}^{n} p_i a_i \sum_{i=1}^{n} p_i b_i \right| \leq (R_1 - r_1)(R_2 - r_2) \sum_{i \in S} p_i \left(\sum_{i=1}^{n} p_i - \sum_{i \in S} p_i \right). \tag{6}$$

3. Main results

In the following theorem we prove the inequality that establishes upper bound for EM_1 in terms of m, d_1, d_n, M_1 and M_2.

Theorem 1. *Let G be a simple graph with n ($n \geq 2$) vertices and m edges. Then*

$$EM_1 \leq \frac{M_1^2}{2m} + 4m + 2M_2 - 4M_1 + 2m(d_1 - d_n)^2 \beta(S), \tag{7}$$

where

$$\beta(S) = \frac{1}{2m}\sum_{i \in S} d_i \left(1 - \frac{1}{2m}\sum_{i \in S} d_i \right), \tag{8}$$

and S is a subset of $I_n = \{1, 2, \ldots, n\}$ which minimizes the expression

$$\left| \sum_{i \in S} d_i - m \right|. \tag{9}$$