Communications in Combinatorics and Optimization
Vol. 8, No. 1 (2023), pp. 13-21
DOI: 10.22049/CCO.2021.27159.1205

CCO
Commun. Comb. Optim.

Research Article

Some new bounds on the modified first Zagreb index

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Received: 26 February 2021; Accepted: 11 August 2021
Published Online: 14 August 2021

Abstract: Let G be a graph containing no isolated vertices. For the graph G, its modified first Zagreb index is defined as the sum of reciprocals of squares of vertex degrees of G. This article provides some new bounds on the modified first Zagreb index of G in terms of some other well-known graph invariants of G. From the obtained bounds, several known results follow directly.

Keywords: Zagreb index, modified first Zagreb index, inverse degree, bounds

AMS Subject classification: 05C07, 05C09, 05C92

1. Introduction

Topological indices are numerical quantities of (chemical) graphs which remain the same under graph isomorphism. There exist many topological indices in literature that found chemical applications. More precisely, in chemical graph theory, topological indices may be helpful in understanding the physical, chemical and biological properties of molecular structures [4, 18, 19].

Throughout this paper, we assume that G is a simple graph with the vertex set $V = \{v_1, v_2, \ldots, v_n\}$, the edge set E, and the vertex–degree sequence $(d_1, d_2, \ldots, d_n)$ satisfying $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, where $n \geq 2$, $|E| = m$ and d_i is the

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degree of the vertex v_i, for $i = 1, 2, \dots, n$. If vertices v_i and v_j are adjacent, we write $i \sim j$.

For the graph G, its first Zagreb index [1], appeared in a study of molecular modeling [6], is defined as

$$M_1(G) = \sum_{i=1}^{n} d_i^2 \,.$$

A problem with the first Zagreb index (and with many other well-known topological indices) is that their contributing parts give greater weights to interior vertices and edges, and smaller weights to terminal vertices and edges of a chemical graph. This contradicts the intuitive reasoning that outer atoms and bonds of the corresponding chemical compound should have greater weights than inner atoms and bonds [17] (see also [11]). In order to overcome this problem, the authors of [17] proposed the modified first Zagreb index, which is denoted by ${}^{m}M_1$ and for the graph G, it is defined as

$${}^{m}M_1(G) = \sum_{i=1}^{n} \frac{1}{d_i^2} \,.$$

The present article is concerned about this topological index. Particularly, some new bounds for the modified first Zagreb index of G are derived in terms of order, size, minimum degree, maximum degree, and/or inverse degree of G, where the inverse degree of G is defined as

$$ID(G) = \sum_{i=1}^{n} \frac{1}{d_i} = \sum_{i \sim j} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2} \right) .$$

The inverse degree first attracted attention through conjectures of the computer program Graffiti [3].

2. Preliminaries

In this section, we recall some results on real number sequences and graph theory that will be used in proofs of theorems in the upcoming section.

Lemma 1. [8, 15] *Let $p = (p_i)$, $i = 1, 2, \dots, n$, be a non-negative real number sequence and let $a = (a_i)$, $i = 1, 2, \dots, n$, be a sequence of positive real numbers. For any real number r satisfying $r \le 0$ or $r \ge 1$, it holds that*

$$\left(\sum_{i=1}^{n} p_i \right)^{r-1} \sum_{i=1}^{n} p_i a_i^r \ge \left(\sum_{i=1}^{n} p_i a_i \right)^{r} . \tag{1}$$

When $0 \le r \le 1$, the opposite inequality sign in (1) holds. Also, the equality sign in (1) holds if and only if $r = 0$, or $r = 1$, or $a_1 = a_2 = \cdots = a_n$, or $p_1 = \cdots = p_t = 0$ and $a_{t+1} = \cdots = a_n$, for some t satisfying $1 \le t \le n-1$.

Lemma 2. [13] *Let T be a tree with the vertex-degree sequence $(d_1, d_2, \ldots, d_n)$ satisfying $d_1 \geq d_2 \geq \cdots \geq d_n$, where $n \geq 3$. If*

$$n - 1 \neq d_2 = \cdots = d_{n-2}\,,$$

then $T \cong P_n$ or $T \cong K_{1,n-1}$ and vice versa.

3. Main results

First, we give an upper/lower bound for ${}^mM_1(G)$ in terms of order, size, inverse degree, and minimum/maximum degree of G, respectively, when G is a non-regular graph without isolated vertices.

Theorem 1. *If G is a non-regular graph without isolated vertices, and with order $n \geq 3$, size m, minimum degree δ, maximum degree Δ, and inverse degree $ID(G)$, then*

$${}^mM_1(G) \geq \frac{1}{\Delta}\left(ID(G) + \frac{(\Delta ID(G) - n)^2}{n\Delta - 2m}\right), \tag{2}$$

and

$${}^mM_1(G) \leq \frac{1}{\delta}\left(ID(G) - \frac{(n - \delta ID(G))^2}{2m - n\delta}\right). \tag{3}$$

Equality sign in either of the inequalities (2) and (3) holds if and only if $\Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = \delta$, for some t, $1 \leq t \leq n-2$.

Proof. Let $(d_1, d_2, \ldots, d_n)$ be the vertex-degree sequence of G such that $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$. Then, we have that

$${}^mM_1(G) - \frac{1}{\Delta}ID(G) = \sum_{i=1}^{n} \frac{\Delta - d_i}{\Delta d_i^2}\,, \tag{4}$$

and

$$\frac{1}{\delta}ID(G) - {}^mM_1(G) = \sum_{i=1}^{n} \frac{d_i - \delta}{\delta d_i^2}\,. \tag{5}$$

On the other hand, for $r = 2$, $p_i = 1 - \frac{d_i}{\Delta}$, $a_i = \frac{1}{d_i}$, $i = 1, 2, \ldots, n$, the inequality (1) transforms into

$$\sum_{i=1}^{n}\left(1 - \frac{d_i}{\Delta}\right)\sum_{i=1}^{n}\frac{1}{d_i^2}\left(1 - \frac{d_i}{\Delta}\right) \geq \left(\sum_{i=1}^{n}\frac{1}{d_i}\left(1 - \frac{d_i}{\Delta}\right)\right)^2,$$

that is

$$\left(n - \frac{2m}{\Delta}\right)\sum_{i=1}^{n}\frac{1}{d_i^2}\left(1 - \frac{d_i}{\Delta}\right) \geq \left(ID(G) - \frac{n}{\Delta}\right)^2. \tag{6}$$

Since G is not regular, it holds that $2m \neq n\Delta$, and hence from (6) we have that

$$\sum_{i=1}^{n} \frac{1}{d_i^2}\left(1-\frac{d_i}{\Delta}\right) \geq \frac{(\Delta ID(G)-n)^2}{\Delta(n\Delta-2m)} .$$

From the above inequality and (4), we arrive at (2).
For $r=2$, $p_i=\frac{d_i}{\delta}-1$, $a_i=\frac{1}{d_i}$, $i=1,2,\dots,n$, the inequality (1) becomes

$$\sum_{i=1}^{n}\left(\frac{d_i}{\delta}-1\right)\sum_{i=1}^{n}\frac{1}{d_i^2}\left(\frac{d_i}{\delta}-1\right) \geq \left(\sum_{i=1}^{n}\frac{1}{d_i}\left(\frac{d_i}{\delta}-1\right)\right)^2 ,$$

that is

$$\left(\frac{2m}{\delta}-n\right)\sum_{i=1}^{n}\frac{1}{d_i^2}\left(\frac{d_i}{\delta}-1\right) \geq \left(\frac{n}{\delta}-ID(G)\right)^2 . \tag{7}$$

Since G is not regular, it holds that $2m \neq n\delta$, and hence from (7) we have

$$\sum_{i=1}^{n}\frac{1}{d_i^2}\left(\frac{d_i}{\delta}-1\right) \geq \frac{(n-\delta ID(G))^2}{\delta(2m-n\delta)} .$$

From the above inequality and (5) we obtain (3).
Since G is not regular, equality in any of the inequalities (6) and (7), and consequently in (2) and (3), hold if and only if $\Delta=d_1=\cdots=d_t>d_{t+1}=\cdots=d_n=\delta$, for some t, $1\leq t\leq n-2$. □

Corollary 1. *If G is a graph without isolated vertices, and with order $n\geq 2$, size m, maximum degree Δ, and inverse degree $ID(G)$, then*

$$^{m}M_1(G) \geq \frac{1}{\Delta}\left(ID(G)+\frac{n^2(n\Delta-2m)}{4m^2}\right) \tag{8}$$

with equality if and only if G is regular.

Proof. Let $(d_1,d_2,\dots,d_n)$ be the vertex-degree sequence of G such that $\Delta=d_1\geq d_2\geq\cdots\geq d_n=\delta>0$. Based on the inequality between arithmetic and harmonic means (see e.g. [16]), we have that

$$\sum_{i=1}^{n} d_i \sum_{i=1}^{n}\frac{1}{d_i} \geq n^2 ,$$

that is

$$ID(G) \geq \frac{n^2}{2m} , \tag{9}$$

with equality if and only if G is regular. From (9) and (2) we obtain (8). □

Corollary 2. *If G is a graph without isolated vertices, and with order $n \geq 2$, size m, maximum degree Δ, and minimum degree δ, then*

$$^{m}M_1(G) \geq \frac{n^3}{4m^2} + \frac{1}{\Delta(\Delta+\delta)} \left(\sqrt{\frac{\Delta}{\delta}} - \sqrt{\frac{\delta}{\Delta}} \right)^2 \tag{10}$$

with equality if and only if G is regular.

Proof. In [5], the following bound on the inverse degree $ID(G)$ was proven

$$ID(G) \geq \frac{n^2}{2m} + \frac{1}{\Delta+\delta} \left(\sqrt{\frac{\Delta}{\delta}} - \sqrt{\frac{\delta}{\Delta}} \right)^2 .$$

From the above inequality and (8), we arrive at (10). □

Since $\left(\sqrt{\frac{\Delta}{\delta}} - \sqrt{\frac{\delta}{\Delta}} \right)^2 \geq 0$, from (10) we obtain the following result.

Corollary 3. *Let G be a graph without isolated vertices and with order $n \geq 2$ and size m. Then*

$$^{m}M_1(G) \geq \frac{n^3}{4m^2} \tag{11}$$

with equality if and only if G is regular.

The inequality (11) was also proven in [7].
In the next theorem, we determine a lower bound on $^{m}M_1(G)$ in terms of size, minimum degree, maximum degree, and inverse degree of G, when G has no isolated vertices.

Theorem 2. *If G is a graph without isolated vertices, and with size m, minimum degree δ, maximum degree Δ, and inverse degree $ID(G)$, then*

$$^{m}M_1(G) \geq \frac{1}{\Delta^2} + \frac{1}{\delta^2} + \sqrt{\frac{\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}\right)^3}{2m - \Delta - \delta}} . \tag{12}$$

Equality in (12) holds if and only if $d_2 = d_3 = \cdots = d_{n-1}$.

Proof. For $r = 3$ the inequality (1) can be rewritten as

$$\left(\sum_{i=2}^{n-1} p_i \right)^2 \sum_{i=2}^{n-1} p_i a_i^3 \geq \left(\sum_{i=2}^{n-1} p_i a_i \right)^3 .$$

Let $(d_1, d_2, \ldots, d_n)$ be the vertex-degree sequence of G such that $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$. For $p_i = \frac{1}{d_i^2}$, $a_i = d_i$, $i = 2, \ldots, n-1$, the above inequality becomes

$$\left(\sum_{i=2}^{n-1} \frac{1}{d_i^2} \right)^2 \sum_{i=2}^{n-1} d_i \geq \left(\sum_{i=2}^{n-1} \frac{1}{d_i} \right)^3 , \tag{13}$$

that is

$$\left({}^mM_1(G) - \frac{1}{\Delta^2} - \frac{1}{\delta^2} \right)^2 (2m - \Delta - \delta) \geq \left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta} \right)^3 ,$$

from which (12) is obtained.
Equality in (13), and therefore in (12), holds if and only if $d_2 = d_3 = \cdots = d_{n-1}$. $\square$

Corollary 4. *If G is a graph without isolated vertices, and with order $n \geq 3$, size m, minimum degree δ, and maximum degree Δ, then*

$$ {}^mM_1(G) \geq \frac{1}{\Delta^2} + \frac{1}{\delta^2} + \frac{(n-2)^3}{(2m - \Delta - \delta)^2} . \tag{14}$$

Equality in (14) holds if and only if $d_2 = d_3 = \cdots = d_{n-1}$.

Proof. Let $(d_1, d_2, \ldots, d_n)$ be the vertex-degree sequence of G such that $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$. From the arithmetic–harmonic mean inequality we have that

$$\sum_{i=2}^{n-1} d_i \sum_{i=2}^{n-1} \frac{1}{d_i} \geq (n-2)^2 ,$$

that is

$$ID(G) - \frac{1}{\Delta} - \frac{1}{\delta} \geq \frac{(n-2)^2}{2m - \Delta - \delta} . \tag{15}$$

From (15) and (12), we arrive at (14).
Equality in (15) holds if and only if $d_2 = d_3 = \cdots = d_{n-1}$, which implies that equality in (14) holds if and only if $d_2 = d_3 = \cdots = d_{n-1}$. $\square$

The inequality (15) was proven in [2] (see also [12]).
The proofs of the next two theorems are analogous to that of Theorem 2, hence omitted.

Theorem 3. *If G is a graph without isolated vertices, and with size m, minimum degree δ, maximum degree Δ, and inverse degree $ID(G)$, then*

$$ {}^mM_1(G) \geq \max \left\{ \frac{1}{\Delta^2} + \sqrt{\frac{\left(ID(G) - \frac{1}{\Delta}\right)^3}{2m - \Delta}} , \frac{1}{\delta^2} + \sqrt{\frac{\left(ID(G) - \frac{1}{\delta}\right)^3}{2m - \delta}} \right\} ,$$

with equality if and only if $d_2 = d_3 = \cdots = d_n$.

Theorem 4. *If G is a graph without isolated vertices, and with size m and inverse degree $ID(G)$, then*

$$ {}^{m}M_1(G) \geq \sqrt{\frac{ID(G)^3}{2m}} \,. \tag{16}$$

Equality in (16) holds if and only if G is regular.

Note that the inequality (16) is stronger than (11).
In the next theorem, we determine a lower bound on the modified first Zagreb index of a tree T in terms of order and inverse degree of T.

Theorem 5. *If T is a tree with order $n \geq 3$, maximum degree Δ and inverse degree $ID(T)$, then*

$$ {}^{m}M_1(T) \geq 2 + \frac{1}{\Delta^2} + \sqrt{\frac{\left(ID(T) - 2 - \frac{1}{\Delta}\right)^3}{2n - 4 - \Delta}} \,. \tag{17}$$

Equality in (17) holds if and only if $T \cong P_n$ or $T \cong K_{1,n-1}$.

Proof. By a similar procedure as in case of inequality (12), one obtains the desired inequality:

$$ {}^{m}M_1(T) \geq 2 + \frac{1}{\Delta^2} + \sqrt{\frac{\left(ID(T) - 2 - \frac{1}{\Delta}\right)^3}{2n - 4 - \Delta}} \,,$$

with equality if and only if $d_2 = d_3 = \cdots = d_{n-2}$; which holds if and only if $T \cong P_n$ or $T \cong K_{1,n-1}$, by Lemma 2. □

Corollary 5. *If T is a tree with order $n \geq 3$ and maximum degree Δ then*

$$ {}^{m}M_1(T) \geq 2 + \frac{1}{\Delta^2} + \frac{(n-3)^3}{(2n - 4 - \Delta)^2} \,. \tag{18}$$

Equality in (18) holds if and only if $T \cong P_n$ or $T \cong K_{1,n-1}$.

Proof. In [14], the following bound on the inverse degree $ID(T)$ was proven

$$ ID(T) \geq 2 + \frac{1}{\Delta} + \frac{(n-3)^2}{2n - 4 - \Delta} \,,$$

with equality if and only if $T \cong P_n$ or $T \cong K_{1,n-1}$. From the above inequality and (17) we obtain (18). □

The proof of the next theorem is analogous to that of Theorem 5, and thus omitted.

Theorem 6. *If T is a tree with order $n \geq 3$ and inverse degree $ID(T)$ then*

$$^{m}M_1(T) \geq 2 + \sqrt{\frac{(ID(T)-2)^3}{2(n-2)}}\,. \tag{19}$$

Equality in (19) holds if and only if $T \cong P_n$.

We have the following corollary of the above theorem.

Corollary 6. *If T is a tree with $n \geq 3$ vertices then*

$$^{m}M_1(T) \geq \frac{n+6}{4}\,, \tag{20}$$

with equality if and only if $T \cong P_n$.

Proof. In [9], the following bound on the inverse degree $ID(T)$ was proven

$$ID(T) \geq \frac{n+2}{2}\,,$$

from this inequality and (19), we arrive at (20). □

We remark here that the inequality (20) was proven in [14] (see also [10]).

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