

Research Article

Some new bounds on the first Zagreb indexStefan D. Stankov¹, Marjan M. Matejić¹, Igor Ž. Milovanović^{1,*}, Emina I. Milovanović¹, Şerife Burcu Bozkurt Altındağ²¹Faculty of Electronic Engineering, University of Niš, 18000 Niš, Serbia²Yenikent Kardelen Konutları, Selçuklu, 42070 Konya, Turkey

(Received: 21 September 2021. Received in revised form: 27 October 2021. Accepted: 27 October 2021. Published online: 28 October 2021.)

© 2021 the authors. This is an open access article under the CC BY (International 4.0) license (www.creativecommons.org/licenses/by/4.0/).**Abstract**

In this paper, new inequalities involving the first Zagreb index, inverse degree index and modified first Zagreb index are established. Some new and old bounds on the first Zagreb index are given as corollaries of the obtained inequalities.

Keywords: vertex degree; topological index; first Zagreb index; modified first Zagreb index; inverse degree index.

2020 Mathematics Subject Classification: 05C07, 05C09, 05C92.

1. Introduction

A graph invariant is any property of graphs that depends only on the abstract structure, not on graph representations such as particular labellings or drawings of the considered graph. A graph invariant may be a polynomial (e.g., the characteristic polynomial), a set of numbers (e.g., the spectrum of a graph), or a numerical value. Numerical graph invariants that quantitate topological characteristics of graphs are called topological indices [2]. Topological indices are powerful tools in the description of chemical and other properties of molecules. Topological indices generally characterize both the size and shape of chemical compounds. Over the years, many topological indices were proposed and studied based on degrees, distances and other parameters of graphs.

Let $G = (V, E)$, $V = \{v_1, v_2, \dots, v_n\}$, be a simple connected graph of order $n \geq 2$ and size m . Denote by

$$\Delta = d_1 \geq d_2 \geq \dots \geq d_n = \delta > 0,$$

the vertex degree sequence of G given in a nonincreasing order, where $d_i = d(v_i)$.

The first Zagreb index is the degree-based index introduced in [17] during the study of total π -electron energy of alternant hydrocarbons. It is defined as

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

During the years, the first Zagreb index became one of the most popular and most extensively studied graph-based molecular structure descriptors. More on its applications and mathematical properties can be found in surveys [1, 3, 14, 16, 41].

A generalization of the first Zagreb index, known as zeroth-order Randić index, is defined [20] as

$${}^0R_\alpha(G) = \sum_{i=1}^n d_i^\alpha, \quad {}^0R_0(G) = n,$$

where α is an arbitrary real number. This index can be found in the literature under the name variable first Zagreb index [26], or first general Zagreb index [30]. Some special cases include the inverse degree index [11] obtained for $\alpha = -1$, that is

$$ID(G) = \sum_{i=1}^n \frac{1}{d_i},$$

and the so called modified first Zagreb index [41] (see also [18, 30]) obtained for $\alpha = -2$, that is

$${}^mM_1(G) = \sum_{i=1}^n \frac{1}{d_i^2}.$$

More on $ID(G)$ and its properties can be found in [8, 10, 36].

In this paper, we consider a relationship between $M_1(G)$, $ID(G)$ and ${}^mM_1(G)$. A number of old/new bounds for $M_1(G)$ are obtained as special cases.

*Corresponding author (igor.milovanovic@elfak.ni.ac.rs)

2. Preliminaries

In this section, we recall some results from the literature that will be used in the subsequent considerations.

Lemma 2.1. [23, 38] *Let $p = (p_i)$, $i = 1, 2, \dots, n$, be a sequence of non-negative real numbers and $a = (a_i)$, $i = 1, 2, \dots, n$, sequence of positive real numbers. Then, for any r , $r \leq 0$ or $r \geq 1$, holds*

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

When $0 \leq r \leq 1$ the opposite inequality is valid. Equality holds if and only if either $r = 0$, or $r = 1$, or $a_1 = a_2 = \dots = a_n$, or $p_1 = p_2 = \dots = p_t = 0$ and $a_{t+1} = \dots = a_n$, or $p_{t+1} = \dots = p_n = 0$ and $a_1 = a_2 = \dots = a_t$, for some t , $1 \leq t \leq n-1$.

The inequality (1) is known in the literature as Jensen's inequality. This is only one of many variations of this inequality. For the history of this inequality one can refer to [39] as well as monograph [37].

The next two results refer to lower and upper bound on the first Zagreb index of connected graphs. In [9] (see also [4, 22, 24, 43]) the following lower bound for $M_1(G)$ was determined.

Lemma 2.2. [9] *Let G be a connected graph with $n \geq 2$ vertices and m edges. Then*

$$M_1(G) \geq \frac{4m^2}{n}. \quad (2)$$

Equality holds if and only if G is a regular graph.

In [6] (see also [15, 19, 21, 25, 32]) the following upper bound was obtained.

Lemma 2.3. [6] *Let G be a connected graph with $n \geq 2$ vertices and m edges. Then*

$$M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta. \quad (3)$$

Equality holds if and only if $d_i \in \{\Delta, \delta\}$, for every i , $1 \leq i \leq n$.

Some generalizations of inequalities (2) and (3) can be found in [3, 5, 12, 28, 28, 29, 31, 33, 34, 40].

3. Main results

In the following theorem, we determine a relationship between $M_1(G)$, ${}^m M_1(G)$ and $ID(G)$.

Theorem 3.1. *Let G be a connected graph with $n \geq 3$ vertices and m edges, and let a be an arbitrary real number. If $d_i = a$ for $i = 2, \dots, n-1$, then*

$$M_1(G) = \Delta^2 + \delta^2 + (n-2)a^2.$$

If $d_i \neq a$, for at least one i , $2 \leq i \leq n-1$, then

$$\begin{aligned} M_1(G) \geq & 4am - a^2n + (\Delta - a)^2 + (\delta - a)^2 + \\ & + \frac{\left(a^2 ID(G) - 2an + 2m - \frac{(\Delta - a)^2}{\Delta} - \frac{(\delta - a)^2}{\delta}\right)^2}{mM_1(G)a^2 - 2aID(G) + n - \frac{(\Delta - a)^2}{\Delta^2} - \frac{(\delta - a)^2}{\delta^2}}. \end{aligned} \quad (4)$$

Equality holds if and only if either $d_2 = \dots = d_{n-1} \neq a$, or $a = d_2 = \dots = d_t > d_{t+1} = \dots = d_{n-1}$, or

$$d_2 = \dots = d_t > d_{t+1} = \dots = d_{n-1} = a,$$

for some t , $2 \leq t \leq n-2$.

Proof. The inequality (1) can be considered in the following form

$$\left(\sum_{i=2}^{n-1} p_i\right)^{r-1} \sum_{i=2}^{n-1} p_i a_i^r \geq \left(\sum_{i=2}^{n-1} p_i a_i\right)^r. \quad (5)$$

For $r = 2$, $p_i = \frac{(d_i - a)^2}{d_i^2}$, $a_i = d_i$, $i = 2, \dots, n-1$, the above inequality becomes

$$\sum_{i=2}^{n-1} \frac{(d_i - a)^2}{d_i^2} \sum_{i=2}^{n-1} (d_i - a)^2 \geq \left(\sum_{i=2}^{n-1} \frac{(d_i - a)^2}{d_i}\right)^2. \quad (6)$$

Since

$$\begin{aligned} \sum_{i=2}^{n-1} \frac{(d_i - a)^2}{d_i^2} &= \sum_{i=1}^n \frac{(d_i - a)^2}{d_i^2} - \frac{(\Delta - a)^2}{\Delta^2} - \frac{(\delta - a)^2}{\delta^2} = \\ &= \sum_{i=1}^n \left(\frac{a^2}{d_i^2} - \frac{2a}{d_i} + 1 \right) - \frac{(\Delta - a)^2}{\Delta^2} - \frac{(\delta - a)^2}{\delta^2} = \\ &= {}^m M_1(G) a^2 - 2a ID(G) + n - \frac{(\Delta - a)^2}{\Delta^2} - \frac{(\delta - a)^2}{\delta^2}, \\ \sum_{i=2}^{n-1} (d_i - a)^2 &= \sum_{i=1}^n (d_i - a)^2 - (\Delta - a)^2 - (\delta - a)^2 = \\ &= \sum_{i=1}^n (d_i^2 - 2ad_i + a^2) - (\Delta - a)^2 - (\delta - a)^2 = \\ &= M_1(G) - 4am + a^2 n - (\Delta - a)^2 - (\delta - a)^2, \end{aligned}$$

and

$$\begin{aligned} \sum_{i=2}^{n-1} \frac{(d_i - a)^2}{d_i} &= \sum_{i=1}^n \frac{(d_i - a)^2}{d_i} - \frac{(\Delta - a)^2}{\Delta} - \frac{(\delta - a)^2}{\delta} = \\ &= \sum_{i=1}^n \left(d_i - 2a + \frac{a^2}{d_i} \right) - \frac{(\Delta - a)^2}{\Delta} - \frac{(\delta - a)^2}{\delta} = \\ &= a^2 ID(G) - 2an + 2m - \frac{(\Delta - a)^2}{\Delta} - \frac{(\delta - a)^2}{\delta}, \end{aligned}$$

from the above results and Equation (6) we get

$$\begin{aligned} &\left({}^m M_1(G) a^2 - 2a ID(G) + n - \frac{(\Delta - a)^2}{\Delta^2} - \frac{(\delta - a)^2}{\delta^2} \right) (M_1(G) - 4am + a^2 n - (\Delta - a)^2 - (\delta - a)^2) \geq \\ &\left(a^2 ID(G) - 2an + 2m - \frac{(\Delta - a)^2}{\Delta} - \frac{(\delta - a)^2}{\delta} \right)^2. \end{aligned} \tag{7}$$

If $d_i = a$ for every i , $2 \leq i \leq n-1$, then equality in (7) is attained. If $d_i \neq a$ for at least one i , $2 \leq i \leq n-1$, then

$${}^m M_1(G) a^2 - 2a ID(G) + n - \frac{(\Delta - a)^2}{\Delta^2} - \frac{(\delta - a)^2}{\delta^2} > 0,$$

and from (7) the inequality (4) is obtained.

If $d_i \neq a$ for at least one i , $2 \leq i \leq n-1$, then equality in (7), and consequently in (4), holds if and only if

$$d_2 = \dots = d_{n-1} \neq a,$$

or

$$a = d_2 = \dots = d_t > d_{t+1} = \dots = d_{n-1},$$

or

$$d_2 = \dots = d_t > d_{t+1} = \dots = d_{n-1} = a,$$

for some t , $2 \leq t \leq n-2$. □

For $a = 0$ we get the following corollary of Theorem 3.1.

Corollary 3.1. *Let G be a connected graph with $n \geq 3$ vertices and m edges. Then*

$$M_1(G) \geq \Delta^2 + \delta^2 + \frac{(2m - \Delta - \delta)^2}{n - 2}, \tag{8}$$

with equality if and only if $d_2 = \dots = d_{n-1}$.

The inequality (8) was proven in [5].

For $a = \Delta$ and $a = \delta$, respectively, we get the following corollary of Theorem 3.1.

Corollary 3.2. *Let G be a connected graph with $n \geq 3$ vertices and m edges. If G is not regular, then*

$$M_1(G) \geq (\Delta - \delta)^2 + \max\{A, B\},$$

where

$$A = 4\Delta m - \Delta^2 n + \frac{\left(\Delta^2 ID(G) - 2n\Delta + 2m - \frac{(\Delta-\delta)^2}{\delta}\right)^2}{mM_1(G)\Delta^2 - 2\Delta ID(G) + n - \frac{(\Delta-\delta)^2}{\delta^2}},$$

and

$$B = 4\delta m - \delta^2 n + \frac{\left(\delta^2 ID(G) - 2n\delta + 2m - \frac{(\Delta-\delta)^2}{\Delta}\right)^2}{mM_1(G)\delta^2 - 2\delta ID(G) + n - \frac{(\Delta-\delta)^2}{\Delta^2}}.$$

Equality holds if and only if $\Delta = d_1 = \dots = d_t > d_{t+1} = \dots = d_{n-1}$, for some t , $1 \leq t \leq n-2$, or

$$d_2 = \dots = d_t > d_{t+1} = \dots = d_n = \delta,$$

for some t , $2 \leq t \leq n-1$.

For $a = 1$ we get the following corollary of Theorem 3.1.

Corollary 3.3. *Let G be a connected graph with $n \geq 3$ vertices and m edges. If $G \cong K_{1,n-1}$ then*

$$M_1(G) = n(n-1).$$

If $G \not\cong K_{1,n-1}$, then

$$M_1(G) \geq 4m - n + (\Delta - 1)^2 + (\delta - 1)^2 + \frac{\left(ID(G) - 2n + 2m - \frac{(\Delta-1)^2}{\Delta} - \frac{(\delta-1)^2}{\delta}\right)^2}{mM_1(G) - 2ID(G) + n - \frac{(\Delta-1)^2}{\Delta^2} - \frac{(\delta-1)^2}{\delta^2}}.$$

Equality holds if and only if $d_2 = \dots = d_t > d_{t+1} = \dots = d_n = \delta = 1$, for some t , $2 \leq t \leq n-1$.

For $a = n-1$ we get the following corollary of Theorem 3.1.

Corollary 3.4. *Let G be a connected graph with $n \geq 3$ vertices and m edges. If $G \cong K_n$ then*

$$M_1(G) = n(n-1)^2.$$

If $G \not\cong K_n$, then

$$M_1(G) \geq 4m(n-1) - n(n-1)^2 + (n-1-\Delta)^2 + (n-1-\delta)^2 + \frac{\left((n-1)^2 ID(G) - 2n(n-1) + 2m - \frac{(n-1-\Delta)^2}{\Delta} - \frac{(n-1-\delta)^2}{\delta}\right)^2}{mM_1(G)(n-1)^2 - 2(n-1)ID(G) + n - \frac{(n-1-\Delta)^2}{\Delta^2} - \frac{(n-1-\delta)^2}{\delta^2}}.$$

Equality holds if and only if $d_2 = \dots = d_{n-1} \neq n-1$, or $n-1 = \Delta = d_1 = \dots = d_t > d_{t+1} = \dots = d_{n-1}$, for some t , $1 \leq t \leq n-2$.

The proofs of the next two theorems are analogous to that of Theorem 3.1, hence omitted.

Theorem 3.2. *Let G be a connected graph with $n \geq 3$ vertices and m edges, and let a be an arbitrary real number. If $d_2 = \dots = d_n = a = \delta$, then*

$$M_1(G) = \Delta^2 + (n-1)\delta^2.$$

If $d_i \neq a$, for at least one i , $2 \leq i \leq n$, then

$$M_1(G) \geq 4am - a^2 n + (\Delta - a)^2 + \frac{\left(a^2 ID(G) - 2na + 2m - \frac{(\Delta-a)^2}{\Delta}\right)^2}{mM_1(G)a^2 - 2aID(G) + n - \frac{(\Delta-a)^2}{\Delta^2}}. \quad (9)$$

Equality holds if and only if either $\Delta = d_1 \geq d_2 = \dots = d_n = \delta \neq a$, or $a = d_2 = \dots = d_t > d_{t+1} = \dots = d_n = \delta$, or $d_2 = \dots = d_t > d_{t+1} = \dots = d_n = \delta = a$, for some t , $2 \leq t \leq n-1$.

Theorem 3.3. *Let G be a connected graph with $n \geq 3$ vertices and m edges, and let a be an arbitrary real number. If $d_i = a$ for every i , $1 \leq i \leq n$, then*

$$M_1(G) = n\Delta^2.$$

If $d_i \neq a$ for at least one i , $1 \leq i \leq n$, then

$$M_1(G) \geq 4am - a^2n + \frac{(a^2ID(G) - 2na + 2m)^2}{mM_1(G)a^2 - 2aID(G) + n}. \quad (10)$$

Equality holds if and only if either $d_1 = d_2 = \dots = d_n \neq a$, or $a = \Delta = d_1 = \dots = d_t > d_{t+1} = \dots = d_n = \delta$, or $\Delta = d_1 = \dots = d_t > d_{t+1} = \dots = d_n = \delta = a$, for some t , $1 \leq t \leq n - 1$.

For $a = 0$, we get the following corollary of Theorem 3.2.

Corollary 3.5. *Let G be a connected graph with $n \geq 2$ vertices and m edges. Then*

$$M_1(G) \geq \Delta^2 + \frac{(2m - \Delta)^2}{n - 1}. \quad (11)$$

Equality holds if and only if $d_2 = d_3 = \dots = d_n = \delta$.

The inequality (11) was proven in [7] (see also [40]). Also, for $a = 0$, from (10) the inequality (2) is obtained.

Corollary 3.6. *Let G be a connected graph with $n \geq 2$ vertices and m edges. If G is regular, then*

$$M_1(G) = \frac{4m^2}{n}.$$

If G is not regular, then

$$M_1(G) \geq \frac{4m^2}{n} + \frac{\left(\frac{2m}{n}ID(G) - n\right)^2}{mM_1(G) - \frac{n^3}{4m^2}}. \quad (12)$$

Proof. In [27] it was proven that

$${}^0R_\alpha(G){}^0R_{-\alpha}(G) \geq n^2,$$

where α is an arbitrary real number. For $\alpha = 1$, we get

$$ID(G) \geq \frac{n^2}{2m}, \quad (13)$$

with equality holding if and only if G is regular. Taking $a = \frac{2m}{n}$, from the above and inequality (10) we arrive at (12). \square

A graph G is regular if and only if $d_1 = d_2 = \dots = d_n > 0$. A connected graph is called irregular if it contains at least two vertices with different degrees. In many applications and problems it is of importance to know how much a given graph deviates from being regular, i.e., how great its irregularity is. For this purpose, various quantitative measure of graph irregularity have been proposed.

Remark 3.1. *Denote with $I(G)$ a topological index such that $I(G) \geq 0$ if G is irregular, and $I(G) = 0$ if and only if G is a regular graph (see e.g. [13, 35]). From the inequality (2) an irregularity measure can be defined as [42]*

$$irr_1(G) = M_1(G) - \frac{4m^2}{n}.$$

Similarly, from the inequality (13), one can define an irregularity measure as

$$irr_2(G) = \frac{2m}{n}ID(G) - n.$$

or, from the inequality

$${}^mM_1(G) \geq \frac{n^3}{4m^2},$$

with equality holding if and only if G is regular, the following irregularity measure is defined

$$irr_3(G) = {}^mM_1(G) - \frac{n^3}{4m^2}.$$

The inequality (12) gives a connection between these irregularity measures, that is

$$irr_2(G) \leq \sqrt{irr_1(G)irr_3(G)}.$$

For $a = 1$ and $G \cong U$, where U is an unicyclic graph, we get the following corollary of Theorem 3.3.

Corollary 3.7. *Let U be a connected unicyclic graph with $n \geq 3$ vertices. Then*

$$M_1(U) \geq 3n + \frac{ID(U)^2}{mM_1(U) - 2ID(U) + n}.$$

Equality holds if and only if $U \cong C_n$, or $\Delta = d_1 = \dots = d_t > d_{t+1} = \dots = d_n = 1$, for some t , $3 \leq t \leq n - \Delta$.

For $a = 1$ and G is a tree, i.e. $G \cong T$, we get the following corollary of Theorem 3.3.

Corollary 3.8. *Let T be a tree with $n \geq 3$ vertices. Then*

$$M_1(T) \geq 3n - 4 + \frac{(ID(T) - 2)^2}{mM_1(T) - 2ID(T) + n}.$$

Equality holds if and only if $\Delta = d_1 = \dots = d_t > d_{t+1} = \dots = d_n = 1$, for some t , $1 \leq t \leq n - 1$.

Theorem 3.4. *Let G be a connected graph with $n \geq 3$ vertices and m edges. If $d_i \in \{\Delta, \delta\}$, for every i , $1 \leq i \leq n$, then*

$$M_1(G) = p\Delta^2 + q\delta^2, \quad p + q = n.$$

If $d_i \notin \{\Delta, \delta\}$, for at least one i , $2 \leq i \leq n - 1$, then

$$M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta - \frac{(n(\Delta + \delta) - 2m - \Delta\delta ID(G))^2}{(\Delta + \delta)ID(G) - n - mM_1(G)\Delta\delta}. \tag{14}$$

Equality holds if and only if $\Delta = d_1 = \dots = d_t > d_{t+1} = \dots = d_r > d_{r+1} = \dots = d_n = \delta$, for some t and r , $1 \leq t \leq n - 2$ and $t + 1 \leq r \leq n - 1$.

Proof. For $r = 2$, $p_i = \frac{(\Delta - d_i)(d_i - \delta)}{d_i^2}$, $a_i = d_i$, $i = 2, \dots, n - 1$, the inequality (5) becomes

$$\sum_{i=2}^{n-1} \frac{(\Delta - d_i)(d_i - \delta)}{d_i^2} \sum_{i=2}^{n-1} (\Delta - d_i)(d_i - \delta) \geq \left(\sum_{i=2}^{n-1} \frac{(\Delta - d_i)(d_i - \delta)}{d_i} \right)^2. \tag{15}$$

Since

$$\begin{aligned} \sum_{i=2}^{n-1} \frac{(\Delta - d_i)(d_i - \delta)}{d_i^2} &= \sum_{i=1}^n \frac{(\Delta - d_i)(d_i - \delta)}{d_i^2} = (\Delta + \delta)ID(G) - n - mM_1(G)\Delta\delta, \\ \sum_{i=2}^{n-1} (\Delta - d_i)(d_i - \delta) &= \sum_{i=1}^n (\Delta - d_i)(d_i - \delta) = 2m(\Delta + \delta) - n\Delta\delta - M_1(G), \\ \sum_{i=2}^{n-1} \frac{(\Delta - d_i)(d_i - \delta)}{d_i} &= \sum_{i=1}^n \frac{(\Delta - d_i)(d_i - \delta)}{d_i} = n(\Delta + \delta) - 2m - \Delta\delta ID(G), \end{aligned}$$

from the above results and Equation (15) we get

$$\begin{aligned} ((\Delta + \delta)ID(G) - n - mM_1(G)\Delta\delta) (2m(\Delta + \delta) - n\Delta\delta - M_1(G)) &\geq \\ &\geq (n(\Delta + \delta) - 2m - \Delta\delta ID(G))^2. \end{aligned} \tag{16}$$

If $d_i \in \{\Delta, \delta\}$, for $1 \leq i \leq n$, then in (16) equality is attained. If $d_i \notin \{\Delta, \delta\}$, for at least one i , $2 \leq i \leq n - 1$, then

$$(\Delta + \delta)ID(G) - n - mM_1(G)\Delta\delta > 0,$$

and from (16) we obtain (14).

If $d_i \notin \{\Delta, \delta\}$, for at least one i , $2 \leq i \leq n - 1$, then equality in (16), and consequently in (14), holds if and only if $\Delta = d_1 = \dots = d_t > d_{t+1} = \dots = d_r > d_{r+1} = \dots = d_n = \delta$, for some t and r , $1 \leq t \leq n - 1$ and $t + 1 \leq r \leq n - 1$. \square

If $d_i \notin \{\Delta, \delta\}$, for at least one i , $2 \leq i \leq n - 1$, then inequality (14) is stronger than (3).

When G is a tree we get the following corollary of Theorem 3.4.

Corollary 3.9. *Let T be a tree with $n \geq 3$ vertices. If $d_i \in \{\Delta, 1\}$, for $1 \leq i \leq n$, then*

$$M_1(T) = p\Delta^2 + q, \quad p + q = n.$$

If $d_i \notin \{\Delta, 1\}$, for at least one i , $2 \leq i \leq n - 1$,

$$M_1(T) \leq (n - 2)\Delta + 2(n - 1) - \frac{(n\Delta - n + 2 - \Delta ID(T))^2}{(\Delta + 1)ID(T) - n - mM_1(T)\Delta}.$$

Equality holds if and only if $\Delta = d_1 = \dots = d_t > d_{t+1} = \dots = d_r > d_{r+1} = \dots = d_n = 1$, for some t and r , $1 \leq t \leq n - \Delta - 1$ and $t + 1 \leq r \leq n - \Delta$.

Acknowledgment

This work was supported by the Serbian Ministry for Education, Science and Technological development.

References

- [1] A. Ali, I. Gutman, E. Milovanović, I. Milovanović, Sum of powers of the degrees of graphs: extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **80** (2018) 5–84.
- [2] S. C. Basak, V. R. Magnuson, G. J. Niemi, R. R. Regal, G. D. Veith, Topological indices: their nature, mutual relatedness, and applications, *Math. Model.* **8** (1987) 300–305.
- [3] B. Borovičanin, K. C. Das, B. Furtula, I. Gutman, Bounds for the Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 17–100.
- [4] D. Caen, An upper bound on the sum of squares of degrees in a graph, *Discrete Math.* **185** (1998) 245–248.
- [5] K. C. Das, Sharp bounds for the sum of the squares of a graph, *Kragujevac J. Math.* **25** (2003) 31–49.
- [6] K. C. Das, Maximizing the sum of squares of the degrees of a graph, *Discrete Math.* **285** (2004) 57–66.
- [7] K. C. Das, K. Xu, J. Nam, On Zagreb indices of graphs, *Front. Math. China* **10** (2015) 567–582.
- [8] K. C. Das, K. Xu, J. Wang, On inverse degree and topological indices of graphs, *Filomat* **30** (2016) 2111–2120.
- [9] C. S. Edwards, The largest vertex degree sum for a triangle in a graph, *Bull. London Math. Soc.* **9** (1977) 203–208.
- [10] S. Elumalai, S. M. Hosamani, T. Monsour, M. A. Rostami, More on inverse degree and topological indices of graphs, *Filomat* **32** (2018) 165–178.
- [11] S. Fajtlowicz, On conjectures of Graffiti-II, *Congr. Numer.* **60** (1987) 187–197.
- [12] A. Ghalavand, A. Ashrafi, I. Gutman, New upper and lower bounds for some degree-based graph invariants, *Kragujevac J. Math.* **44** (2020) 181–188.
- [13] I. Gutman, Topological indices and irregularity measures, *Bull. Int. Virtual Inst.* **8** (2018) 469–475.
- [14] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.
- [15] I. Gutman, K. C. Das, B. Furtula, E. Milovanović, I. Milovanović, Generalizations of Szökefalvi Nagy and Chebyshev inequalities with applications in spectral graph theory, *Appl. Math. Comput.* **313** (2017) 235–244.
- [16] I. Gutman, E. Milovanović, I. Milovanović, Beyond the Zagreb indices, *AKCE Int. J. Graph Comb.* **17** (2020) 74–85.
- [17] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.
- [18] J. Hao, Theorems about Zagreb indices and modified Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 659–670.
- [19] S. M. Hosamani, B. Basavangoud, New upper bounds for the first Zagreb index, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 97–101.
- [20] Y. Hu, X. Li, Y. Shi, T. Xu, I. Gutman, On molecular graphs with smallest and greatest zeroth-order general Randić index, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 425–434.
- [21] A. Ilić, M. Ilić, B. Liu, On the upper bounds for the first Zagreb index, *Kragujevac J. Math.* **35** (2011) 173–182.
- [22] A. Ilić, D. Stevanović, On comparing Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 681–687.
- [23] J. L. Jensen, Sur les fonctions convexes et les intégralities entre les valeurs moyennes, *Acta Math.* **30** (1906) 175–193.
- [24] A. K. Kaksari, M. Ghorbani, On the forgotten topological index, *Iranian J. Math. Chem.* **8** (2017) 327–338.
- [25] J. Li, W. C. Shiu, A. Chong, On the Laplacian Estrada index of graph, *Appl. Anal. Discrete Math.* **3** (2009) 147–156.
- [26] X. Li, J. Zhang, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 185–208.
- [27] B. Liu, I. Gutman, On general Randić indices, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 147–154.
- [28] M. Matejić, E. Milovanović, I. Milovanović, R. Khoelilar, A note on the first Zagreb index and coindex of graphs, *Commun. Comb. Optim.* **6** (2021) 41–51.
- [29] M. M. Matejić, P. D. Milošević, E. I. Milovanović, I. Ž. Milovanović, Remark on general zeroth-order Randić and general sum-connectivity indices, *Sci. Publ. State Univ. Novi Pazar, Ser. A: Math. Inform. Mechan.* **11** (2019) 11–20.
- [30] A. Milićević, S. Nikolić, On variable Zagreb indices, *Croat. Chem. Acta* **77** (2004) 97–101.
- [31] P. Milošević, I. Milovanović, E. Milovanović, M. Matejić, Some inequalities for the general zeroth-order Randić index, *Filomat* **33** (2019) 5251–5260.
- [32] E. I. Milovanović, M. M. Matejić, I. Ž. Milovanović, Remark on lower bound for forgotten topological index, *Sci. Publ. State Univ. Novi Pazar, Ser. A: Math. Inform. Mechan.* **9** (2017) 19–24.
- [33] E. I. Milovanović, I. Ž. Milovanović, Sharp bounds for the first Zagreb index and first Zagreb coindex, *Miskolc Math. Notes* **16** (2015) 1017–1024.
- [34] I. Ž. Milovanović, V. M. Čirić, I. Z. Milentijević, E. I. Milovanović, On some spectral, vertex and edge degree-based graph invariants, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 177–188.
- [35] I. Ž. Milovanović, E. I. Milovanović, V. Čirić, N. Jovanović, On some irregularity measures of graphs, *Sci. Publ. State Univ. Novi Pazar, Ser. A: Math. Inform. Mechan.* **8** (2016) 21–34.
- [36] I. Ž. Milovanović, E. I. Milovanović, M. M. Matejić, Some properties of the inverse degree index and coindex, *Filomat*, In press.
- [37] D. S. Mitrinović, J. E. Pečarić, A. M. Fink, *Inequalities Involving Functions and Their Integrals and Derivatives*, Kluwer, Dordrecht, 1991.
- [38] D. S. Mitrinović, J. E. Pečarić, A. M. Fink, *Classical and New Inequalities in Analysis*, Kluwer, Dordrecht, 1993.
- [39] D. S. Mitrinović, P. M. Vasić, The centroid method in inequalities, *Univ. Beograd Publ. Elektrotehn. Fak. Ser. Mat. Fiz.* **498-541** (1975) 3–16.
- [40] T. Monsour, M. A. Rostami, E. Suresh, G. B. A. Xavier, New sharp lower bounds for the first Zagreb index, *Sci. Publ. State Univ. Novi Pazar, Ser. A: Math. Inform. Mechan.* **8** (2016) 11–19.
- [41] S. Nikolić, G. Kovačević, A. Milićević, N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113–124.
- [42] T. Réti, A. Ali, On the variance-type graph irregularity measures, *Commun. Comb. Optim.* **5** (2020) 169–178.
- [43] Y. S. Yoon, J. K. Kim, A relationship between bounds on the sum of squares of degrees of a graph, *J. Appl. Math. Comput.* **21** (2006) 233–238.