Communications in Mathematical and in Computer Chemistry

ISSN 0340 - 6253

Some New Inequalities for the Forgotten Topological Index and Coindex of Graphs

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(Received February 16, 2020)

Abstract

Let G = (V, E), $V = \{v_1, v_2, \ldots, v_n\}$ be a simple connected graph with n vertices, m edges and a sequence of vertex degrees $d_1 \ge d_2 \ge \cdots \ge d_n > 0$, $d_i = d(i)$. If vertices v_i and v_j are adjacent in G we write $i \sim j$, otherwise $i \approx j$. A so called forgotten topological index is defined as $F(G) = \sum_{i=1}^n d_i^3 = \sum_{i \sim j} (d_i^2 + d_j^2)$, and its corresponding coindex as $\overline{F}(G) = \sum_{i \approx j} (d_i^2 + d_j^2)$. Several inequalities involving lower and upper bounds for the F(G) and $\overline{F}(G)$ are derived. Also, relationships between F(G) and $\overline{F}(G)$ and some other topological indices are determined. In addition, a number of results for F(G) and $\overline{F}(G)$ when a graph has tree structure, are obtained.

1 Introduction

A topological index of a graph is a numerical quantity which is invariant under automorphisms of the graph. Topological indices are important and useful tools in mathematical chemistry, nanomaterials, pharmaceutical engineering, etc. used for quantifying information on molecules. Molecules and molecular compounds are modelled as molecular graphs, in which vertices correspond to the atoms and edges to the chemical bonds between them. Hundreds of various topological indices have been introduced in mathematical chemistry literature in order to describe physical and chemical properties of molecules, especially for studying quantitative structure–activity relationships (QSAR) and quantitative structure–property relationships (QSPR) for predicting different properties of chemical compounds (see for example [42–44]). Many of them are defined as simple functions of the degrees of the vertices of (molecular) graph. Various mathematical properties of topological indices have been investigated, as well.

Let G be a simple graph, that is graph without multiple, directed, or weighted edges, and without self-loops, with vertex set V(G) and edge set E(G), where |V(G)| = n and |E(G)| = m. The number of first neighbors of the vertex $v_i \in V(G)$ is its degree, and will be denoted by $d_i = d(v_i)$. Denote by $\Delta = d_1 \ge d_2 \ge \cdots \ge d_n = \delta > 0$ the sequence of vertex degrees of G. The complement of G has the same vertex set V(G), and two vertices are adjacent in \overline{G} if and only if they are not adjacent in G, that is $\overline{G} = (V, \overline{E})$. If vertices v_i and v_j of G are adjacent, we write $i \sim j$. On the other hand, if v_i and v_j are adjacent in \overline{G} , we write $i \approx j$.

The first and second Zagreb indices are vertex-degree-based graph invariants defined as

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

and

$$M_2(G) = \sum_{i \sim j} d_i d_j.$$

The quantity $M_1(G)$ was first time considered in 1972 [20], whereas $M_2(G)$ in 1975 [21]. These terms were recognized to be a measure of the extent of branching of the carbon– atom skeleton of the underlying molecule. The first Zagreb index became one of the most popular and most extensively studied graph-based molecular structure descriptors.

In [20], another quantity, the sum of cubes of vertex degrees

$$F(G) = \sum_{i=1}^{n} d_i^3 = \sum_{i \sim j} (d_i^2 + d_j^2),$$

was encountered, as well. This quantity is also a measure of branching and it was found that its predictive ability is quite similar to that of $M_1(G)$. However, for the unknown reasons, it did not attracted any attention until 2015 when it was reinvented in [15] and named the *forgotten topological index*. In the case of entropy and acentric factor, both $M_1(G)$ and F(G) gain correlation coefficients larger than 0.95 [15]. For other physicochemical properties, neither $M_1(G)$ nor F(G) are satisfactorily correlated. However, its linear combination

$$M_1(G) + \lambda F(G) \tag{1}$$

yields a highly accurate mathematical model of certain physico-chemical properties of alkanes. A significant improvement with the above model was obtained in the case of octanol-water partition coefficient. It is worth noting that the paper [15] was cited more than 300 times so far. More on mathematical properties and chemical applications of the forgotten topological index can be found in [2,4,5,19,23,24,28,31–33,35].

In [38] (see also [9]) it was shown that $M_1(G)$ can be also represented as

$$M_1(G) = \sum_{i \sim j} (d_i + d_j).$$

Inspired by the above identity, in [10] a concept of coindices was introduced. In this case the sum runs over the edges of the complement of G. Thus, the first Zagreb coindex is defined as

$$\overline{M}_1(G) = \sum_{i \approx j} (d_i + d_j),$$

and, analogously, the forgotten topological coindex, or F-coindex, as [16] (see also [8])

$$\overline{F}(G) = \sum_{i \approx j} (d_i^2 + d_j^2) \,.$$

The *F*-coindex has almost the same predictive ability for a chemically relevant property of a non-trivial class of molecules as (1) (see [45]). The authors of [45] use the name Lanzhou index for the *F*-coindex.

It was discovered that the following connection between F-coindex, $M_1(G)$ and F(G) exists [8, 16, 40]

$$\overline{F}(G) = (n-1)M_1(G) - F(G).$$
(2)

Various generalizations of the first Zagreb index have been proposed. In [25] a so called general zeroth–order Randić index was introduced. It is defined as

$${}^{0}\!R_{\alpha}(G) = \sum_{i=1}^{n} d_{i}^{\alpha},$$

where α is an arbitrary real number. It is also met under the names the first general Zagreb index [29] and variable first Zagreb index [31]. More about this topological index can be found in [2, 36].

For specific values of α , specific notations and names are being used. Thus, for $\alpha = -1$, the inverse degree index [13]

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

is obtained.

In this paper we further discuss some properties of the forgotten index and coindex. Considering the fact that obtaining the exact and easy to compute formula for various topological indices is not always possible, it is useful to know approximating expressions. We obtain some inequalities related to the forgotten index and coindex and other graphical parameters. The rest of the paper is organized as follows. In Section 2, we recall some analytical inequalities for real number sequences that are used in the proofs of theorems. Section 3 is devided into three subsections. In Subsections 3.1 and 3.2 several inequalities involving lower and upper bounds for the F(G) and $\overline{F}(G)$ are derived. Also, we establish some relations between the F-index and/or F-coindex and some of the aforementioned indices. As the structures of many molecules are tree like, in Subsection 3.3 we obtain a number of results for forgotten index and coindex when a graph has tree structure.

2 Preliminaries

In this section we recall a couple of analytical inequalities that will be frequently used in proofs of theorems throughout the paper.

Let $p = (p_i)$, i = 1, 2, ..., n, be a sequence of non-negative real numbers, and $a = (a_i)$, i = 1, 2, ..., n, a sequence of positive real numbers. Then for any real $r, r \le 0$ or $r \ge 1$, holds [27] (see also [37])

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

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

Let $x = (x_i)$ and $a = (a_i)$, i = 1, 2, ..., n, be positive real number sequences. Then for all $r, r \ge 0$, holds [41]

$$\sum_{i=1}^{n} \frac{x_i^{r+1}}{a_i^r} \ge \frac{\left(\sum_{i=1}^{n} x_i\right)^{r+1}}{\left(\sum_{i=1}^{n} a_i\right)^r},\tag{4}$$

with equality holding if and only if r = 0 or $\frac{x_1}{a_1} = \frac{x_2}{a_2} = \cdots = \frac{x_n}{a_n}$.

3 Main results

3.1 Bounds for the forgotten topological index

In the next theorem we determine upper bound for F(G) depending on $M_1(G)$ and ID(G).

Theorem 1. Let G be a simple (n, m)-graph without isolated vertices. Then

$$F(G) \le \min\left\{ (\Delta + 3\delta)M_1(G) - 6m\delta(\Delta + \delta) + n\delta^2(\delta + 3\Delta) - \Delta\delta^3 ID(G), \\ (\delta + 3\Delta)M_1(G) - 6m\Delta(\Delta + \delta) + n\Delta^2(\Delta + 3\delta) - \Delta^3\delta ID(G) \right\}.$$
(5)

Equality holds if and only if $\Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_n = \delta$, for some t, $1 \le t \le n-1$.

Proof. For any vertex $v_i \in V(G)$ we have that

$$(\Delta - d_i)(d_i - \delta) \ge 0,$$

that is

$$d_i + \frac{\Delta\delta}{d_i} \le \Delta + \delta. \tag{6}$$

After multiplying the above inequality by $(d_i - \delta)^2$ and summing over i, i = 1, 2, ..., n, we get

$$\sum_{i=1}^n (d_i - \delta)^2 d_i + \Delta \delta \sum_{i=1}^n \frac{(d_i - \delta)^2}{d_i} \le (\Delta + \delta) \sum_{i=1}^n (d_i - \delta)^2,$$

that is

$$F(G) - 2\delta M_1(G) + 2m\delta^2 + \Delta\delta(\delta^2 ID(G) + 2m - 2n\delta) \le (\Delta + \delta)(M_1(G) - 4m\delta + n\delta^2),$$

from which the first inequality in (5) is obtained.

Similarly, after multiplying (6) by $(\Delta - d_i)^2$ and summing over i, i = 1, 2, ..., n, we obtain

$$\sum_{i=1}^{n} (\Delta - d_i)^2 d_i + \Delta \delta \sum_{i=1}^{n} \frac{(\Delta - d_i)^2}{d_i} \le (\Delta + \delta) \sum_{i=1}^{n} (\Delta - d_i)^2,$$

that is

$$F(G) - 2\Delta M_1(G) + 2m\Delta^2 + \Delta\delta(\Delta^2 ID(G) + 2m - 2n\Delta) \le (\Delta + \delta)(M_1(G) - 4m\Delta + n\Delta^2),$$

from which the second inequality in (5) is obtained.

Equality in (6) is attained if and only if $d_i \in \{\delta, \Delta\}$ for every i, i = 1, 2, ..., n, which implies that equality in (5) holds if and only if $\Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_n = \delta$, for some $t, 1 \le t \le n-1$.

Remark 1. After multiplying (6) by the appropriate expressions involving d_i and summing over *i*, like in the case of Theorem 1, many inequalities for different vertex-degree-based topological indices are obtained. We illustrate this with a few examples. For instance,

after multiplying (6) by d_i , $\Delta - d_i$, $d_i - \delta$, d_i^2 , $(\Delta - d_i)d_i$ and $(d_i - \delta)d_i$, respectively, and summing over i, i = 1, 2, ..., n, we get

$$M_{1}(G) \leq 2m(\Delta + \delta) - n\Delta\delta,$$

$$M_{1}(G) \geq \Delta^{2}\delta ID(G) + 2m(\delta + 2\Delta) - n\Delta(\Delta + 2\delta),$$

$$M_{1}(G) \leq \Delta\delta^{2}ID(G) + 2m(2\delta + \Delta) - n\delta(2\Delta + \delta),$$

$$F(G) \leq M_{1}(G)(\Delta + \delta) - 2m\Delta\delta,$$

$$F(G) \geq (2\Delta + \delta)M_{1}(G) + n\Delta^{2}\delta - 2m\Delta(\Delta + 2\delta),$$
(9)

$$F(G) \le (\Delta + 2\delta)M_1(G) + n\Delta\delta^2 - 2m\delta(2\Delta + \delta).$$
(10)

The inequality (7) was proven in [6], while inequalities (9) and (10) in [18, Theorem 2.3]. From (7) and (8), the following inequality follows

$$F(G) \le 2m(\Delta^2 + \Delta\delta + \delta^2) - n\Delta\delta(\Delta + \delta), \tag{11}$$

which was proven in [33].

The inequality (8) was proven in [26] (see also [33]). In [5] it was proven that

$$F(G) \le (\Delta + \delta)M_1(G) - 2m\Delta\delta + \frac{1}{2}(\Delta - \delta)\sum_{i \sim j} |d_i - d_j|,$$

The inequality (8) is stronger than the above one.

The next inequality is a direct consequence of (8)

$$F(G) \leq \frac{M_1(G)^2}{8m} \left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2$$

This inequality was proven in [33] (see also [1]).

Closely related to (8) is the inequality

$$F(G) \le 2(\Delta + \delta)M_1(G) - 4m\Delta\delta - 2M_2(G),$$

which was proven in [14] (see also [11,46]). Its direct consequence is the inequality

$$F(G) \leq \frac{M_1(G)^2}{4m} \left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2 - 2M_2(G),$$

which was proven in [14] (see also [46]). A more general inequality was proven in [32] and [34].

In [12] it was proven that

$$F(G) \le (\Delta + \delta)(M_1(G) - n) + 2m - \Delta\delta(2m - ID(G)).$$

This upper bound for F(G) and the one given by (5) depend on the same parameters. We have performed a number of tests for various classes of graphs and did not find any graph for which the above inequality is stronger than (5).

In the next theorem we prove inequalities which reveal relations between $M_1(G)$ and F(G).

Theorem 2. Let G be a simple (n, m)-graph of size $n \ge 2$. Then

 $((n-1)\Delta - 2m + \delta)(\Delta M_1(G) - F(G) - (\Delta - \delta)\delta^2) \ge ((2m - \delta)\Delta - M_1(G) + \delta^2)^2$ (12) and

$$(2m - \Delta - (n - 1)\delta)(F(G) - \delta M_1(G) - (\Delta - \delta)\Delta^2) \ge (M_1(G) - (2m - \Delta)\delta - \Delta^2)^2.$$
(13)

Equality in (12) holds if and only if $\Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_{n-1} \ge d_n = \delta$, for some $t, 1 \le t \le n-2$. Equality in (13) is attained if and only if $\Delta = d_1 \ge d_2 = \cdots = d_t \ge d_{t+1} = \cdots = d_n = \delta$, for some $t, 2 \le t \le n-1$.

Proof. For r = 2, the inequality (3) can be considered in the following form

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

Now, for $p_i = \Delta - d_i$, $a_i = d_i$, i = 1, 2, ..., n - 1, the above inequality transforms into

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

that is

$$\left(\sum_{i=1}^{n} (\Delta - d_i) - (\Delta - \delta)\right) \left(\sum_{i=1}^{n} (\Delta - d_i)d_i^2 - (\Delta - \delta)\delta^2\right) \\
\geq \left(\sum_{i=1}^{n} (\Delta - d_i)d_i - (\Delta - \delta)\delta\right)^2,$$
(14)

from which we obtain (12).

Similarly, for r = 2 the inequality (3) can be considered as

$$\sum_{i=2}^{n} p_i \sum_{i=2}^{n} p_i a_i^2 \ge \left(\sum_{i=2}^{n} p_i a_i\right)^2.$$

For $p_i = d_i - \delta$, $a_i = d_i$, i = 2, 3, ..., n, this inequality becomes

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

that is

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

from which (13) is obtained.

Equality in (14), and consequently in (12), holds if and only if $\Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_{n-1} \ge d_n = \delta$, for some $t, 1 \le t \le n-2$.

Equality in (15), and, hence, in (13), holds if and only if $\Delta = d_1 \ge d_2 = \cdots = d_t \ge d_{t+1} = \cdots = d_n = \delta$, for some $t, 2 \le t \le n - 1$.

3.2 Bounds for the forgotten topological coindex

In the next theorem we determine a connection between condices $\overline{F}(G)$ and $\overline{M}_1(G)$ and index ID(G).

Theorem 3. Let G be a simple (n, m)-graph, $n \ge 2$, without isolated vertices. Then

$$\overline{F}(G) \le (\Delta + 2\delta)\overline{M}_1(G) + \Delta\delta^2 ((n-1)ID(G) - n) - \delta(2\Delta + \delta)(n(n-1) - 2m).$$
(16)

Equality holds if and only if $\Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_n = \delta$, for some t, $1 \le t \le n-1$.

Proof. After multiplying (6) by $(n - 1 - d_i)(d_i - \delta)$ and summing over i, i = 1, 2, ..., n, we get

$$\sum_{i=1}^{n} (n-1-d_i)(d_i-\delta)d_i + \Delta\delta \sum_{i=1}^{n} \frac{(n-1-d_i)(d_i-\delta)}{d_i} \le (\Delta+\delta) \sum_{i=1}^{n} (n-1-d_i)(d_i-\delta),$$

that is

$$\overline{F}(G) - \delta \overline{M}_1(G) + \Delta \delta (n(n-1) - 2m - \delta(n-1)ID(G) + n\delta) \leq (\Delta + \delta)(\overline{M}_1(G) - \delta(n(n-1) - 2m)),$$

from which (16) is obtained.

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Remark 2. In [19] the following inequality was proved

$$\overline{F}(G) \le (\Delta + \delta)\overline{M}_1(G) - \Delta\delta(n(n-1) - 2m).$$

We have performed a number of tests for various types of graphs, and did not find any graph for which the above inequality is stronger than (16).

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By the similar arguments as in case of Theorem 3, the following result can be proven.

Theorem 4. Let G be a simple (n, m)-graph without isolated vertices. Then

$$\overline{F}(\overline{G}) \le (\Delta + \delta)M_1(\overline{G}) - \Delta\delta((n-1)^2 ID(G) - 2n(n-1) + 2m).$$

Equality holds if and only if $\Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_n = \delta$, for some t, $1 \le t \le n-1$.

In the following theorem we reveal a connection between $\overline{F}(G)$ and ID(G).

Theorem 5. Let G be a simple (n, m)-graph, $n \ge 3$, without isolated vertices. Then

$$\left((n-1)\left(ID(G) - \frac{\Delta + \delta}{\Delta\delta}\right) - n + 2 \right)^2 \left(\overline{F}(G) - (n-1)(\Delta^2 + \delta^2) + \Delta^3 + \delta^3\right)$$

$$\geq ((n-1)(n-2) - 2m + \delta + \Delta)^3.$$
(17)

Equality holds if and only if $\Delta = d_1 \ge d_2 = \cdots = d_{n-1} \ge d_n = \delta$, or $n-1 = \Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_{n-1} \ge d_n = \delta$, for some $t, 1 \le t \le n-2$.

Proof. For r = 3, the inequality (3) can be considered in the following form

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

For $p_i = \frac{n-1-d_i}{d_i}$, $a_i = d_i$, i = 2, 3, ..., n-1, the above inequality transforms into

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

that is

$$\left(\sum_{i=1}^{n} \frac{n-1-d_{i}}{d_{i}} - \frac{n-1-\Delta}{\Delta} - \frac{n-1-\delta}{\delta}\right)^{2} \times \left(\sum_{i=1}^{n} (n-1-d_{i})d_{i}^{2} - (n-1-\Delta)\Delta^{2} - (n-1-\delta)\delta^{2}\right)$$

$$\geq \left(\sum_{i=1}^{n} (n-1-d_{i}) - (n-1-\Delta) - (n-1-\delta)\right)^{3},$$
(18)

from which we obtain (17).

Equality in (18), and consequently in (17), holds if and only if $d_2 = \cdots = d_{n-1}$, or $n-1 = \Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_{n-1} \ge d_n = \delta$, for some $t, 1 \le t \le n-2$.

In the following theorem we establish relationship between topological coindices $\overline{F}(G)$ and $\overline{ID}(G)$. **Theorem 6.** Let G be a simple (n, m)-graph, $n \ge 3$, without isolated vertices. Then

$$\left(\overline{ID}(G) - \frac{n-1-\Delta}{\Delta^2} - \frac{n-1-\delta}{\delta^2}\right) \left(\overline{F}(G) - (n-1-\Delta)\Delta^2 - (n-1-\delta)\delta^2\right)$$

$$\geq (2\overline{m} - 2(n-1) + \Delta + \delta)^2.$$
(19)

Equality holds if and only if $\Delta = d_1 \ge d_2 = \cdots = d_{n-1} \ge d_n = \delta$, or $n-1 = \Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_{n-1} \ge d_n = \delta$, for some $t, 2 \le t \le n-1$.

Proof. For r = 2, the inequality (3) can be considered as

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

Now, for $p_i = \frac{n-1-d_i}{d_i^2}$, $a_i = d_i^2$, i = 2, 3, ..., n-1, the above inequality transforms into

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

that is

$$\left(\sum_{i=1}^{n} \frac{n-1-d_i}{d_i^2} - \frac{n-1-\Delta}{\Delta^2} - \frac{n-1-\delta}{\delta^2}\right) \times \left(\sum_{i=1}^{n} (n-1-d_i)d_i^2 - (n-1-\Delta)\Delta^2 - (n-1-\delta)\delta^2\right)$$
(20)
$$\geq \left(\sum_{i=1}^{n} (n-1-d_i) - (n-1-\Delta) - (n-1-\delta)\right)^2.$$

Since

$$\overline{ID}(G) = \sum_{i \not\sim j} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2} \right) = \sum_{i=1}^n \frac{n-1-d_i}{d_i^2} \quad \text{and} \quad \overline{F}(G) = \sum_{i=1}^n (n-1-d_i)d_i^2,$$

from the above we obtain (19).

Equality in (20), and therefore in (19), holds if and only if $d_2 = \cdots = d_{n-1}$, or $n-1 = \Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_{n-1} \ge d_n = \delta$, for some $t, 2 \le t \le n-1$.

In the following theorem we establish relationship between topological indices F(G)and ID(G) and coindices $\overline{F}(G)$ and $\overline{ID}(G)$.

Theorem 7. Let G be a simple (n, m)-graph without isolated vertices. Then

$$\sqrt{ID(G)F(G)} + \sqrt{\overline{ID}(G)\overline{F}(G)} \ge n(n-1).$$
(21)

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

Proof. Let G be a simple (n, m)-graph such that $d_i \neq 0$ and $d_i \neq n - 1$. Then we have that

$$\overline{ID}(G) = \sum_{i \neq j} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2} \right) = \sum_{i=1}^n \frac{n-1-d_i}{d_i^2} = \sum_{i=1}^n \frac{(n-1-d_i)^2}{(n-1-d_i)d_i^2}.$$
(22)

On the other hand, for r = 1, $x_i = n - 1 - d_i$, $a_i = (n - 1 - d_i)d_i^2$, i = 1, 2, ..., n, the inequality (4) becomes

$$\sum_{i=1}^{n} \frac{(n-1-d_i)^2}{(n-1-d_i)d_i^2} \ge \frac{\left(\sum_{i=1}^{n} (n-1-d_i)\right)^2}{\sum_{i=1}^{n} (n-1-d_i)d_i^2}.$$
(23)

From (22) and (23) we get

$$\overline{ID}(G) \ge \frac{(n(n-1)-2m)^2}{\overline{F}(G)},$$

i.e.

$$\sqrt{\overline{ID}(G)\overline{F}(G)} \ge n(n-1) - 2m.$$
(24)

Further, for r = 2, $p_i = \frac{1}{d_i}$, $a_i = d_i^2$, i = 1, 2, ..., n, the inequality (3) transforms into

$$\sum_{i=1}^{n} \frac{1}{d_i} \sum_{i=1}^{n} d_i^3 \ge \left(\sum_{i=1}^{n} d_i\right)^2,$$

wherefrom it follows

$$\sqrt{ID(G)F(G)} \ge 2m. \tag{25}$$

The inequality (21) is obtained by combining (24) and (25).

Equality in (24) holds if and only if $\frac{1}{d_1^2} = \cdots = \frac{1}{d_n^2}$, $d_i \neq 0$ and $d_i \neq n-1$. Since for $G \cong K_n$ the equality is attained in (21), it follows that equality in (21) holds if and only if G is a regular graph.

In the same manner as in Theorem 7, the following result can be proved.

Theorem 8. Let G be a simple (n,m)-graph without isolated vertices such that \overline{G} is without isolated vertices as well. Then

$$\sqrt{ID(G)F(G)} + \sqrt{ID(\overline{G})F(\overline{G})} \ge n(n-1)$$

and

$$\sqrt{ID(G)\overline{F}(\overline{G})} + \sqrt{ID(\overline{G})\overline{F}(G)} \ge n(n-1).$$

Equalities hold if and only if G is a regular graph.

3.3 Bounds of the forgotten index and coindex for graphs with tree structure

In this section we present results for the forgotten index and coindex when graph G is a tree.

The next theorem establishes bounds for F(T) in terms of order n and maximal vertex degree Δ .

Theorem 9. Let T be a tree with n vertices. If $n \ge 4$, then

$$F(T) \ge \Delta^3 + 2 + \frac{(2(n-2) - \Delta)^3}{(n-3)^2}.$$
(26)

Equality holds if and only if a tree T is such that $\Delta = d_1 \ge d_2 = \cdots = d_{n-2} \ge d_{n-1} = d_n = \delta = 1.$

Proof. For r = 2 the inequality (3) can be considered as

$$\sum_{i=2}^{n-2} p_i \sum_{i=2}^{n-2} p_i a_i^2 \ge \left(\sum_{i=2}^{n-2} p_i a_i\right)^2.$$
(27)

For $p_i = a_i = d_i$, i = 2, 3, ..., n - 2, this inequality becomes

$$\sum_{i=2}^{n-2} d_i \sum_{i=2}^{n-2} d_i^3 \ge \left(\sum_{i=1}^{n-2} d_i^2\right)^2,$$

that is

$$\left(\sum_{i=1}^{n} d_{i} - \Delta - d_{n-1} - \delta\right) \left(\sum_{i=1}^{n} d_{i}^{3} - \Delta^{3} - d_{n-1}^{3} - \delta^{3}\right)$$
$$\geq \left(\sum_{i=1}^{n} d_{i}^{2} - \Delta^{2} - d_{n-1}^{2} - \delta^{2}\right)^{2},$$

from which we get

$$F(G) \ge \Delta^3 + d_{n-1}^3 + \delta^3 + \frac{\left(M_1(G) - \Delta^2 - d_{n-1}^2 - \delta^2\right)^2}{2m - \Delta - d_{n-1} - \delta}.$$
(28)

On the other hand, for $p_i = 1, a_i = d_i, i = 2, 3, ..., n-2$, the inequality (27) becomes

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

wherefrom we obtain

$$M_1(G) \ge \Delta^2 + d_{n-1}^2 + \delta^2 + \frac{(2m - \Delta - d_{n-1} - \delta)^2}{n - 3}.$$
(29)

From (28) and (29) it follows

$$F(G) \ge \Delta^3 + d_{n-1}^3 + \delta^3 + \frac{(2m - \Delta - d_{n-1} - \delta)^3}{(n-3)^2}.$$
(30)

Let $G \cong T$ be a tree with $n \ge 4$ vertices. Since every tree has at least two vertices of degree 1, for m = n - 1, $d_{n-1} = \delta = 1$, from (30) we arrive at (26).

Equality in (29), i.e. in (30), holds if and only if $d_2 = \cdots = d_{n-2}$, which implies that equality in (26) holds if and only if T is a tree with the property $\Delta = d_1 \ge d_2 = \cdots = d_{n-2} \ge d_{n-1} = d_n = \delta = 1$.

Corollary 1. Let T be an arbitrary tree with $n \ge 2$ vertices. Then

$$8n - 14 \le F(T) \le (n - 1)(n^2 - 2n + 2).$$
(31)

Equality in the left-hand side of (31) holds if and only if $T \cong P_n$, whereas in the right-hand side if and only if $T \cong K_{1,n-1}$.

Proof. The function $f(x) = x^3 + 2 + \frac{(2(n-2)-x)^3}{(n-3)^2}$, $n \ge 4$, is an increasing function for $x \ge 2$. Since $\Delta \ge 2$, it follows that $f(\Delta) \ge f(2)$, and from (26) the left-hand side of (31) is obtained.

From (11) we have that

$$F(T) \le 2(n-1) + \Delta(\Delta + 1).$$
 (32)

Now, consider the function g(x) = 2(n-1) + (n-2)x(x+1). It is an increasing function for $x \ge 1$. For $\Delta \le n-1$, we have that $g(\Delta) \le g(n-1)$, and from (32) we get the right-hand side of (31).

The inequalities (31) were proven in [30].

In [17] it was proven that

$$16n - 30 - 2M_2(T) \le F(T) \le n^2(n-1) - 2M_2(T)$$
.

The inequalities (31) are stronger than the above ones.

By the similar arguments as in case of Theorem 9, according to (29) and (7), the following result is obtained.

Theorem 10. Let T be a tree with n vertices. If $n \ge 4$, then

$$M_1(T) \ge \Delta^2 + 2 + \frac{(2(n-2) - \Delta)^2}{n-3}.$$
(33)

If $n \geq 2$, then

$$M_1(T) \le 2(n-1) + (n-2)\Delta.$$
 (34)

Equality in (33) holds if and only if T is a tree with the property $\Delta = d_1 \ge d_2 = \cdots = d_{n-2} \ge d_{n-1} = d_n = \delta = 1$. Equality in (34) is attained if and only if a tree T is such that $\Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_n = \delta = 1$, for some t, $2 \le t \le n-2$.

Remark 3. The inequality (34) is stronger than inequality

$$M_1(T) \le n(n-3) + 2(\Delta + 1),$$

proven in [7].

Corollary 2. Let T be an arbitrary tree with $n \ge 2$ vertices. Then

$$4n - 6 \le M_1(T) \le n(n-1). \tag{35}$$

Equality in the left-hand side of (35) holds if and only if $T \cong P_n$, while in the right-hand side if and only if $T \cong K_{1,n-1}$.

Remark 4. The inequalities (35) were proven in [22] (see also [30]).

Corollary 3. Let T be an arbitrary tree with n vertices. If $n \ge 4$, then

$$F(T) + \overline{F}(T) \ge (n-1)\left(\Delta^2 + 2 + \frac{(2(n-2) - \Delta)^2}{n-3}\right).$$

If $n \geq 2$, then

$$F(T) + \overline{F}(T) \le (n-1)(2(n-1) + (n-2)\Delta)$$

Equality in the first inequality holds if and only if T is a tree such that $\Delta = d_1 \ge d_2 = \cdots = d_{n-2} \ge d_{n-1} = d_n = \delta = 1$. Equality in the second inequality is attained if and only if a tree T is such that $\Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_n = \delta = 1$, for some t, $2 \le t \le n-1$.

Corollary 4. Let T be an arbitrary tree with n vertices. Then

$$2(n-1)(2n-3) \le F(T) + \overline{F}(T) \le n(n-1)^2.$$

Equality in the left-hand side holds if and only if $T \cong P_n$, while in the right-hand side if and only if $T \cong K_{1,n-1}$. -733-

Theorem 11. Let T be an arbitrary tree with n vertices. If $n \ge 4$, then

$$F(\overline{T}) + \overline{F}(\overline{T}) \ge (n-1)\left((n-1)^2(n-4) + \Delta^2 + 2 + \frac{(2(n-2)-\Delta)^2}{n-3}\right).$$
 (36)

If $n \geq 2$, then

$$F(\overline{T}) + \overline{F}(\overline{T}) \le (n-1)((n-1)^2(n-4) + 2(n-1) + (n-2)\Delta).$$
(37)

Equality in (36) holds if and only if a tree T is such that $\Delta = d_1 \ge d_2 = \cdots = d_{n-2} \ge d_{n-1} = d_n = \delta = 1$. Equality in (37) is attained if and only if a tree T has a property $\Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_n = \delta = 1$, for some t, $2 \le t \le n-1$.

Proof. Since [16]

$$F(\overline{T}) + \overline{F}(\overline{T}) = (n-1)M_1(\overline{T})$$

and

$$M_1(\overline{T}) = (n-1)^2(n-4) + M_1(T),$$

we have that

$$F(\overline{T}) + \overline{F}(\overline{T}) = (n-1)((n-1)^2(n-4) + M_1(T)).$$

From the above and (33) and (34), we get (36) and (37).

Corollary 5. Let T be an arbitrary tree with $n \ge 2$ vertices. Then

$$(n-1)(n-2)(n^2-4n+5) \le F(\overline{T}) + \overline{F}(\overline{T}) \le (n-1)^2(n-2)^2.$$

Equality in the left-hand side holds if and only if $T \cong P_n$, and in the right-hand side if and only if $T \cong K_{1,n-1}$.

In what follows we prove inequalities of the Nordhaus–Gaddum type [39] for F(G)and $\overline{F}(G)$ when G has a tree structure.

Theorem 12. Let T be an arbitrary tree with n vertices. If $n \ge 4$, then

$$F(T) + F(\overline{T}) \ge (n-1)\left((n-6)(n-1)^2 + 3\Delta^2 + 6 + \frac{3(2(n-2)-\Delta)^2}{n-3}\right).$$
 (38)

If $n \geq 2$, then

$$F(T) + F(\overline{T}) \le (n-1)((n-6)(n-1)^2 + 6(n-1) + 3(n-2)\Delta).$$
(39)

Equality in (38) holds if and only if tree T is such that $\Delta = d_1 \ge d_2 = \cdots = d_{n-2} \ge d_{n-1} = d_n = \delta = 1$. Equality in (39) is attained if and only if tree T is such that $\Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_n = \delta = 1$, for some t, $1 \le t \le n-2$.

Proof. In [16] (see also [8]) it was proven that

$$F(G) + F(\overline{G}) = (n-1)(n(n-1)^2 - 6m(n-1) + 3M_1(G)),$$

therefore for $G \cong T$ we have that

$$F(T) + F(\overline{T}) = (n-1)((n-6)(n-1)^2 + 3M_1(T)).$$

From the above and (33) and (34) we obtain (38) and (39).

Corollary 6. Let T be an arbitrary tree with $n \ge 2$ vertices. Then

$$(n-1)(n^3 - 8n^2 + 25n - 24) \le F(T) + F(\overline{T}) \le (n-1)^2(n^2 - 4n + 6).$$

Equality in the left-hand side holds if and only if $T \cong P_n$, and in the right-hand side if and only if $T \cong K_{1,n-1}$.

In a similar way, the following results are obtained.

Theorem 13. Let T be an arbitrary tree with n vertices. If $n \ge 2$, then

$$\overline{F}(T) + \overline{F}(\overline{T}) \ge (n-1)(n-2)(2n-2-\Delta).$$
(40)

If $n \geq 4$, then

$$\overline{F}(T) + \overline{F}(\overline{T}) \le (n-1) \left(2(n-1)^2 - \Delta^2 - 2 - \frac{(2(n-2) - \Delta)^2}{n-3} \right).$$
(41)

Equality in (40) is attained if and only if tree T is such that $\Delta = d_1 = \cdots = d_t \ge d_{t+1} = \cdots = d_n = \delta = 1$, for some t, $1 \le t \le n-2$. Equality in (41) holds if and only if tree T is such that $\Delta = d_1 \ge d_2 = \cdots = d_{n-2} \ge d_{n-1} = d_n = \delta = 1$.

Corollary 7. Let T be an arbitrary tree with $n \ge 2$ vertices. Then

$$(n-1)^2(n-2) \le \overline{F}(T) + \overline{F}(\overline{T}) \le 2(n-1)(n-2)^2.$$

Equality in the left-hand side holds if and only if $T \cong K_{1,n-1}$, and in the right-hand side if and only if $T \cong P_n$.

Acknowledgment: This paper was supported by the Serbian Ministry of Education, Science and Technological development.

J. B. Liu was supported by the National Science Foundation of China under Grant No. 11601006.

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