NEW UPPER AND LOWER BOUNDS FOR SOME DEGREE-BASED GRAPH INVARIANTS

A. GHALAVAND, A. ASHRAFI, AND I. GUTMAN

Abstract. For a simple graph $G$ with vertex set $V(G)$ and edge set $E(G)$, let $\deg(u)$ be the degree of the vertex $u \in V(G)$. The forgotten index of $G$ and its coindex are defined as $F(G) = \sum_{v \in V(G)} \deg^3(v)$ and $\overline{F}(G) = \sum_{uv \in E(G)} [\deg(u) + \deg^2(v)]$. New bounds for the first Zagreb index $M_1(G) = \sum_{v \in V(G)} \deg(v)^2$, forgotten index, and its coindex are obtained.

1. Introduction

Throughout this paper, all graphs considered are assumed to be simple, i.e., without directed, weighted, or multiple edges, without self-loops and with a finite number of vertices. Let $G$ be such a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. A graph with $n$ vertices and $m$ edges will be referred to as an $(n, m)$-graph.

By $\deg(v)$ or $\deg_G(v)$ is denoted the degree of the vertex $v \in V(G)$. Let $D(G) = \{\deg(v_1), \deg(v_2), \ldots, \deg(v_n)\}$. If $D(G) = \{r\}$, then $G$ is said to be $r$-regular. If $D(G) = \{r, s\}$, then we say that $G$ is $(r, s)$-biregular. This includes the case of regular graphs if $r = s$. Analogously, if $D(G) = \{r, s, t\}$, then the graph $G$ will be said to be $(r, s, t)$-triregular. Let, in addition, $\Delta = \max_{v \in V(G)} \deg(v)$ and $\delta = \min_{v \in V(G)} \deg(v)$.

The first Zagreb index $M_1(G)$ is defined as [13]

$$M_1 = M_1(G) = \sum_{v \in V(G)} \deg^2(v) = \sum_{uv \in E(G)} [\deg(u) + \deg(v)].$$

It is the oldest and most studied degree-based graph invariant; details of its mathematical theory and chemical applications can be found in the surveys [5, 11, 17].

Key words and phrases. Degree (of vertex), coindex, forgotten index, $F$-index, Zagreb index.

2010 Mathematics Subject Classification. Primary: 05C07. Secondary: 05C90.

Received: March 6, 2018.

Accepted: March 22, 2018.
In the paper [13], $M_1$ was used for designing approximate expressions for total $\pi$-electron energy. In the same paper, also the sum of cubes of vertex degrees ($F$) was used for the same purpose. However, whereas $M_1$ eventually gained much popularity [5,11,17], no attention was paid to $F$. Only more than forty years later, the invariant $F$ attracted some interest, thanks to the discovery of its applicability in physical chemistry [4]. For this reason it was named forgotten index and is defined as [4]:

$$F = F(G) = \sum_{v \in V(G)} \deg(v)^3 = \sum_{uv \in E(G)} [\deg(u)^2 + \deg(v)^2].$$

In the last few years, numerous mathematical studies of the forgotten index have been published, see [1–3,6,7,10,12,16]. Some of pharmacological applications of the $F$-index were also attempted [15].

Both $M_1$ and $F$ are special cases of the so-called first general Zagreb index, defined as

$$M_1^\alpha = M_1^\alpha(G) = \sum_{u \in V(G)} \deg(u)^\alpha = \sum_{uv \in E(G)} [\deg(u)^{\alpha-1} + \deg(v)^{\alpha-1}],$$

where $\alpha$ is an arbitrary real number [15,18].

The coindex of $M_1^\alpha$ is defined as [18]

$$\overline{M}_1^\alpha(G) = \sum_{uv \notin E(G)} [\deg(u)^{\alpha-1} + \deg(v)^{\alpha-1}].$$

The special case of this expressions for $\alpha = 3$ is the coindex of the forgotten index [8,14]

$$\overline{F}(G) = \sum_{uv \notin E(G)} [\deg(u)^2 + \deg(v)^2].$$

2. Main Results

We first state results that improve those reported in [12]. Denote by $\overline{G}$ the complement of the graph $G$.

**Theorem 2.1.** Let $G$ be an $(n,m)$-graph. Then

$$F(G) + F(\overline{G}) = n^4 + M_1(G)(3n - 3) - 2m(3n^2 - 6n + 3) - n(3n^2 - 3n + 1)$$

and

$$F(G) \times F(\overline{G}) = n^4 F(G) + (3n - 3)F(G) M_1(G) - 2m(3n^2 - 6n + 3)F(G) - n(3n^2 - 3n + 1)F(G) - F(G)^2.$$
Proof. By definition of a graph complement, we have
\[ F(G) = \sum_{u \in V(G)} \deg_G(u)^3 = \sum_{u \in V(G)} \left[ n - 1 - \deg_G(u)^3 \right] \]
\[ = \sum_{u \in V(G)} \left[ n^3 + \deg_G(u)^3(3n - 3) - \deg_G(u)(3n^2 - 6n + 3) \right] \]
\[ = -3n^2 + 3n - \deg_G(u)^3 \]
\[ = n^4 + M_1(G)(3n - 3) - 2m(3n^2 - 6n + 3) - n(3n^2 - 3n + 1) - F(G). \]

**Theorem 2.2.** Let \( G \) be an \((n, m)\)-graph. Then
\[ F(G) \leq n\Delta^3 + 3\Delta M_1(G) - 6m\Delta^2 \]
and
\[ F(G) \geq n\delta^3 + 3\delta M_1(G) - 6m\delta^2, \]
with equalities if and only if \( G \) is regular.

**Proof.** Define an auxiliary function \( Y_1(G) = \sum_{u \in V(G)} [\deg(u) - k]^3 \), where \( k \) is a real number. Then,
\[ Y_1(G) = \sum_{u \in V(G)} \left[ \deg(u)^3 - k^3 - 3\deg(u)^2k + 3\deg(u)k^2 \right] \]
\[ = F(G) - nk^3 - 3kM_1(G) + 6mk^2. \]
If \( k = \Delta \), then \( Y_1(G) \leq 0 \) and \( F(G) \leq n\Delta^3 + 3\Delta M_1(G) - 6m\Delta^2 \). For \( k = \delta \), \( Y_1(G) \geq 0 \) and \( F(G) \geq n\delta^3 + 3\delta M_1(G) - 6m\delta^2 \). The equalities hold if and only if \( G \) is regular.

**Theorem 2.3.** Let \( G \) be an \((n, m)\)-graph. Then
\[ F(G) \geq M_1(G)(\delta + 2\Delta) - \Delta^2(2m - n\delta) - 4m\Delta\delta \]
and
\[ F(G) \leq M_1(G)(\Delta + 2\delta) - \delta^2(2m - n\Delta) - 4m\delta\Delta \]
with equalities if and only if \( G \) is \((\Delta, \delta)\)-biregular.

**Proof.** Define \( Y_2(G) = \sum_{u \in V(G)} [\deg(u) - k]^2 [\deg(u) - h] \), where \( k \) and \( h \) are real numbers. Then,
\[ Y_2(G) = \sum_{u \in V(G)} \left[ \deg(u)^2 + k^2 - 2\deg(u)k \right] [\deg(u) - h] \]
\[ = \sum_{u \in V(G)} \left[ \deg(u)^3 - \deg(u)^2h + \deg(u)k^2 - k^2h - 2\deg(u)^2k + 2\deg(u)kh \right] \]
\[ = F(G) - M_1(G)(h + 2k) + k^2(2m - nh) + 4mkh. \]
If \( k = \Delta \) and \( h = \delta \), then \( Y_2(G) \geq 0 \) and \( F(G) \geq M_1(G)(\delta + 2\Delta) - \Delta^2(2m - n\delta) - 4m\Delta\delta \). For \( k = \delta \) and \( h = \Delta \), we have \( Y_2(G) \leq 0 \) and \( F(G) \leq M_1(G)(\Delta + 2\delta) - \delta^2(2m - n\Delta) - 4m\delta\Delta \). The equalities hold if and only if \( G \) is \((\Delta, \delta)\)-biregular.

**Theorem 2.4.** Let \( G \) be an \((n, m)\)-graph. Then \( F(G) \geq 2[M_1(G) + m - n] \). If \( G \) is connected, then equality holds if and only if \( G \cong P_n \) or \( G \cong C_n \).
Proof. Define the auxiliary function \( Y_3(G) = \sum_{u \in V(G)} [\deg(u)^2 - 1][\deg(u) - 2] \) and note that \( Y_3(G) = 0 \) if and only if \( \Delta(G) \leq 2 \). In case of connected graphs, this will occur if either \( G \cong P_n \) or \( G \cong C_n \).

Now,

\[
Y_3(G) = \sum_{u \in V(G)} [\deg(u)^3 - 2\deg(u)^2 - \deg(u) + 2]
= F(G) - 2M_1(G) - 2m + 2n.
\]

Since \( Y_3(G) \geq 0 \), \( F(G) \geq 2[M_1(G) + m - n] \) with equality for connected graphs if and only if \( G \cong P_n \) or \( G \cong C_n \). \( \square \)

**Theorem 2.5.** Let \( G \) be an \((n, m)\)-graphs. Then

\[
F(G) \leq (3\Delta - 3)M_1(G) - 2m(3\Delta^2 - 6\Delta + 2) + n\Delta(\Delta - 1)(\Delta - 2)
\]

and

\[
F(G) \geq (3\delta + 3)M_1(G) - 2m(3\delta^2 + 6\delta + 2) + n\delta(\delta + 1)(\delta + 2).
\]

The equalities holds if and only if \( G \) is \((\delta, \delta + 1, \delta + 2)\)-triregular.

**Proof.** Define \( Y_4(G) = \sum_{u \in V(G)} [\deg(u) - a][\deg(u) - b][\deg(u) - c] \), where \( a \), \( b \), and \( c \) are real numbers. Then,

\[
Y_4(G) = \sum_{u \in V(G)} [\deg(u)^3 - \deg(u)^2(a + b + c) + \deg(u)(ab + ac + bc) - abc]
= F(G) - (a + b + c)M_1(G) + 2m(ab + ac + bc) - nabc.
\]

If \( a = \Delta, b = \Delta - 1 \) and \( c = \Delta - 2 \), then \( Y_4(G) \leq 0 \) and \( F(G) \leq (3\Delta - 3)M_1(G) - 2m(3\Delta^2 - 6\Delta + 2) + n\Delta(\Delta - 1)(\Delta - 2) \). For \( a = \delta, b = \delta + 1 \) and \( c = \delta + 2 \), \( Y_4(G) \geq 0 \) and \( F(G) \geq (3\delta + 3)M_1(G) - 2m(3\delta^2 + 6\delta + 2) + n\delta(\delta + 1)(\delta + 2) \). The equalities hold if and only if \( G \) is \((\delta, \delta + 1, \delta + 2)\)-triregular. \( \square \)

For the sake of completeness, we mention here a result from [18].

**Theorem 2.6.** [18] Let \( G \) be an \((n, m)\)-graph. Then for \( \alpha \geq 1 \),

\[
M_1'^{(\alpha + 1)}(G) = (n - 1)M_1^\alpha(G) - M_1^{\alpha + 1}(G).
\]

**Theorem 2.7.** Let \( G \) be an \((n, m)\)-graph. Then

\[
\overline{F}(G) \geq 2m[2\Delta(n - 1) + 3\Delta^2] - n[(n - 1)\Delta^2 + \Delta^3] - 3\Delta M_1(G).
\]

The equality holds if and only if \( G \) is regular.

**Proof.** Define

\[
Y_5(G) = (n - 1) \sum_{u \in V(G)} [\deg(u) - \Delta]^2 - \sum_{u \in V(G)} [\deg(u) - \Delta]^3.
\]
Then,
\[
Y_5(G) = (n-1) \sum_{u \in V(G)} \left[ \deg(u)^2 + \Delta^2 - 2\deg(u) \right] \\
- \sum_{u \in V(G)} \left[ \deg(u)^3 - \Delta^3 - 3\deg(u)^2 + 3\Delta^2 \deg(u) \right] \\
= (n-1)M_1(G) - F(G) + n \left[ (n-1)\Delta^2 + \Delta^3 \right] \\
- 2m \left[ 2\Delta(n-1) + 3\Delta^2 \right] + 3\Delta M_1(G).
\]

Since \(Y_5(G) \geq 0\), one can see that
\[
(n-1)M_1(G) - F(G) \geq 2m \left[ 2\Delta(n-1) + 3\Delta^2 \right] - n \left[ (n-1)\Delta^2 + \Delta^3 \right] - 3\Delta M_1(G).
\]

The equality holds if and only if \(G\) is a regular graph. Therefore, by Theorem 2.6,
\[
F(G) \geq 2m \left[ 2\Delta(n-1) + 3\Delta^2 \right] - n \left[ (n-1)\Delta^2 + \Delta^3 \right] - 3\Delta M_1(G)
\]
with equality if and only if \(G\) is regular. \(\square\)

**Theorem 2.8.** Let \(G\) be an \((n,m)\)-graph. Then
\[
F(G) \geq 2m \left[ (n-1)(2\Delta - 1) + \Delta^2 + 2\Delta(\Delta - 1) \right] - M_1(G)(3\Delta - 1) \\
- n \left[ (n-1)\Delta(\Delta - 1) + \Delta^2(\Delta - 1) \right].
\]
The equality holds if and only if \(G\) is \((\Delta, \Delta - 1)\)-biregular.

**Proof.** We define the auxiliary function
\[
Y_6(G) = (n-1) \sum_{u \in V(G)} \left[ \deg(u) - \Delta \right] \left[ \deg(u) - (\Delta - 1) \right] \\
- \sum_{u \in V(G)} \left[ \deg(u) - \Delta \right]^2 \left[ \deg(u) - (\Delta - 1) \right].
\]

Then,
\[
Y_6(G) = (n-1) \sum_{u \in V(G)} \left[ \deg(u)^2 - \deg(u)(2\Delta - 1) + \Delta(\Delta - 1) \right] \\
- \sum_{u \in V(G)} \left[ \deg(u)^3 - \deg(u)^2(3\Delta - 1) + \deg(u)\Delta^2 - \Delta^2(\Delta - 1) + 2\deg(u)\Delta(\Delta - 1) \right] \\
= (n-1)M_1(G) - 2m(n-1)(2\Delta - 1) + n(n-1)\Delta(\Delta - 1) \\
- F(G) + M_1(G)(3\Delta - 1) - 2m\Delta^2 + n\Delta^2(\Delta - 1) - 4m\Delta(\Delta - 1) \\
= (n-1)M_1(G) - F(G) - 2m \left[ (n-1)(2\Delta - 1) + \Delta^2 + 2\Delta(\Delta - 1) \right] \\
+ n \left[ (n-1)\Delta(\Delta - 1) + \Delta^2(\Delta - 1) \right] + M_1(G)(3\Delta - 1).
\]
Since \( Y_0(G) \geq 0 \),
\[
(n - 1)M_1(G) - F(G) \geq 2m \left[ (n - 1)(2\Delta - 1) + \Delta^2 + 2\Delta(\Delta - 1) \right] \\
- n \left[ (n - 1)\Delta(\Delta - 1) + \Delta^2(\Delta - 1) \right] - (3\Delta - 1)M_1(G),
\]
with equality if and only if \( G \) is a \((\Delta, \Delta - 1)\)-biregular graph. We now apply Theorem 2.6 to show that
\[
F(G) \geq 2m \left[ (n - 1)(2\Delta - 1) + \Delta^2 + 2\Delta(\Delta - 1) \right] \\
- n \left[ (n - 1)\Delta(\Delta - 1) + \Delta^2(\Delta - 1) \right] - (3\Delta - 1)M_1(G)
\]
with equality if and only if \( G \) is \((\Delta, \Delta - 1)\)-biregular. \(\square\)

**Theorem 2.9.** Let \( G \) be an \((n, m)\)-graph. Then
\[
F(G) \leq 2m \left[ (n - 1)(\delta + \Delta) + \Delta^2 + 2\Delta\delta \right] - n \left[ (n - 1)\Delta\delta + \Delta^2\delta \right] - (\delta + 2\Delta)M_1(G).
\]
The equality holds if and only if \( G \) is \((\Delta, \delta)\)-biregular.

**Proof.** Define the function
\[
Y_\gamma(G) = (n - 1) \sum_{u \in V(G)} [\deg(u) - \Delta] [\deg(u) - \delta] - \sum_{u \in V(G)} [\deg(u) - \Delta]^2 [\deg(u) - \delta].
\]
Then,
\[
Y_\gamma(G) = (n - 1) \sum_{u \in V(G)} [\deg(u)^2 - \deg(u)(\delta + \Delta) + \Delta\delta] \\
- \sum_{u \in V(G)} [\deg(u)^3 - \deg(u)^2(\delta + 2\Delta) + \deg(u)\Delta^2 - \Delta^2\delta + 2\deg(u)\Delta\delta] \\
= (n - 1)M_1(G) - 2m(n - 1)(\delta + \Delta) + n(n - 1)\Delta\delta \\
- F(G) + M_1(G)(\delta + 2\Delta) - 2m\Delta^2 + n\Delta^2\delta - 4m\Delta\delta \\
= (n - 1)M_1(G) - F(G) - 2m \left[ (n - 1)(\delta + \Delta) + \Delta^2 + 2\Delta\delta \right] \\
+ n \left[ (n - 1)\Delta\delta + \Delta^2\delta \right] + (\delta + 2\Delta)M_1(G).
\]
Since \( Y_\gamma(G) \leq 0 \),
\[
(n - 1)M_1(G) - F(G) \leq 2m \left[ (n - 1)(\delta + \Delta) + \Delta^2 + 2\Delta\delta \right] \\
- n \left[ (n - 1)\Delta\delta + \Delta^2\delta \right] - (\delta + 2\Delta)M_1(G),
\]
and the equality holds if and only if \( G \) is a \((\Delta, \delta)\)-biregular graph. We now apply Theorem 2.6 to show that,
\[
F(G) \leq 2m \left[ (n - 1)(\delta + \Delta) + \Delta^2 + 2\Delta\delta \right] - n \left[ (n - 1)\Delta\delta + \Delta^2\delta \right] - (\delta + 2\Delta)M_1(G),
\]
with equality holding if and only if \( G \) is \((\Delta, \delta)\)-biregular. \(\square\)

**Theorem 2.10.** Let \( G \) be an \((n, m)\)-graph. Then the following holds.
(a) \(M_1(G) \leq 2m(\delta + \Delta) - n\Delta\delta\), with equality if and only if \(G\) is \((\Delta, \delta)\)-biregular.
(b) \(M_1(G) \geq 2m(2\Delta - 1) - n\Delta(\Delta - 1)\) and \(M_1(G) \geq 2m(2\delta + 1) - n\delta(\delta + 1)\). The equalities hold if and only if \(G\) is \((\delta, \delta + 1)\)-biregular.
(c) Let \(r\) be a real number. Then \(M_1(G) \geq 4ma - nr^2\), with equality if and only if \(G\) is an \(r\)-regular graph.

**Proof.** Consider the function \(Y_8(G) = \sum_{u \in V(G)} \left[ \deg(u) - a \right] \left[ \deg(u) - b \right]\), where \(a\) and \(b\) are real numbers. Then we have,
\[
Y_8(G) = \sum_{u \in V(G)} \left[ \deg(u)^2 - \deg(u)b - \deg(u)a + ab \right] = M_1(G) - 2m(a + b) + nab.
\]
If \(a = \Delta\) and \(b = \delta\), then \(Y_8(G) \leq 0\) and \(M_1(G) \leq 2m(\delta + \Delta) - n\Delta\delta\). Now the equality holds if and only if \(G\) is a \((\Delta, \delta)\)-biregular graph. This completes the part (a).

Suppose that \(a = \Delta\) and \(b = \Delta - 1\). Then \(Y_8(G) \geq 0\) and \(M_1(G) \geq 2m(2\Delta - 1) - n\Delta(\Delta - 1)\). For \(a = \delta\) and \(b = \delta + 1\), \(Y_8(G) \geq 0\) and \(M_1(G) \geq 2m(2\delta + 1) - n\delta(\delta + 1)\). The equalities hold if and only if \(G\) is \((\delta, \delta + 1)\)-biregular, which completes the proof of part (b).

Finally, assume that \(a = b = r\). Then \(Y_8(G) \geq 0\) and \(M_1(G) \geq 4ma - nr^2\). The equality holds if and only if \(G\) is \(r\)-regular. \(\square\)

**Acknowledgements.** The research of the first two authors was partially supported by the University of Kashan under grant no 364988/111.

**References**

188  A. GHALAVAND, A. ASHRAFI, AND I. GUTMAN


1Department of Pure Mathematics, Faculty of Mathematical Science, University of Kashan, Kashan 87317-51167, I. R. Iran
Email address: ali.ghalavand.kh@gmail.com
Email address: ashrafi@kashanu.ac.ir

2Faculty of Science, University of Kragujevac, 34000 Kragujevac, Serbia
Email address: gutman@kg.ac.rs