Kragujevac Journal of Mathematics
Volume 44(2) (2020), Pages 181–188.

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

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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 $\overline{F}(G) = \sum_{uv\notin E(G)} \left[\deg^2(u) + \deg^2(v)\right]$. New bonds 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 $V(G) = \{v_1, v_2, \dots, v_n\}$ 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 $D(G) = \{\deg(v_1), \deg(v_2), \dots, \deg(v_n)\}$. 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]

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

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 π-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]:

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

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

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

where α is an arbitrary real number [15, 18].

The coindex of M_1^α is defined as [18]

$$\overline{M_1^\alpha}(G) = \sum_{\substack{uv\notin E(G)\\ u\neq v}} \left[\deg(u)^{\alpha-1} + \deg(v)^{\alpha-1}\right].$$

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

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

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

$$\begin{aligned} F(G) \times F(\overline{G}) =& n^4F(G) + (3n-3)F(G)\,M_1(G) - 2m(3n^2-6n+3)F(G) \\ & - n(3n^2-3n+1)F(G) - F(G)^2. \end{aligned}$$

Proof. By definition of a graph complement, we have

$$F(\overline{G}) = \sum_{u\in V(G)} \deg_{\overline{G}}(u)^3 = \sum_{u\in V(G)} \Big[n-1-\deg_G(u)\Big]^3$$
$$= \sum_{u\in V(G)} \Big[n^3 + \deg_G(u)^2(3n-3) - \deg_G(u)(3n^2-6n+3)$$
$$-3n^2+3n-1-\deg_G(u)^3\Big]$$
$$= n^4 + M_1(G)(3n-3) - 2m(3n^2-6n+3) - n(3n^2-3n+1) - F(G). \quad \square$$

Theorem 2.2. *Let G be an (n,m)-graph. Then*

$$F(G) \le n\Delta^3 + 3\Delta M_1(G) - 6m\Delta^2 \text{ and } F(G) \ge n\delta^3 + 3\delta M_1(G) - 6m\delta^2,$$

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,

$$Y_1(G) = \sum_{u\in V(G)} \Big[\deg(u)^3 - k^3 - 3\deg(u)^2k + 3\deg(u)k^2\Big]$$
$$= F(G) - nk^3 - 3kM_1(G) + 6mk^2.$$

If $k=\Delta$, then $Y_1(G)\le 0$ and $F(G) \le n\Delta^3+3\Delta M_1(G)-6m\Delta^2$. For $k=\delta$, $Y_1(G)\ge 0$ and $F(G)\ge n\delta^3+3\delta M_1(G)-6m\delta^2$. The equalities hold if and only if G is regular. $\square$

Theorem 2.3. *Let G be an (n,m)-graph. Then*

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

and

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

with equalities if and only if G is (Δ,δ)-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,

$$Y_2(G) = \sum_{u\in V(G)} \Big[\deg(u)^2 + k^2 - 2\deg(u)k\Big] [\deg(u)-h]$$
$$= \sum_{u\in V(G)} \Big[\deg(u)^3 - \deg(u)^2h + \deg(u)k^2 - k^2h - 2\deg(u)^2k + 2\deg(u)kh\Big]$$
$$= F(G) - M_1(G)(h+2k) + k^2(2m-nh) + 4mkh.$$

If $k=\Delta$ and $h=\delta$, then $Y_2(G)\ge 0$ and $F(G) \ge M_1(G)(\delta+2\Delta) - \Delta^2(2m-n\delta) - 4m\Delta\delta$. For $k=\delta$ and $h=\Delta$, we have $Y_2(G)\le 0$ and $F(G)\le M_1(G)(\Delta+2\delta) - \delta^2(2m-n\Delta) - 4m\delta\Delta$. The equalities hold if and only if G is (Δ,δ)-biregular. $\square$

Theorem 2.4. *Let G be an (n,m)-graph. Then $F(G)\ge 2[M_1(G)+m-n]$. 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,

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

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 $G \cong C_n$. □

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,

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

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. □

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 $\alpha \geq 1$,*

$$\overline{M_1^{\alpha+1}}(G) = (n - 1)M_1^{\alpha}(G) - M_1^{\alpha+1}(G)\,.$$

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,

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

Since $Y_5(G)\geq 0$, one can see that

$$(n-1)M_1(G)-F(G)\geq 2m\Big[2\Delta(n-1)+3\Delta^2\Big]-n\Big[(n-1)\Delta^2+\Delta^3\Big]-3\Delta\, M_1(G).$$

The equality holds if and only if G is a regular graph. Therefore, by Theorem 2.6,

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

with equality if and only if G is regular. □

Theorem 2.8. *Let G be an (n,m)-graph. Then*

$$\begin{aligned}\overline{F}(G)\geq& 2m\left[(n-1)(2\Delta-1)+\Delta^2+2\Delta(\Delta-1)\right]-M_1(G)(3\Delta-1)\\&-n\left[(n-1)\Delta(\Delta-1)+\Delta^2(\Delta-1)\right].\end{aligned}$$

The equality holds if and only if G is $(\Delta,\Delta-1)$-biregular.

Proof. We define the auxiliary function

$$\begin{aligned}Y_6(G) =&(n-1)\sum_{u\in V(G)}\left[\deg(u)-\Delta\right]\left[\deg(u)-(\Delta-1)\right]\\&-\sum_{u\in V(G)}\left[\deg(u)-\Delta\right]^2\left[\deg(u)-(\Delta-1)\right].\end{aligned}$$

Then,

$$\begin{aligned}Y_6(G) =&(n-1)\sum_{u\in V(G)}\Big[\deg(u)^2-\deg(u)(2\Delta-1)+\Delta(\Delta-1)\Big]\\&-\sum_{u\in V(G)}\Big[\deg(u)^3-\deg(u)^2(3\Delta-1)+\deg(u)\Delta^2\\&-\Delta^2(\Delta-1)+2\deg(u)\Delta(\Delta-1)\Big]\\=&(n-1)M_1(G)-2m(n-1)(2\Delta-1)+n(n-1)\Delta(\Delta-1)\\&-F(G)+M_1(G)(3\Delta-1)-2m\Delta^2+n\Delta^2(\Delta-1)-4m\Delta(\Delta-1)\\=&(n-1)M_1(G)-F(G)-2m\left[(n-1)(2\Delta-1)+\Delta^2+2\Delta(\Delta-1)\right]\\&+n\left[(n-1)\Delta(\Delta-1)+\Delta^2(\Delta-1)\right]+M_1(G)(3\Delta-1).\end{aligned}$$

Since $Y_6(G) \geq 0$,

$$(n-1)M_1(G) - F(G) \geq 2m\left[(n-1)(2\Delta-1) + \Delta^2 + 2\Delta(\Delta-1)\right] - n\left[(n-1)\Delta(\Delta-1) + \Delta^2(\Delta-1)\right] - (3\Delta-1)M_1(G),$$

with equality if and only if G is a $(\Delta, \Delta-1)$-biregular graph. We now apply Theorem 2.6 to show that

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

with equality if and only if G is $(\Delta, \Delta-1)$-biregular. □

Theorem 2.9. *Let G be an (n,m)-graph. Then*

$$\overline{F}(G) \leq 2m\left[(n-1)(\delta+\Delta) + \Delta^2 + 2\Delta\delta\right] - n\left[(n-1)\Delta\delta + \Delta^2\delta\right] - (\delta+2\Delta)M_1(G).$$

The equality holds if and only if G is (Δ, δ)-biregular.

Proof. Define the function

$$Y_7(G) = (n-1)\sum_{u\in V(G)}[\deg(u)-\Delta][\deg(u)-\delta] - \sum_{u\in V(G)}[\deg(u)-\Delta]^2[\deg(u)-\delta].$$

Then,

$$\begin{aligned} Y_7(G) =& (n-1)\sum_{u\in V(G)}\left[\deg(u)^2 - \deg(u)(\delta+\Delta) + \Delta\delta\right] \\ &- \sum_{u\in V(G)}\left[\deg(u)^3 - \deg(u)^2(\delta+2\Delta) + \deg(u)\Delta^2 - \Delta^2\delta + 2\deg(u)\Delta\delta\right] \\ =& (n-1)M_1(G) - 2m(n-1)(\delta+\Delta) + n(n-1)\Delta\delta \\ & -F(G) + M_1(G)(\delta+2\Delta) - 2m\Delta^2 + n\Delta^2\delta - 4m\Delta\delta \\ =& (n-1)M_1(G) - F(G) - 2m\left[(n-1)(\delta+\Delta) + \Delta^2 + 2\Delta\delta\right] \\ & + n\left[(n-1)\Delta\delta + \Delta^2\delta\right] + (\delta+2\Delta)M_1(G). \end{aligned}$$

Since $Y_7(G) \leq 0$,

$$(n-1)M_1(G) - F(G) \leq 2m\left[(n-1)(\delta+\Delta) + \Delta^2 + 2\Delta\delta\right] - n\left[(n-1)\Delta\delta + \Delta^2\delta\right] - (\delta+2\Delta)M_1(G),$$

and the equality holds if and only if G is a (Δ, δ)-biregular graph. We now apply Theorem 2.6 to show that,

$$\overline{F}(G) \leq 2m\left[(n-1)(\delta+\Delta) + \Delta^2 + 2\Delta\delta\right] - n\left[(n-1)\Delta\delta + \Delta^2\delta\right] - (\delta+2\Delta)M_1(G),$$

with equality holding if and only if G is (Δ, δ)-biregular. □

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* (Δ, δ)*-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 holds if and only if* G *is* $(\delta, \delta + 1)$*-biregular.*
(c) *Let* r *be a real number. Then* $M_1(G) \geq 4ma - n\,r^2$, *with equality if and only if* G *is an* r*-regular graph.*

Proof. Consider the function $Y_8(G) = \sum_{u \in V(G)} \Big[\deg(u) - a\Big]\Big[\deg(u) - b\Big]$, where a and b are real numbers. Then we have,

$$\begin{aligned} Y_8(G) = & \sum_{u \in V(G)} \Big[\deg(u)^2 - \deg(u)b - \deg(u)a + ab\Big] \\ = & M_1(G) - 2m(a + b) + nab. \end{aligned}$$

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 (Δ, δ)-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 $M_1(G) \geq 4ma - n\,r^2$. The equality holds if and only if G is r-regular. ☐

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

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