Bulletin T.CXLVIII de l'Académie serbe des sciences et des arts − 2015
Classe des Sciences mathématiques et naturelles
Sciences mathématiques, № 40

ON AN OLD/NEW DEGREE–BASED TOPOLOGICAL INDEX

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(Presented at the 3rd Meeting, held on April 24, 2015)

A b s t r a c t. *Let G be a graph with vertex sex $V(G)$ and let $d(x)$ be the degree of the vertex $x \in V(G)$. The graph invariant $F = \sum\limits_{x \in V(G)} d(x)^3$ played some role in a paper published in 1972, but has not attracted any attention until quite recently. In 2014 an unexpected chemical application of the F-index was discovered, which motivated us to establish its basic mathematical properties. Results obtained along these lines are presented.*

AMS Mathematics Subject Classification (2000): 05C07, 92E10, 05C90.

Key Words: F-index, forgotten topological index, degree (of vertex), Zagreb indices, degree–based topological indices.

1. *Introduction*

Let G be a simple graph with n vertices and m edges, with vertex set $V(G)$ and edge set $E(G)$. The edge connecting the vertices x and y will be denoted by xy.

The degree of the vertex x, denoted by $d(x)$, is the number of first neighbors of x in the underlying graph. Since the 1970s, two degree–based graph invariants have been extensively studied. These are the *first Zagreb index* M_1 and the *second Zagreb* *index* M_2 , defined as

$$M_1 = M_1(G) = \sum_{x \in V(G)} d(x)^2, \tag{1.1}$$

$$M_2 = M_2(G) = \sum_{xy \in E(G)} d(x)\, d(y)\,. \tag{1.2}$$

Details on the two Zagreb topological indices, including their history, can be found in the reviews [26, 15, 5] published on the occasion of their 30th anniversary, and in the recent articles [13, 16]. The Zagreb index M_1 was first time encountered in a paper published in 1972 [19] where a series of approximate formulas for total π-electron energy E were deduced. By means of these formulas, several structural details have been identified, on which E depends. Among these was the sum of squares of the vertex degrees of the underlying molecular graph (in [19] denoted by $\Sigma\sigma_1^2$). Eventually, it attracted much attention, has been subject of hundreds of researches, and became traditionally called the *first Zagreb index* and denoted by M_1 (for details see [13]).

In the same paper [19], in the same approximate formulas for E, there was also a term equal to the sum of cubes of the vertex degrees (in [19] denoted by $\Sigma\sigma_1^3$). For reasons not easy to comprehend, this latter term did not attract any attention, and in the next more than 40 years was completely ignored by scholars doing research on degree–based topological indices. Recall that nowadays several dozens of degree–based topological indices are in the focus of interest of mathematicians and mathematical chemists, with a legion of published papers; for details see the books [30, 31, 28] and the surveys [18, 11, 12, 32].

In connection with the preparation of the article [13], we became interested in the "forgotten" topological index

$$F = F(G) = \sum_{x \in V(G)} d(x)^3\,. \tag{1.3}$$

What first had to be decided was if this degree–based graph invariant deserves to be studied at all. Under "deserves" is meant that it has some outstanding application or unexpected mathematical property. After a number of failures, we discovered a remarkable fact that the linear combination $M_1 + \lambda F$ yields a highly accurate mathematical model of certain physico–chemical properties of alkanes [10]. This success encouraged us to search for mathematical properties of the F-index. The present article outlines the main results obtained so far.

2. *Encountering the F-index in previous works*

The claim that between 1972 and 2014, the degree–based topological index F, Eq. (1.3), was completely ignored, needs to be somewhat corrected.

2.1. Measures of irregularity

A graph whose all vertex degrees are mutually equal is said to be regular. If some vertex degrees differ, then the graph is irregular. Several approaches were proposed to measure the irregularity of a graph [17, 1]. Of those based on vertex degrees, the most thoroughly investigated are the Albertson index [2, 9]

$$\sum_{xy \in E(G)} |d(x) - d(y)|$$

and the Bell index [4]

$$\sum_{x \in V(G)} \left(d(x) - \frac{2m}{n} \right)^2 .$$

Interestingly, one of the most obvious such measures, namely

$$IRM(G) := \sum_{xy \in E(G)} \big[d(x) - d(y) \big]^2$$

seems to have been never mentioned in the literature.[1] It is easy to show that

$$IRM(G) = F(G) - 2\, M_2(G)\,. \tag{2.1}$$

2.2. Reformulated Zagreb index

In 2004, Miličević et al. [24] defined the "*reformulated Zagreb indices*" in which vertex degrees were replaced by edge degrees. These are just the ordinary Zagreb indices, Eqs. (1.1), (1.2), of the line graph $L(G)$ of the underlying graph G. It is immediate to show that

$$M_1(L(G)) = \sum_{xy \in E(G)} \big[d(x) + d(y) - 2 \big]^2$$

which leads to

$$M_1(L(G)) = 4m - 2\, M_1(G) + 2\, M_2(G) + F(G)$$

an expression reported in [33].

[1] The quantity IRM was considered by the authors of [17], but was not included into their publication because of the occurrence of the "disturbing" term F in Eq. (2.1).

2.3. Third Zagreb index

In a recent paper [27], several degree–based topological indices were considered, and one of them named "*third Zagreb index*". It was defined as

$$\sum_{xy \in E(G)} \big[d(x)+d(y)\big]^2 .$$

In fact, this quantity is equal to $F(G) + 2\,M_2(G)$.

2.4. Generalized first Zagreb index

Several authors (e.g., [21, 22, 29, 14, 25, 3, 20, 23]) came to the obvious idea to generalize the first Zagreb index, Eq. (1.1), as

$$M_1^{(p)}(G) = \sum_{x \in V(G)} d(x)^p$$

with p being a positive real–number (not necessarily an integer). Evidently, our F-index is the special case of $M_1^{(p)}$ for $p = 3$. Several properties of the generalized first Zagreb index were shown to hold irrespective of the value of the exponent p, thus holding also for the F-index. This, in particular, is the case of graphs (belonging to some specified class, e.g., trees, unicyclic graphs, bicyclic graphs, ...), extremal w.r.t. $M_1^{(p)}$. In what follows, such properties will not be considered.

Let $x \in V(G)$ and let $f(x)$ be any function of the vertex x. Then the following identity is obeyed [7]:

$$\sum_{x \in V(G)} f(x) = \sum_{xy \in E(G)} \left[\frac{f(x)}{d(x)} + \frac{f(y)}{d(y)}\right] . \tag{2.2}$$

Special cases of (2.2) for $f(x) = d(x)^2$ and $f(x) = d(x)^3$ are

$$M_1(G) = \sum_{xy \in E(G)} \big[d(x)+d(y)\big] \tag{2.3}$$

and

$$F(G) = \sum_{xy \in E(G)} \big[d(x)^2+d(y)^2\big] \tag{2.4}$$

and these relations will be frequently used in the subsequent considerations.

3. *Coindices*

In 2006, bearing in mind Eqs. (1.2) and (2.3), Došlić [6] put forward the concept of first and second Zagreb coindices, defined as

$$\overline{M}_1 = \overline{M}_1(G) = \sum_{xy \notin E(G)} \big[d(x) + d(y)\big] \tag{3.1}$$

and

$$\overline{M}_2 = \overline{M}_2(G) = \sum_{xy \notin E(G)} d(x)\, d(y) \tag{3.2}$$

respectively. In formulas (3.1) and (3.2) it is assumed that $x \neq y$.

The Zagreb coindices of a graph G and of its complement $\overline{G}$ can be expressed in terms of the Zagreb indices of G. The respective formulas are collected in the survey [16].

In full analogy with Eqs. (3.1) and (3.2), relying on Eq. (2.4), we can now define the F-coindex as

$$\overline{F}(G) = \sum_{xy \notin E(G)} \big[d(x)^2 + d(y)^2\big]\,. \tag{3.3}$$

Theorem 3.1. *Let G be a graph with n vertices and m edges. Let $\overline{G}$ be the complement of G. Then*

$$F(\overline{G}) = n(n-1)^3 - 6m(n-1)^2 + 3(n-1)\, M_1(G) - F(G), \tag{3.4}$$

$$\overline{F}(G) = (n-1)\, M_1(G) - F(G), \tag{3.5}$$

$$\overline{F}(\overline{G}) = 2m(n-1)^2 - 2(n-1)\, M_1(G) + F(G)\,. \tag{3.6}$$

PROOF. If the degree of the vertex x in G is d, then the degree of the same vertex in $\overline{G}$ is $n-1-d$. Bearing this in mind, from Eq. (1.3) we get

$$\begin{aligned} F(\overline{G}) &= \sum_{x \in V(G)} \big[n-1-d(x)\big]^3 \\ &= \sum_{x \in V(G)} \big[(n-1)^3 - 3(n-1)^2\, d(x) + 3(n-1)\, d(x)^2 - d(x)^3\big] \end{aligned}$$

and Eq. (3.4) follows from (1.1), (1.3), and the fact the the sum of vertex degrees is equal to $2m$.

Denote for brevity $d(x)^2 + d(y)^2$ by $\gamma_{x,y}$. Then in view of Eqs. (2.4), (3.3), and (1.1),

$$\begin{aligned}\sum_{x\in V}\sum_{y\in V} F(x,y) &= \sum_{xy\in E}\gamma_{x,y} + \sum_{xy\notin E}\gamma_{x,y} + \sum_{x\in V}\gamma_{x,x} \\ &= F(G) + \overline{F}(G) + 2\,M_1(G)\,.\end{aligned}$$

On the other hand,

$$\sum_{x\in V}\sum_{y\in V}\left[d(x)^2 + d(y)^2\right] = n\sum_{x\in V} d(x)^2 + n\sum_{y\in V} d(y)^2 = 2n\,M_1(G)\,.$$

Therefore,

$$F(G) + \overline{F}(G) + 2\,M_1(G) = 2n\,M_1(G)$$

and Eq. (3.5) follows.

In order to arrive at the Eq. (3.6), combine (3.4) and (3.5). By (3.5),

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

whereas $F(\overline{G})$ can be expressed by means of (3.4). Eq. (3.6) is then obtained by using the following relation

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

from [16].

Remark 3.1. In [16] it was proven that $\overline{M}_1(\overline{G}) = \overline{M}_1(G)$. From Theorem 3.1 we see that an analogous identity for the forgotten topological index, namely $\overline{F}(\overline{G}) = \overline{F}(G)$, does not hold.

4. *Identities for the F-index*

Using the same notation as in [13], we denote by $\sigma_G(H)$ the number of distinct subgraphs of the graph G that are isomorphic to H. In particular, we are interested in $\sigma_G(S_3)$ and $\sigma_G(S_4)$, where S_n stands for the n-vertex star.

Theorem 4.1. *Let G be a graph with n vertices and m edges, and let $\sigma_G(S_3)$ and $\sigma_G(S_4)$ be as specified above. Then*

$$F(G) = 6\,\sigma_G(S_3) + 6\,\sigma_G(S_4) + 2m. \tag{4.1}$$

PROOF. Note that

$$\sigma_G(S_p) = \sum_{x \in V(G)} \binom{d(x)}{p-1},$$

which implies

$$\sigma_G(S_3) = \sum_{x \in V(G)} \binom{d(x)}{2} = \frac{1}{2}\big[M_1(G) - 2m\big]$$

$$\sigma_G(S_4) = \sum_{x \in V(G)} \binom{d(x)}{3} = \frac{1}{6}\big[F(G) - 3\,M_1(G) + 4m\big]\,.$$

Therefore,

$$\sigma_G(S_3) + \sigma_G(S_4) = \frac{1}{6}\,F(G) - \frac{1}{3}\,m,$$

which directly leads to Eq. (4.1).

Theorem 4.2. *Let G be a graph with n vertices and m edges. Then*

$$F(G) = \sum_{xy \in E(G)} \big[d(x) - d(y)\big]^2 + 2\,M_2(G)\,. \tag{4.2}$$

If, in addition, the graph G is triangle–free, then

$$F(G) = \sum_{xy \in E(G)} \big[d(x) - d(y)\big]^2 - 2\,M_1(G) + 4m + \sum_{i=1}\sum_{j=1} \big(\mathbf{A}^3\big)_{ij}, \tag{4.3}$$

where $\mathbf{A}$ is the adjacency matrix of G.

PROOF. Eq. (4.2) is a straightforward consequence of (1.2) and (2.4) and Eq. (4.3) is obtained from (4.2) by substituting into it the result of Lemma 4.1.

Lemma 4.1. *Let G be a triangle–free graph of order n and let $\mathbf{A}$ be its adjacency matrix. Then*

$$\sum_{i=1}^{n}\sum_{j=1}^{n} \big(\mathbf{A}^3\big)_{ij} = 2\,M_1(G) + 2\,M_2(G) - 4m\,. \tag{4.4}$$

PROOF. Let x and y be adjacent vertices of the graph G and xy the edge connecting them.

As well known, $\big(\mathbf{A}^3\big)_{ij}$ is equal to the number of walks of length 3 in the graph G, starting at vertex i and ending at vertex j. We first determine the number of walks of length 3, which go over the edge xy.

For the sake of brevity, denote $d(x)-1$ and $d(y)-1$ by p and q, respectively. Let the first neighbors of the vertex x be y and $x_1, x_2, \ldots, x_p$. Let the first neighbors of the vertex y be x and $y_1, y_2, \ldots, y_q$. Because G is triangle–free, the vertices $x_1, x_2, \ldots, x_p, y_1, y_2, \ldots, y_q$ are distinct.

The walks of length 3 that go over the edge xy can be classified as indicated in the following table:

type			count
$x_i x y y_j$	&	$y_j y x x_i$	$pq+pq$
$x_i x y x$	&	$x y x x_i$	$p+p$
$y_j y x y$	&	$y x y y_j$	$q+q$
$x x_i x y$	&	$y y_j y x$	$p+q$
$x y x x_i$	&	$y x y y_j$	$p+q$
$xyxyx$	&	$yxyxy$	$1+1$

Thus, the total count of such walks is

$$\begin{aligned}
(pq+pq) &+ (p+p)+(q+q)+(p+q)+(p+q)+(1+1) \\
&= 2pq+4(p+q)+2 \\
&= 2\big[d(x)-1\big]\big[d(y)-1\big]+4\big[d(x)+d(y)-2\big]+2 \\
&= 2d(x)\,d(y)+2\big[d(x)+d(y)\big]-4,
\end{aligned}$$

which after summation over all edges of G and by taking into account Eqs. (1.2) and (2.3) yields the relation (4.4).

5. *Bounds for the F-index*

In [10], the following bounds for the forgotten topological index were established:[2]

$$F(G) \geq \frac{1}{2m}\,M_1(G), \tag{5.1}$$

$$F(G) \geq \frac{1}{m}\,M_1(G)^2 - 2\,M_2(G), \tag{5.2}$$

$$F(G) \leq 2\,M_2(G) + m(n-1)^2\,. \tag{5.3}$$

Equality in (5.1) and (5.2) is attained if and only if the graph G is regular. Equality in (5.3) holds if and only if $G \cong S_n$.

[2] In [10], there is a printing error in the proof and formulation of inequality (5.3).

An improvement of (5.1), namely

$$F(G) \geq \frac{2m}{n} M_1(G) \tag{5.4}$$

is obtained from (1.3), by using the Chebyshev inequality:

$$\sum_{x \in V(G)} d(x)^3 = \sum_{x \in V(G)} d(x)\, d(x)^2 \geq \frac{1}{n} \left(\sum_{x \in V(G)} d(x) \right) \left(\sum_{x \in V(G)} d(x)^2 \right).$$

Equality in (5.4) holds also for regular graphs.

Elphic and Réti [8] have recently shown that $M_2 \leq m(2m-n+1)$. By combining this result with (5.3), we get

$$F(G) \leq m(n^2 - 6n + 4m + 6)$$

with equality if $G \cong S_n$.

Let δ and Δ be the smallest and greatest degree of the graph G. From another inequality in [8], namely $M_2 \leq m\big[2m - n + 1 - (\delta - 1)(n - 1 - \Delta)\big]$, we get

$$F(G) \leq m\big[(n-2)^2 + 4m - 2(\delta - 1)(n - 1 - \Delta)\big]$$

with equality if $G \cong S_n$.

Let $a_1, a_2, \ldots, a_n$ be non-negative real numbers, such that

$$a_1 + a_2 + \cdots + a_n = 1.$$

Then according to a result by Motzkin and Straus [25], for any graph G of order n and clique number ω,

$$\sum_{ij \in E(G)} a_i\, a_j \leq \frac{\omega - 1}{2\omega}\,. \tag{5.5}$$

If we set $a_i = d(i)^2 / M_1(G)$, $i = 1, 2, \ldots, n$, then the conditions required by the Motzkin–Straus theorem are satisfied. Starting with Eq. (2.4), we have

$$\begin{aligned}
F(G) &= \sum_{ij \in E(G)} \left[d(i)^2 + d(j)^2\right] \\
&= M_1(G) \sum_{ij \in E(G)} \left[a_i + a_j\right] \\
&= M_1(G) \sum_{ij \in E(G)} a_i\, a_j \left[\frac{1}{a_i} + \frac{1}{a_j}\right] \\
&= M_1(G)^2 \sum_{ij \in E(G)} a_i\, a_j \left[\frac{1}{d(i)^2} + \frac{1}{d(j)^2}\right] \\
&\leq 2\, M_1(G)^2 \sum_{ij \in E(G)} a_i\, a_j
\end{aligned}$$

which by the Motzkin–Straus inequality (5.5) yields

$$F(G) \leq \frac{\omega - 1}{\omega}\, M_1(G)^2\,.$$

For triangle–free graphs, $\omega = 2$, and then

$$F(G) \leq \frac{1}{2}\, M_1(G)^2\,.$$

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