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Abstract

The two Zagreb indices $M_1 = \sum_v d(v)^2$ and $M_2 = \sum_{uv} d(u)\,d(v)$ are vertex-degree-based graph invariants that have been introduced in the 1970s and extensively studied ever since. In the last few years, a variety of modifications of M_1 and M_2 were put forward. The present survey of these modified Zagreb indices outlines their main mathematical properties, and provides an exhaustive bibliography.

Keywords: Degree (of vertex); Zagreb index; Vertex-degree-based graph invariants; Zagreb-type indices

Contents

1. Introduction

In this paper we are concerned with simple graphs, that is graphs without multiple, directed, or weighted edges, and without self-loops. Let G be such a graph with vertex set $V(G)$ and edge set $E(G)$. Let $|V(G)| = n$ and $|E(G)| = m$.

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If two vertices u and v of the graph G are adjacent, then the edge connecting them will be denoted by uv.

The number of first neighbors of the vertex $u \in V(G)$ is its degree, and will be denoted by $d(u)$.

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

$$M_1 = M_1(G) = \sum_{u \in V(G)} d(u)^2 \tag{1}$$

and

$$M_2 = M_2(G) = \sum_{uv \in E(G)} d(u)\, d(v)\,. \tag{2}$$

The quantity M_1 was first time considered in 1972 [1], whereas M_2 in 1975 [2]. These were named *Zagreb group indices* [3] (in view of the fact that the authors of [1,2] were members of the "Rudjer Bošković" Institute in Zagreb, Croatia). Eventually, the name was shortened into *first Zagreb index* and *second Zagreb index* [4].

An alternative expression for the first Zagreb index is [5]

$$M_1 = \sum_{uv \in E(G)} \big[d(u) + d(v)\big]\,, \tag{3}$$

which happens to be a special case of a more general identity [6]

$$\sum_{u \in V(G)} \gamma(d(u)) = \sum_{uv \in E(G)} \left[\frac{\gamma(d(u))}{d(u)} + \frac{\gamma(d(v))}{d(v)}\right]$$

which is valid for any function $\gamma(x)$, defined for $x = d(u)\,,\ u \in V(G)$.

Let $d(uv)$ be the degree of the edge uv, equal to the number of edges that are incident to uv. It is immediate that $d(uv) = d(u) + d(v) - 2$, and thus by Eq. (3),

$$\sum_{uv \in E(G)} d(uv) = M_1(G) - 2m$$

i.e.,

$$M_1 = \sum_{uv \in E(G)} \big[d(uv) + 2\big]\,. \tag{4}$$

Accordingly, the first Zagreb index can be considered as edge-degree-based topological index as well.

The two Zagreb indices attracted much interest and a plethora of their mathematical properties and chemical applications were reported. As an illustration of how extensive these studies have been, and still are, we mention that the articles [1] and [2] are quoted in (at least) 54 and 70 books, which means well over 1000 times in published papers.

Details of the theory and applications of the two Zagreb indices can be found in several surveys [7–13] and in the references quoted therein.

After most of the results on Zagreb indices were established, the inevitable occurred: Their various modifications have been proposed, thus opening the possibility to do analogous research and publish numerous additional papers. In what follows, we outline the main directions of scholarly activities along these lines.

2. General Zagreb indices

The most direct and most straightforward modification of the Zagreb-index-concept is to introduce in their definition a variable parameter:

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

and

$$M_2^{(\alpha)} = \sum_{uv \in E(G)} \big[d(u)\, d(v)\big]^\alpha,$$

where α is a real number. These generalizations of the Zagreb indices seem to be first considered by Li et al. [14,15], and then followed by countless other publications. $M_1^{(\alpha)}$ and $M_2^{(\alpha)}$ are called *general Zagreb indices* (see e.g., [16–19])

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or *variable Zagreb indices* (see e.g., [20–23]). In addition, $M_1^{(\alpha)}$ is also studied under the name *zeroth-order general Randić index* (see e.g., [24–26]), whereas $M_2^{(\alpha)}$ under the name *general Randić index* (see e.g., [27–29]).

Based on (3) and (4), in [30] the following generalization of the first Zagreb index was introduced

$$H_\alpha = H_\alpha(G) = \sum_{uv\in E(g)} \big[d(u)+d(v)\big]^\alpha = \sum_{uv\in E(G)} \big[d(uv)+2\big]^\alpha, \qquad \alpha \in R$$

under the name *general sum-connectivity index*.

Let $\Delta = \max_{u\in V(G)}\{d(u)\}$, $\delta = \min_{u\in V(G)}\{d(u)\}$, $\Delta_{e_1} = \max_{uv\in E(G)}\{d(uv)+2\}$ and $\delta_{e_1} = \min_{uv\in E(G)}$ $\{d(uv)+2\}$. Then the following inequalities for $M_1^{(\alpha)}$ and H_α are valid (see for example [31–33])

$$M_1^{(\alpha+1)} - \big(\Delta+\delta\big)M_1^{(\alpha)} + \Delta\delta M_1^{(\alpha-1)} \le 0\,,$$
$$H_{\alpha+1} - \big(\Delta_{e_1}+\delta_{e_1}\big)H_\alpha + \Delta_{e_1}\delta_{e_1}H_{\alpha-1} \le 0\,,$$
$$M_1^{(\alpha+1)} \ge \frac{M_1^\alpha}{(2m)^{\alpha-1}}\,, \qquad \alpha \le 0 \text{ or } \alpha \ge 1\,,$$
$$H_{\alpha+1} \ge \frac{\big(F+2M_2\big)^\alpha}{M_1^{\alpha-1}}\,, \qquad \alpha \le 0 \text{ or } \alpha \ge 1\,,$$

where F is the forgotten index defined as

$$F = \sum_{u\in V(G)} d(u)^3.$$

When $0 \le \alpha \le 1$, the sense of the last two inequalities reverses. These inequalities are general and by the appropriate choice of parameter α upper and lower bounds for a number of Zagreb type topological indices can be obtained.

It happens occasionally, that author(s) propose a new topological index and that it turns out to be already defined under a different name. Thus, for example, in [34] the authors defined a new index, named general harmonic index, H_α^*, as

$$H_\alpha^* = H_\alpha^*(G) = \sum_{uv\in E(G)} \left[\frac{2}{d(u)+d(v)}\right]^\alpha.$$

However, since

$$H_\alpha^* = 2^\alpha H_{-\alpha}$$

this obviously is not a new topological index.

Similarly, in [35] a so called Re-defined version of Zagreb indices, $ReZG_1$, $ReZG_2$,and $ReZG_3$, were introduced and defined as

$$ReZG_1 = ReZG_1(G) = \sum_{uv\in E(G)} \frac{d(u)+d(v)}{d(u)\,d(v)}\,,$$
$$ReZG_2 = ReZG_2(G) = \sum_{uv\in E(G)} \frac{d(u)\,d(v)}{d(u)+d(v)}\,,$$
$$ReZG_3 = ReZG_3(G) = \sum_{uv\in E(G)} \big[d(u)\,d(v)\big]\big[d(u)+d(v)\big]\,.$$

However, since $ReZG_1 = n$, it is not a topological index at all. On the other hand, $ReZG_2 = ISI$, where $ISI = ISI(G)$, is the *inverse sum indeg index*, earlier defined in [36]. The index $ReZG_3$ was named *re-defined third Zagreb index*. A few years later the same index was proposed in [37] under the name *second Gourava index*, obtained as a special case of the *generalized Zagreb index* $M_{r,s}$ introduced in [38]:

$$M_{r,s} = M_{r,s}(G) = \sum_{uv\in E(G)} \big[d(u)^r\,d(v)^s + d(v)^r\,d(u)^s\big].$$

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Maybe the following generalization of Zagreb indices would also make sense:

$$M_{\alpha,\beta} = M_{\alpha,\beta}(G) = \sum_{uv \in E(G)} \frac{\left[d(u)\, d(v)\right]^{\alpha}}{\left[d(u) + d(v)\right]^{\beta}},$$

where α and β are arbitrary real numbers. It can be easily observed that $M_{0,-1} = M_1$, $M_{1,0} = M_2$, $M_{\alpha,0} = M_2^{\alpha}$ and $M_{0,-\beta} = H_{\beta}$.

2.1. Special cases

If $\alpha = 2$, then the general first Zagreb index $M_1^{(\alpha)}$ coincide with its ordinary version. The same happens with $M_2^{(\alpha)}$ if $\alpha = 1$. Some other special cases deserved particular interest and have been examined separately.

$M_1^{(\alpha)}$ for $\alpha = -2$ is the *modified first Zagreb index*, ${}^{m}M_1$,

$${}^{m}M_1 = {}^{m}M_1(G) = \sum_{u \in V(G)} \frac{1}{d(u)^2}.$$

It was first defined in [39].

$M_1^{(\alpha)}$ for $\alpha = -1$ is the *inverse degree*, ID,

$$ID = ID(G) = \sum_{u \in V(G)} \frac{1}{d(u)}.$$

This index is also known under names *modified total adjacency index* and *sum of reciprocals of degrees*. It has first attracted attention through a conjecture-generating computer program Graffiti [40,41]. The name *inverse degree* was first introduced in 2005 [42], followed by half-a-dozen papers [43–49].

$M_1^{(\alpha)}$ for $\alpha = -1/2$ is the *zeroth-order Randić index*,

$$M_1^{(-1/2)} = M_1^{(-1/2)}(G) = \sum_{u \in V(G)} \frac{1}{\sqrt{d(u)}},$$

a quantity conceived already in 1976 [50], but which was examined only in a relatively small number of subsequent papers (see e.g., [51–53]). Most results on $M_1^{(-1/2)}$ are found in studies concerned with the zeroth-order general Randić index (see e.g., [24–26]).

$M_1^{(\alpha)}$ for $\alpha = 3$ can be found already in the paper [1], but neither in the 1970s nor in next 40 years did it attract any attention. Only in 2015, some of its unusual features (in quantitative structure–property chemical applications) have been recognized [54], after which this structure-descriptor suddenly became attractive to mathematical chemists [55–68]. This graph invariant was named *forgotten topological index* or F-index. Thus,

$$F = F(G) = \sum_{u \in V(G)} d(u)^3 = \sum_{uv \in E(G)} \left[d(u)^2 + d(v)^2\right]. \tag{5}$$

$M_2^{(\alpha)}$ for $\alpha = -1/2$ is the classical Randić (or connectivity) index,

$$R = R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)\, d(v)}},$$

put forward by Randić in 1975 [69]. It is probably the most popular and most thoroughly investigated molecular-structure descriptor. Details of its mathematical theory and physico-chemical usages go beyond the ambit of the present survey; these can be found in the books [50,70–73].

$M_2^{(\alpha)}$ for $\alpha = -1$ was first time examined in 1998 by Bollobás and Erdős [74,75], and is nowadays usually referred to as the *Randić index* R_{-1} (see e.g., [76–79])

$$R_{-1} = R_{-1}(G) = \sum_{uv \in E(G)} \frac{1}{d(u)\, d(v)}.$$

It is also known under the name *modified second Zagreb index* [80] and *first order overall index* [81] .

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$M_2^{(\alpha)}$ for $\alpha = 1/2$ is the *reciprocal Randić index*,

$$RR = RR(G) = \sum_{uv \in E(G)} \sqrt{d(u)\, d(v)},$$

introduced in [71,72].

H_α for $\alpha = -1/2$ is the *sum-connectivity index*, χ,

$$\chi = \chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u) + d(v)}} = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(uv) + 2}},$$

introduced in [82]. More on this index can be found in [83–85].

For $\alpha = -1$ we have that $2H_{-1} = H$, where

$$H = H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)},$$

is the *harmonic index* proposed in [40]. Details on its mathematical theory and applications can be found in [31,86].

H_α for $\alpha = 2$ becomes the *hyper-Zagreb index*

$$HM(G) = \sum_{uv \in E(G)} \left[d(u) + d(v)\right]^2 = \sum_{uv \in E(G)} \left[d(u) + d(v)\right]^2,$$

introduced by Shirdel et al. in 2013 [87].

Although it is elementary to show that

$$HM(G) = F(G) + 2\, M_2(G)$$

the properties of the hyper-Zagreb index were nevertheless investigated in a few recent papers [88–95]. Emphasis was on bounds for HM, its coindices, and on its change under graph operations.

3. Sigma index

In order to provide a quantitative measure of graph irregularity, i.e., of the deviation of a graph from being regular, Albertson introduced the irregularity index [96]

$$Alb(G) = \sum_{uv \in E(G)} \left|d(u) - d(v)\right|.$$

This index was also considered in [97] under the name *third Zagreb index*.

In order to avoid the absolute value in the above formula, in a recent paper [98], the *sigma index* was put forward, defined as

$$\sigma(G) = \sum_{uv \in E(G)} \left[d(u) - d(v)\right]^2.$$

The following identity is immediate:

$$\sigma(G) = F(G) - 2\, M_2(G).$$

The properties of σ are analogous to that of the Albertson index. Yet, there exist pairs of graphs G_1, G_2, such that $Alb(G_1) > Alb(G_2)$ whereas $\sigma(G_1) < \sigma(G_2)$ [99].

It can be shown that the following interplay between $Alb(G)$ and $\sigma(G)$ holds:

$$Alb(G) \le \sqrt{m\sigma(G)}.$$

4. Reformulated Zagreb indices

In 2004, Miličević et al. [100] proposed variants of the Zagreb indices using edge degrees instead of vertex degrees. Let, as before, $d(uv)$ be the degree of the edge uv.

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The so-called *reformulated Zagreb indices* are then defined in analogy to Eqs. (1) and (2) as [100]

$$RM_1(G) = \sum_{uv \in E(G)} d(uv)^2 \qquad \text{and} \qquad RM_2(G) = \sum_{e,e' \in E(G)} d(e)\, d(e')$$

where e, e' are pairs of incident edges of the graph G.

It is trivially evident that the reformulated Zagreb indices of the graph G coincide with the ordinary Zagreb indices of the line graph of the graph G, and thus are nothing new. In spite of this, quite a few papers [101–110] have been devoted to the study of the indices RM_1 and RM_2, often "forgetting" to observe their close relation with the ordinary Zagreb indices.

A less trivial result along these lines is the identity [101]

$$RM_1(G) = F(G) + 2\, M_2(G) - 4\, M_1(G) + 4m.$$

In a recent paper [111], the concept of reformulated F-index was introduced:

$$RF = RF(G) = \sum_{uv \in E(G)} d(uv)^3.$$

In [68] it was proved that

$$RF = \sum_{uv \in E(G)} \big(d(uv) + 2\big)^3 - 6\big(F + 2M_2\big) + 12M_1 - 8m,$$

which was exploited in [68,112] to determine lower bounds for RF.

5. Banhatti indices

In 2016, the Indian scholar Kulli put forward the following combination of ordinary and reformulated Zagreb indices [113,114]:

$$B_1(G) = \sum_{u,e} \big[d(u) + d(e)\big] \qquad \text{and} \qquad B_2(G) = \sum_{u,e} d(u)\, d(e)$$

where the summations go over pairs of a vertex u and edge e, such that e is incident to u. The author of [113,114] proposed that the new graph invariants be named *K Banhatti indices*, with Banhatti being a city in India whereas K might hint towards "Kulli".

Unfortunately, the two Banhatti indices satisfy the identities [115]:

$$B_1(G) = 3\, M_1(G) - 4m \qquad \text{and} \qquad B_2(G) = HM(G) - 2\, M_1(G)$$

which reduce them to earlier known Zagreb-type indices.

Kulli proposed also *hyper-K Banhatti indices*, defined as [116]

$$HB_1(G) = \sum_{u,e} \big[d(u) + d(e)\big]^2 \qquad \text{and} \qquad HB_2(G) = \sum_{u,e} \big[d(u)\, d(e)\big]^2$$

whose properties await to be elaborated in the future.

6. Coindices and non-neighbor Zagreb indices

Let $J(G)$ be any vertex-degree-based graph invariant of the form

$$J(G) = \sum_{uv \in E(G)} \Gamma\big[d(u), d(v)\big]$$

such that $\Gamma(x, y) = \Gamma(y, x)$. Then the *coindex* of $J(G)$ is defined as

$$\overline{J}(G) = \sum_{\substack{uv \notin E(G) \\ u \neq v}} \Gamma\big[d(u), d(v)\big]$$

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or, what is the same, as

$$\overline{J}(G) = \sum_{uv \in E(\overline{G})} \Gamma\big[d(u), d(v)\big]$$

where $\overline{G}$ is the complement of the graph G.

The concept of coindices was invented by Došlić in 2008 [117] and was first applied to the two Zagreb indices. Thus,

$$\overline{M}_1(G) = \sum_{\substack{uv \notin E(G) \\ u \neq v}} \big[d(u) + d(v)\big] \qquad \text{and} \qquad \overline{M}_2(G) = \sum_{\substack{uv \notin E(G) \\ u \neq v}} d(u)\, d(v).$$

By direct calculation it can be shown that the Zagreb coindices are in a simple relation with the Zagreb indices, viz.,

$$\overline{M}_1(G) = 2m(n-1) - M_1(G)\,,$$

$$\overline{M}_2(G) = 2m^2 - \frac{1}{2}\, M_1(G) - M_2(G)\,,$$

$$\overline{M}_1(\overline{G}) = 2m(n-1) - M_1(G)\,, \tag{6}$$

$$\overline{M}_2(\overline{G}) = m(n-1)^2 - (n-1)M_1(G) + M_2(G)\,. \tag{7}$$

In spite of this, in the recent literature [118–132] much work has been devoted to Zagreb coindices. For a review see [11].

Coindices of other Zagreb-type indices could also be determined. For instance [88]:

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

Rizwana et al. [133] considered the *non-neighbor Zagreb indices*, based on the number of non-neighbors of a vertex, denoted by $\overline{d}(u)$. Evidently, for a graph of order n, $\overline{d}(u) = n - 1 - d(u)$. Therefore, if the non-neighbor Zagreb indices are defined as [133]

$$M_1^{nn}(G) = \sum_{u \in V(G)} \overline{d}(u)^2 \qquad \text{and} \qquad M_2^{nn}(G) = \sum_{uv \in E(G)} \overline{d}(u)\,\overline{d}(v)$$

then

$$M_1^{nn}(G) = 2m(n-1) - M_1(G)$$

and

$$M_2^{nn}(G) = m(n-1)^2 - (n-1)M_1(G) + M_2(G).$$

However, according to (6) and (7) it is obvious that

$$M_1^{nn}(G) = \overline{M}_1(\overline{G}) \qquad \text{and} \qquad M_2^{nn} = \overline{M}_2(\overline{G}),$$

so M_1^{nn} and M_2^{nn} cannot be considered as new topological indices.

7. Reduced Zagreb indices

From Eqs. (2) and (3) it immediately follows that

$$M_2(G) - M_1(G) = \sum_{uv \in E(G)} [d(u) - 1][d(v) - 1] - m.$$

From the analysis in the paper [134] it appeared to be purposeful to consider the quantity

$$RM_2 = RM_2(G) = \sum_{uv \in E(G)} [d(u) - 1][d(v) - 1]$$

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as the *reduced second Zagreb index*. It can be easily observed that (see [135])

$$RM_2(G) = M_2(G) - M_1(G) + m.$$

Further studies along these lines can be found in [135–138].

A *reduced reciprocal Randić index* was defined in [135] as

$$RRR = RRR(G) = \sum_{uv \in E(G)} \sqrt{\big(d(u)-1\big)\big(d(v)-1\big)}$$

The authors of [135] proved that for any connected graph with n vertices, the following inequalities are valid:

$$RR(P_n) \le RR(G) \le RR(K_n),$$
$$RM_2(S_n) \le RM_2(G) \le RM_2(K_n),$$
$$RRR(S_n) \le RRR(G) \le RRR(K_n),$$

where P_n is a path, S_n a star graph, and K_n a complete graph.

It should be noted that the idea of "reduction", i.e., replacement $d(u) \to d(u) - 1$, can be extended to any vertex-degree-based graph invariant [135].

8. Leap Zagreb indices

In a recent paper [139], Naji et al. elaborated the idea of using the second degree of a vertex, $d_2(u)$, namely the number of second neighbors. This leads to three *leap Zagreb indices*, defined as

$$LM_1(G) = \sum_{u \in V(G)} d_2(u)^2,$$
$$LM_2(G) = \sum_{uv \in E(G)} d_2(u)\, d_2(v),$$
$$LM_3(G) = \sum_{u \in V(G)} d(u)\, d_2(u).$$

It is interesting that as early as in 2008, Yamaguchi discovered an equality [140]

$$LM_3(G) = M_2(G) - \frac{1}{2}\, M_1(G)$$

that holds for triangle- and quadrangle-free graphs.

In [139] the bounds

$$LM_1(G) \le M_1(G) + n(n-1)^2 - 4m(n-1),$$
$$LM_2(G) \le M_2(G) - (n-1)M_1(G) + m(n-1)^2,$$
$$LM_3(G) \le 2m(n-1) - M_1(G)$$

were established. Equality holds if and only if $diam(G) \le 2$.

9. What is missing?

There are other directions in which Zagreb indices have been modified. These violate too much from the original concept, and have been left out from the present survey. Yet, we mention the main ideas.

Instead of summation, multiplication can be used in Eqs. (1)–(3) and elsewhere, resulting in *multiplicative Zagreb indices*. In particular, the multiplicative version of Eq. (1) is

$$\prod_{v \in V(G)} d(v)^2 = \left[\prod_{v \in V(G)} d(v) \right]^2 \equiv [NK(G)]^2$$

which is just the square of the Narumi–Katayama index NK, put forward already in the 1980s [141].

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Bearing in mind Eq. (3), we may define the first Zagreb matrix $Z^{(1)}$ as

$$\left(Z^{(1)}\right)_{ij} = \begin{cases} d(v_i) + d(v_j) & \text{if } v_i v_j \in E(G) \\ 0 & \text{otherwise}. \end{cases}$$

If the eigenvalues of $Z^{(1)}$ are $\zeta_i^{(1)}$, $i = 1, 2, \ldots, n$, then the *first Zagreb energy* would be [142]

$$ZE_1(G) = \sum_{i=1}^{n} |\zeta_i^{(1)}|.$$

Analogously, in view of Eq. (2), the *second Zagreb energy* could be defined as

$$ZE_2(G) = \sum_{i=1}^{n} |\zeta_i^{(2)}|$$

where $\zeta_i^{(2)}$, $i = 1, 2, \ldots, n$, are the eigenvalues of the second Zagreb matrix $Z^{(2)}$, whose elements are

$$\left(Z^{(2)}\right)_{ij} = \begin{cases} d(v_i)\, d(v_j) & \text{if } v_i v_j \in E(G) \\ 0 & \text{otherwise}. \end{cases}$$

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