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ON THE ORIGIN OF TWO DEGREE–BASED TOPOLOGICAL INDICES

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A b s t r a c t. *Let G be a graph with vertex sex $V(G)$ and edge set $E(G)$. Two much studied and in chemistry much applied graph invariants are the first Zagreb index $M_1 = \sum_{x \in V(G)} d(x)^2$ and the second Zagreb index $M_2 = \sum_{xy \in E(G)} d(x)\, d(y)$, where $d(x)$ is the degree of the vertex $x \in V(G)$. We analyze the way how these invariants were conceived in the 1970s and clarify some missing details.*

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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.

As usual, the path, cycle, and star on n vertices will be denoted by P_n, S_n, and C_n, respectively.

Let G and H be graphs. We denote by $\sigma_G(H)$ the number of distinct subgraphs of the graph G which are isomorphic to H. In particular, the graph G has $\sigma_G(P_1)$ vertices, $\sigma_G(P_2)$ edges, $\sigma_G(C_3)$ triangles, and $\sigma_G(P_2 \cup P_2)$ pairs of independent edges.

In this paper we are concerned with two degree–based graph invariants, called Zagreb indices. The *first Zagreb index* M_1 and the *second Zagreb index* M_2 are defined as

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

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

The Zagreb indices belong among the oldest and most studied molecular structure descriptors and found noteworthy applications in chemistry. It is generally accepted that these have been conceived in 1972 by Trinajstić and the present author, and first published in the much quoted paper [22]. The nowadays standard notation M_1 and M_2, as well as the definitions (1.1) and (1.2) were first time used in the paper [21].

Details on these vertex–based topological indices can be found in the reviews [28, 17, 7] published on the occasion of their 30th anniversary, as well as in a recent surveys [16, 20].

Nowadays, there exist hundreds of papers on Zagreb indices and related matter.[1]

The first survey on topological indices appeared in 1983 [1]. In it also M_1 and M_2 were mentioned and commented. The authors of [1] named them "*Zagreb group indices*", bearing in mind that these resulted from the work of a group of scholars at the "Rudjer Bošković" institute in Zagreb. The name remained, except that "*group*" was eventually dropped.

Although much is known on Zagreb indices, some details concerning their discovery and relation to other topological indices deserve to be commented and clarified.

[1] By a recent literature search we found 90 papers whose title contain *Zagreb index* or *Zagreb indices*, in which count are not included papers dealing with augmented, general, modified, reformulated, multiplicative, variable Zagreb indices, Zagreb coindices, and Zagreb eccentricity index.

2. *Before Zagreb indices*

The first graph–based molecular structure descriptors (topological indices) were invented in 1947 [30, 33]. Of these, the Platt index I_{Pl} is the count of the edges incident to an edge of the underlying graph, and its sum over all edges [30]:

$$I_{Pl} = I_{Pl}(G) = \sum_{xy \in E(G)} [d(x) + d(y) - 2] \ . \tag{2.1}$$

What was completely overlooked by the authors of the papers [22, 21], was the following generally valid identity

$$M_1 = I_{Pl} + 2m$$

which straightforwardly follows from (2.1) and the relation

$$M_1(G) = \sum_{xy \in E(G)} [d(x) + d(y)] \ . \tag{2.2}$$

In the 1970s and 1980s, the relation (2.2) was not known. It seems to be first time explicitly mentioned in a paper published in 2011 [9].

We now see that the first Zagreb index is essentially the same as the much older Platt index.

In 1964, Gordon and Scantelbury [12] considered a graph invariant that sometimes is referred to as the Gordon–Scantelbury index I_{GS}. By definition, it is equal to the number of acyclic P_3-subgraphs contained in the graph G. For triangle–free graphs,

$$I_{GS} = I_{GS}(G) = \sigma_G(P_3)$$

which because of $\sigma_G(P_3) = \sum_{x \in V(G)} \binom{d(x)}{2}$, is related with M_1 . Direct calculation yields the simple identity

$$M_1 = 2\, I_{GS} + 2m$$

which implies that the first Zagreb index is essentially the same as the somewhat older Gordon–Scantelbury index. This too was missed by the authors of [22, 21].

The sum of squares of vertex degrees (which, of course, is same as the first Zagreb index) was also independently studied in the mathematical literature, see, for instance [8, 29, 3, 27].

In 1947, Wiener introduced two topological indices [33]. The first is what nowadays is referred to as the Wiener index, equal to the sum of distances between all pairs of vertices of the graph G. The second, named by Wiener "*polarity number*" and denoted here by W_P, is the number of pairs of vertices whose distance is three.

In order to show that W_P is also closely related to the Zagreb indices needs some preparations.

Define the *reduced second Zagreb index* as [11, 18]

$$RM_2 = RM_2(G) = \sum_{xy \in E(G)} [d(x)-1][d(y)-1] \ . \tag{2.3}$$

Bearing in mind Eqs. (1.2) and (2.2), one straightforwardly obtains

$$RM_2(G) = M_2(G) - M_1(G) + m \ . \tag{2.4}$$

As it could be expected, relation (2.4) was encountered within studies of the difference between the two Zagreb indices [2, 26, 11, 20]. In addition, the reduced second Zagreb index, Eq. (2.3), plays an important role in the theory of Wiener polarity number W_P .

The following Theorems 2.1 and 2.2 from Ref. [20] are important for themselves, but we need them in the considerations in Section 3. In order that our paper be self–contained, we reproduce these two theorems, in whose proofs some minor improvements have been included.

Theorem 2.1. *If the graph G contains $\sigma_G(P_4)$ 4-vertex path subgraphs and $\sigma_G(C_3)$ triangles, then*

$$RM_2 = \sigma_G(P_4) + 3\,\sigma_G(C_3) \ . \tag{2.5}$$

Proof. Let xy be an edge of the graph G, connecting the vertices x and y . Then in addition to the edge xy, there are $d(x)-1$ other edges incident to x, and $d(y)-1$ other edges incident to y. Let $u \neq y$ be a vertex adjacent to x . Let $v \neq x$ be a vertex adjacent to y. We have to distinguish between two cases.

If $u \neq v$, then the four vertices u, x, y, v form a 4-vertex path which is as subgraph contained in G.

If $u = v$, then the three vertices u, x, y form a triangle which is as subgraph contained in G.

Then the term $[d(x)-1][d(y)-1]$ counts the number of 4-vertex paths in G whose central edge is xy, plus the number of triangles to which the edge xy belongs.

Summing $[d(x) - 1][d(y) - 1]$ over all edges of G, we get the count of all 4-vertex path subgraphs of G, plus three times the number of triangles of G, i.e., we arrive at Eq. (2.5). □

Formula (2.5) seems to have been first reported in [26]. Its special case for triangle–free graphs and trees was reported or used several times [32, 25, 23, 10].

Every pair of vertices at distance 3 corresponds to at least one 4-vertex path subgraph, but the opposite is not generally true. Therefore, in the general case, $W_P \leq \sigma_G(P_4)$, implying [25]

$$W_P \leq M_2 - M_1 + m \ . \tag{2.6}$$

Equality in (2.6) is characterized by the following:

Theorem 2.2. *Let G be a graph with first and second Zagreb indices M_1 and M_2, and with m edges. Then its Wiener polarity number obeys the identity*

$$W_P = M_2 - M_1 + m \tag{2.7}$$

if and only if G is either acyclic or if its girth (size of the smallest cycle) is greater than 6.

Proof. Without loss of generality we may assume that G is connected. If G is acyclic (i.e., G is a tree) then there is a one-to-one correspondence between a pair of vertices at distance 3 and a 4-vertex path subgraph. Consequently, $W_P = \sigma_G(P_4)$ holds for trees and thus Eq. (2.7) holds.

If the graph G is the triangle (C_3) then $M_2 = M_1$, $m = 3$, whereas $W_P = 0$. Thus, in the case $G \cong C_3$, Eq. (2.7) is violated.

Let u and v be a pair of vertices of G, being the endpoints of a 4-vertex path subgraph u, x, y, v. If the distance between u and v is less than 3, then $W_P < \sigma_G(P_4)$ and Eq. (2.7) is violated.

We have to separately consider the cases when the distance between u and v is one and two, when also $W_P < \sigma_G(P_4)$ and Eq. (2.7) is violated.

Suppose that the distance between u and v is one. Then the vertices u, x, y, v form a quadrangle, i.e., the girth of G is 4 or less.

Suppose that the distance between u and v is two. Then there are two possibilities.

(i) The vertices u and y are connected, in which case the vertices u, x, y form a triangle, or (what is the same) the vertices x and v are connected, in which case the vertices x, y, v form a triangle. Then the girth of G is three.

(ii) There is a fifth vertex w, adjacent to u and v. Then the vertices u, x, y, v, w form a pentagon, i.e., the girth of G is 5 or less.

Remains to consider the case when the distance between the vertices u and x is 3, but the path connecting them is not unique. If so, then again $W_P < \sigma_G(P_4)$ and Eq. (2.7) is violated.

Suppose that u, x, y, v is not the only shortest path between u and v. Let u, x', y', v be another such path. If $x \neq x'$ and $y \neq y'$, then u, x, y, v, y', x' form a hexagon and the girth of G is 6 or less.

If $x = x'$, then x, y, v, y' form a quadrangle. Analogously, if $y = y'$, then u, x, y, x' form a quadrangle. The girth of G is 4 or less.

We thus see that a one-to-one correspondence between a pair of vertices at distance 3 and a 4-vertex path subgraph exists if and only if G is either a tree or if its girth is greater than 6. □

Special cases of Theorem 2.2 were reported in [10, 23]. Its correct statement, but with an incomplete proof, is found in [25]. Anyway, the relation between Wiener polarity index (from the 1970s) and the Zagreb indices was recognized only around 2010.

3. *Origin of the Zagreb indices*

The paper [22] was an early attempt by the present author and his supervisor Trinajstić to analyze the structure–dependency of total π-electron energy. Eventually, this direction of research has been elaborated in much detail, and evolved in the (mathematical) theory of graph energy (for details see [14, 19, 24]).

With today's knowledge, we see that the results of the paper [22] are insignificant, and its mathematical methods are not sound. No surprise, this mathematical approach to graph energy was abandoned soon after 1972. Yet, [22] is one of Ivan Gutman's most cited publications. This happened not because of its results on graph energy, but because of the universally accepted belief that the two Zagreb indices were first time introduced in [22]. In the countless later published papers on Zagreb indices, it became customary to quote [22] as their source.[2]

[2]Ref. [22] is quoted in at least 35 textbooks and monographs by authors other than I.G., whereas Ref. [21] is quoted in at least 48 such publications. The number of papers published in scientific journals, in which Refs. [22, 21] are quoted (in connection with the Zagreb indices), might tenfold exceed these values.

Let us therefore scrutinize the contents of the paper [22].

The definition of total π-electron energy used in [22] coincides with the modern definition of graph energy, namely with [14, 19, 24]

$$\mathcal{E} = \mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|,$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of the graph G [5, 6].

In [22], approximate expressions were deduced for $\mathcal{E}$ in terms of the first few coefficients of the characteristic polynomial of the underlying graph. Let this polynomial be of the form $\sum\limits_{k\geq 0} a_k\, \lambda^{n-2k}$. Then the formulas reported in [22] are as follows:

$$\mathcal{E}^{(0)} = g\, n, \tag{3.1}$$

$$\mathcal{E}^{(1)} = g\left(\frac{n}{2} - \frac{a_2}{g^2}\right), \tag{3.2}$$

$$\mathcal{E}^{(2)} = g\left(\frac{3n}{8} - \frac{3a_2}{2g^2} + \frac{a_4}{4g^4} - \frac{a_2^2}{4g^4}\right), \tag{3.3}$$

$$\mathcal{E}^{(3)} = g\left(\frac{5n}{16} - \frac{15a_2}{8g^2} + \frac{5a_4}{4g^4} - \frac{5a_2^2}{8g^4} - \frac{3a_6}{8g^6} + \frac{3a_2\, a_4}{8g^6} - \frac{a_2^3}{8g^6}\right), \tag{3.4}$$

where g is an (unspecified) fitting parameter.

In the time when the paper [22] was written, it was already known how the coefficients of the characteristic polynomial depend on the structure of the underlying graph [31, 4, 13, 15]. The idea of the paper [22] was to use this knowledge and the approximations (3.1)–(3.4), and deduce the main features of the structure–dependency of $\mathcal{E}$. For this the explicit dependence of the coefficients a_2, a_4, and a_6 on the structure of the underlying graph had to be established.

Using the Sachs theorem [5, 6, 31, 4, 13] it is immediate to see that $a_2 = -\sigma_G(P_2) = -m$ and $a_4 = \sigma_G(P_2 \cup P_2) - 2\,\sigma_G(C_4)$. Now,

$$\sigma_G(P_2 \cup P_2) = \binom{m}{2} - \sum_{v \in V(G)} \binom{d(v)}{2} \tag{3.5}$$

since the graph G has a total of $\binom{m}{2}$ pairs of edges, of which

$$\sum_{v \in V(G)} \binom{d(v)}{2}$$

are pairwise incident. Expanding the right–hand side of (3.5), and bearing in mind Eq. (1.1), we get

$$a_4 = \binom{m+1}{2} - \frac{1}{2} M_1 - 2\,\sigma_G(C_4)$$

in which the first Zagreb index is encountered. Via formula (3.3), the is first Zagreb index is related with graph energy. The same, but in a much more complicated manner, happens also in formula (3.4).

In Ref. [21], the two topological indices M_1 and M_2 are defined in the same manner as as in the present Eqs. (1.1) and (1.2). In Ref. [21], it is claimed that in the previous article [22] "*it was shown that M_1 and M_2 appear in a topological formula for total π-electron energy*". As we just have shown, this indeed is the case with M_1.

On the other hand, by a careful scrutiny of the paper [22], we established that in the approximate formulas for $\mathcal{E}$ reported in [22], there is no term that would be equivalent or even similar to the right–hand side of Eq. (1.2). We must therefore conclude that [22] is erroneously considered to be the source of the second Zagreb index. The several hundred quotations of [22] reveal the sad fact that most of those who cited the paper [22], did not read it.

Anyway, a term identical to the second Zagreb index occurs in the combinatorial expression for the coefficient a_6 and therefore in the approximate formula (3.4). In what follows we demonstrate this fact for the first time (with a delay of ca 40 years!).

According to the Sachs theorem,

$$a_6 = -\sigma_G(P_2 \cup P_2 \cup P_2) + 2\,\sigma_G(C_4 \cup P_2) + 4\,\sigma_G(C_3 \cup C_3) - 2\,\sigma_G(C_6). \quad (3.6)$$

For the sake of completeness, we briefly mention the structural interpretation of the last three terms on the right–hand side of Eq. (3.6). The meaning of $\sigma_G(C_6)$ and $\sigma_G(C_3 \cup C_3)$ is straightforward: the former is the number of hexagons, the latter is the number of pairwise disjoint triangles contained in the graph G. In addition,

$$\sigma_G(C_4 \cup P_2) = \sum_{C_4} m(G - C_4)$$

where $m(G - C_4)$ is the number of edges of the subgraph of G, obtained by deleting the quadrangle C_4, and the summation goes over all quadrangles contained in G.

We now focus our attention to the first term in formula (3.6), namely to the number of selections of three mutually independent edges.

There are exactly five mutually non-isomorphic graphs with three edges and without isolated vertices, H_1, H_2, H_3, H_4, H_5 (see Fig. 1).

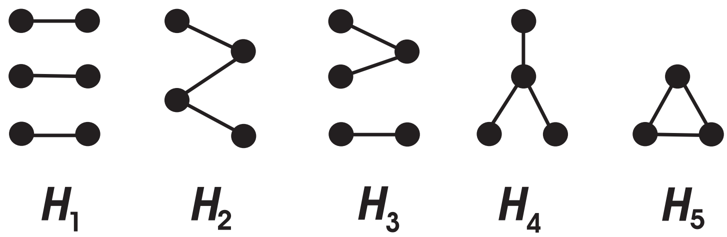

Fig. 1. Graphs with $m = 3$ and no isolated vertices: $H_1 \cong P_2 \cup P_2 \cup P_2$, $H_2 \cong P_4$, $H_3 \cong P_3 \cup P_2$, $H_4 \cong S_4$, and $H_5 \cong C_3$

If the graph G has m edges, then three edges in it can be selected in $\binom{m}{3}$ different ways, and

$$\binom{m}{3} = \sigma_G(H_1) + \sigma_G(H_2) + \sigma_G(H_3) + \sigma_G(H_4) + \sigma_G(H_5). \tag{3.7}$$

The quantity $\sigma_G(H_2) = \sigma_G(P_4)$ has been determined in Theorem 2.1,

$$\sigma_G(H_2) = RM_2(G) - 3\,\sigma_G(C_3). \tag{3.8}$$

In addition, it is evident that

$$\sigma_G(H_4) = \sum_{x \in V(G)} \binom{d(x)}{3} \qquad \text{and} \qquad \sigma_G(H_5) = \sigma_G(C_3). \tag{3.9}$$

In order to calculate $\sigma_G(H_3)$, we notice that each of the graphs H_2, H_3, H_4, H_5 is constructed by adding a new edge to the 2-edge path P_3. By this construction we have to add to P_3 one among $m - 2$ remaining edges of the graph G. If x is the central vertex of P_3, then the construction can be done in $\binom{d(x)}{2} \cdot (m-2)$ ways, and the total number of distinct constructions is $\sum_{x \in V(G)} \binom{d(x)}{2} \cdot (m-2)$.

Whereas the construction $P_2 \to H_3$ can be performed in a single manner, the construction leading to H_2, H_4, and H_5 can be, respectively, done in 2, 3, and 3 different ways. In view of this,

$$(m-2) \sum_{x \in V(G)} \binom{d(x)}{2} = 2\,\sigma_G(H_2) + \sigma_G(H_3) + 3\,\sigma_G(H_4) + 3\,\sigma_G(H_5). \quad (3.10)$$

Substituting Eqs. (3.8) and (3.9) back into (3.10), we can express $\sigma_G(H_3)$ as

$$\sigma_G(H_3) = (m-2) \sum_{x \in V(G)} \binom{d(x)}{2} - 3 \sum_{x \in V(G)} \binom{d(x)}{3} - 2\,RM_2 + 3\,\sigma_G(C_3). \quad (3.11)$$

Substituting Eqs. (3.8), (3.9), and (3.11) back into (3.7) we get

$$\sigma_G(H_1) = \binom{m}{3} - (m-2) \sum_{x \in V(G)} \binom{d(x)}{2} + 2 \sum_{x \in V(G)} \binom{d(x)}{3} + RM_2 - \sigma_G(C_3)$$

$$= \frac{m}{6}(m^2 + 3m - 2) - \frac{m}{2} \sum_{x \in V(G)} d(x)^2 + \frac{1}{3} \sum_{x \in V(G)} d(x)^3 + RM_2 - \sigma_G(C_3),$$

which in view of Eqs. (1.1), (1.2), and (2.4) yields

$$\sigma_G(H_1) = \frac{m}{6}(m^2 + 3m + 4) - \frac{m+2}{2} M_1 + M_2 + \frac{1}{3} \sum_{x \in V(G)} d(x)^3 - \sigma_G(C_3).$$

Returning to the Sachs–type expression for a_6, Eq. (3.6), we arrive at:

Theorem 3.1. *The coefficient a_6 of the characteristic polynomial of a graph G depends on the structure of G in the following manner*

$$a_6 = -\frac{m}{6}(m^2 + 3m + 4) + \frac{m+2}{2} M_1(G) - M_2(G) - \frac{1}{3} \sum_{x \in V(G)} d(x)^3$$

$$+ 2\,\sigma_G(C_4 \cup P_2) + 4\,\sigma_G(C_3 \cup C_3) - 2\,\sigma_G(C_6)\,. \quad (3.12)$$

Via formula (3.12), the approximate expression (3.4) for graph energy is related with both first and second Zagreb indices.

Three special cases of Theorem 3.1 are worth to be pointed out:

Corollary 3.1. *The coefficient a_6 of the characteristic polynomial of a tree T of order n, depends on the structure of T in the following manner:*

$$a_6 = -\frac{n-1}{6}\,(n^2+n+2) + \frac{n+1}{2}\,M_1(T) - M_2(T) - \frac{1}{3}\sum_{x\in V(T)} d(x)^3 .$$

Corollary 3.2. *The coefficient a_6 of the characteristic polynomial of a triangle– and quadrangle–free graph G depends on the structure of G in the following manner:*

$$a_6 = -\frac{m}{6}\,(m^2+3m+4) + \frac{m+2}{2}\,M_1(G) - M_2(G) - \frac{1}{3}\sum_{x\in V(G)} d(x)^3 - 2\,\sigma_G(C_6) .$$

Corollary 3.3. *The number of selections of three independence edges in the graph G depends on the first and second Zagreb indices of G in the following manner:*

$$\frac{m}{6}\,(m^2+3m+4) - \frac{m+2}{2}\,M_1(G) + M_2(G) + \frac{1}{3}\sum_{x\in V(G)} d(x)^3 .$$

4. *Concluding remarks*

In the present paper we have demonstrated that in an approximate expression for graph energy, reported as early as in 1972 [22], there exists a term that is nowadays referred to as the “second Zagreb index”. Curiously, however, in the paper [22], this detail is not found (although, perhaps, it was known to its authors). Therefore, the true source of the second Zagreb index is not the paper [22] from 1972, but the later paper [21] from 1975.

In the expressions deduced in the paper [22], there are terms equal to the sum of squares of vertex degrees. Recognizing that this sum represents a measure of the extent of branching, it was proposed in [21] to be used as a topological index, and was eventually named “first Zagreb index”. In the very same expressions examined in the paper [22], there was a term equal to the sum of cubes of vertex degrees. This sum is also a measure of the extent of branching. Yet, it eluded the attention of the authors of [22], and until now nobody ever considered it as a separate degree–based topological index.

The proper degree–based graph invariant on which the coefficient a_6, and therefore also the approximate formula $\mathcal{E}^{(\ni)}$, depend is not the second

Zagreb index M_2, Eq. (1.2), but the reduced second Zagreb index RM_2, Eq. (2.3). This detail was also not recognized by the authors of [22, 21], and the graph invariant RM_2 did not attract any attention until quite recently [11, 18].

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