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On Vertex–Degree–Based Molecular Structure Descriptors

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Abstract

If $G = (\mathbf{V}\ \mathbf{E})$ is a molecular graph, and d_u is the degree of its vertex u, then the first and second Zagreb indices are $\sum\limits_{u\in\mathbf{V}} d_u^2$ and $\sum\limits_{uv\in\mathbf{E}} d_u\, d_v$, respectively. These molecular structure descriptors, introduced in the 1970s, have been much studied. Yet, a number of their properties, that seem to have evaded attention so far, are established in this work for the first time. Also a more recent degree–based descriptor, the geometric–arithmetic index, equal to $\sum\limits_{uv\in\mathbf{E}} \sqrt{d_u\, d_v}/[(d_u + d_v)/2]$, is analyzed. It is demonstrated that instead of the ratio of geometric and arithmetic means, almost any other means could be used.

1. Introduction

In the recent years, in mathematical chemistry it became a popular practice to introduce novel molecular structure descriptors (topological indices), see, for instance, [1–20]. In this paper we show that there still exist numerous unexplored features of the old topological indices, in particular of those that are simple functions of the degrees of the vertices of the molecular graph.

Let $G = (\mathbf{V}, \mathbf{E})$ be a molecular graph with vertex set $\mathbf{V}$ and edge set $\mathbf{E}$. The edge connecting the vertices u and v will be denoted by uv and then $uv \in \mathbf{E}$. The degree (= number of first neighbors) of the vertex u is denoted by d_u. Note that if $uv \in \mathbf{E}$, then $d_u \geq 1$ and $d_v \geq 1$.

In this work we are mainly concerned with the two oldest vertex–degree–based structure descriptors, nowadays known under the name *first* and *second Zagreb indices*. These are defined as

$$Zg_1 = Zg_1(G) = \sum_{u \in \mathbf{V}} d_u^2 \qquad \text{and} \qquad Zg_2 = Zg_2(G) = \sum_{uv \in \mathbf{E}} d_u \, d_v \, .$$

The Zagreb indices were first time considered in [21] and since then studied in hundreds of papers, see [22–24] and the references cited therein. It should be noted that in [21] these indices were not defined *ad hoc*, but were recognized as terms occurring in a power–series expansion of the total π-electron energy.

In what follows we shall need the standard means of positive real numbers $x_1, x_2, \ldots, x_n$. Let p be a real number. For $p \neq 0$, the mean M_p is defined as

$$M_p = M_p(x_1, x_2, \ldots, x_n) = \left(\frac{1}{n} \sum_{i=1}^{n} (x_i)^p \right)^{1/p} . \tag{1}$$

It can be shown that

$$M_0 = M_0(x_1, x_2, \ldots, x_n) = \lim_{p \to 0} M_p = \left(\prod_{i=1}^{n} x_i \right)^{1/n} . \tag{2}$$

The best known of these means are M_1, M_0, and M_{-1} called, respectively, arithmetic, geometric, and harmonic mean. If $p > q$, then $M_p > M_q$. More details on means can be found in the monographs [25, 26].

2. Some elementary results

Let the graph G considered possess n_0 isolated vertices (= vertices of degree zero) and let $\mathbf{V}_0$ be the set of these vertices. Recall that for molecular graphs $n_0 = 0$ and $\mathbf{V}_0 = \emptyset$.

Lemma 1. The identity

$$\sum_{uv \in \mathbf{E}} [f(d_u) + f(d_v)] = \sum_{u \in \mathbf{V} \setminus \mathbf{V}_0} d_u\, f(d_u) \tag{3}$$

holds for any graph G and any function f.

Proof. Every summand $f(d_x)$ in the left–hand side summation occurs as many times as many neighbors the vertex x has, i. e., d_x times. ■

As two special cases of Lemma 1 we mention

$$\sum_{uv \in \mathbf{E}} (d_u + d_v) = \sum_{u \in \mathbf{V} \setminus \mathbf{V}_0} d_u^2 = \sum_{u \in \mathbf{V}} d_u^2 = Zg_1(G) \tag{4}$$

and

$$\sum_{uv \in \mathbf{E}} \left(\frac{1}{d_u} + \frac{1}{d_v} \right) = \sum_{u \in \mathbf{V} \setminus \mathbf{V}_0} d_u \cdot \frac{1}{d_u} = n - n_0 \ . \tag{5}$$

Formula (4) is well known and was employed already in [21]; its formal proof can be found in [27]. Formula (5) has also been previously used [28]. It is worth noting that in a recent paper [29], formula (4) was considered as the *definition* of the first Zagreb index.

In another recent work [30] the *Zagreb coindices* were introduced, defined as

$$\overline{Zg}_1 = \overline{Zg}_1(G) = \sum_{uv \notin \mathbf{E}} (d_u + d_v) \qquad \text{and} \qquad \overline{Zg}_2 = \overline{Zg}_2(G) = \sum_{uv \notin \mathbf{E}} d_u\, d_v \ .$$

Bearing in mind that the sum of vertex degrees is equal to twice the number of edges, it is easy to show [30] that for a graph G with n vertices and m edges,

$$\begin{aligned} Zg_1(G) + \overline{Zg}_1(G) &= 2m(n-1) \\ Zg_2(G) + \overline{Zg}_2(G) &= 2m^2 - \frac{1}{2}\, Zg_1 \ . \end{aligned}$$

Denote by $\#P_k(G)$ the number of k-vertex paths that are, as subgraphs, contained in G. It is evident that $\#P_1(G) = n$ and $\#P_2(G) = m$. We now show that $\#P_3$ and $\#P_4$ are closely related to the Zagreb indices, namely that

$$\#P_3(G) = \frac{1}{2}\, Zg_1(G) - m \tag{6}$$

and

$$\#P_4(G) = Zg_2(G) - Zg_1(G) + m - 3t \tag{7}$$

where t is the number of triangles in G.

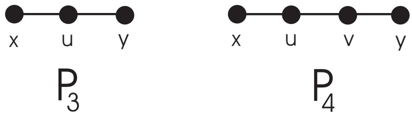

Fig. 1. Diagrams used for proving Eqs. (6) and (7).

In order to prove Eq. (6), consider the 3-vertex path depicted in Fig. 1 and consider its central vertex u. Since there are $\binom{d_u}{2}$ vertex pairs x, y, in the graph G there are $\binom{d_u}{2}$ three-vertex paths centered at u. Consequently,

$$\#P_3(G) = \sum_{u \in \mathbf{V}} \binom{d_u}{2} = \frac{1}{2} \sum_{u \in \mathbf{V}} d_u^2 - \frac{1}{2} \sum_{u \in \mathbf{V}} d_u$$

and Eq. (6) follows from the fact that the sum of vertex degrees is equal twice the number of edges.

In order to prove Eq. (7), consider the 4-vertex path depicted in Fig. 1 and consider its central edge uv. The vertex u has $d_u - 1$ neighbors besides v. Analogously, the vertex v has $d_v - 1$ neighbors besides u. If the edge uv belongs to t_{uv} triangles, then in exactly t_{uv} cases the vertices x and y coincide. Therefore, there are $(d_u - 1)(d_v - 1) - t_{uv}$ four-vertex paths centered at uv. Consequently,

$$\begin{aligned}\#P_4(G) = \sum_{uv \in \mathbf{E}} [(d_u - 1)(d_v - 1) - t_{uv}] \quad &= \quad \sum_{uv \in \mathbf{E}} d_u\, d_v - \sum_{uv \in \mathbf{E}} (d_u + d_v) \\ &+ \quad \sum_{uv \in \mathbf{E}} 1 - \sum_{uv \in \mathbf{E}} t_{uv} \;.\end{aligned}$$

Eq. (7) follows now by taking into account the identity (4) and the fact that since each triangle has three edges, $\sum t_{uv} = 3t$.

3. Zagreb indices and means

Directly from identity (4) it follows that the first Zagreb index can be written in terms of arithmetic means as

$$Zg_1(G) = 2 \sum_{uv \in \mathbf{E}} M_1(d_u, d_v) \;.$$

To find an analogous expression for the second Zagreb index is a bit more difficult.

Theorem 2. The identity

$$Zg_2(G) = \sum_{uv \in \mathbf{E}} M_p(d_u, d_v) \cdot M_{-p}(d_u, d_v) \tag{8}$$

is valid for any value of p. Thus, in particular, the second Zagreb index can be expressed in terms of arithmetic and harmonic means:

$$Zg_2(G) = \sum_{uv \in \mathbf{E}} M_1(d_u, d_v) \cdot M_{-1}(d_u, d_v) \ .$$

Proof. Consider the product $M_p(d_u, d_v) \cdot M_{-p}(d_u, d_v)$. We have

$$\begin{aligned}
M_p(d_u, d_v) \cdot M_{-p}(d_u, d_v) &= \left\{ \frac{1}{2} \left[(d_u)^p + (d_v)^p \right] \right\}^{1/p} \left\{ \frac{1}{2} \left[\left(\frac{1}{d_u} \right)^p + \left(\frac{1}{d_v} \right)^p \right] \right\}^{-1/p} \\
&= \left[\frac{(d_u)^p + (d_v)^p}{\left(\frac{1}{d_u} \right)^p + \left(\frac{1}{d_v} \right)^p} \right]^{1/p} \\
&= \left[(d_u)^p \ (d_v)^p \right]^{1/p} = d_u \, d_v = \left[M_0(d_u, d_v) \right]^2
\end{aligned}$$

from which the identity (8) follows straightforwardly. ■

Considerations based on means make it possible to conceive the following partition of the first Zagreb index into two components. In view of

$$\begin{aligned}
\lim_{p \to \infty} M_p(x_1, x_2, \ldots, x_n) &= \max(x_1, x_2, \ldots, x_n) \\
\lim_{p \to -\infty} M_p(x_1, x_2, \ldots, x_n) &= \min(x_1, x_2, \ldots, x_n)
\end{aligned}$$

we can decompose Zg_1 as $Zg_{1a} + Zg_{1b}$ where

$$\begin{aligned}
Zg_{1a} = Zg_{1a}(G) &= \sum_{uv \in \mathbf{E}} \lim_{p \to \infty} M_p(d_u, d_v) = \sum_{uv \in \mathbf{E}} \max\{d_u, d_v\} \\
Zg_{1b} = Zg_{1b}(G) &= \sum_{uv \in \mathbf{E}} \lim_{p \to -\infty} M_p(d_u, d_v) = \sum_{uv \in \mathbf{E}} \min\{d_u, d_v\} \ .
\end{aligned}$$

Theorem 3. Let G be a graph with maximal vertex degree Δ. Then

$$\begin{aligned}
Zg_2(G) &\leq Zg_{1a}(G) \, Zg_{1b}(G) \\
Zg_2(G) &\leq \Delta \sqrt{Zg_{1a}(G) \, Zg_{1b}(G)} \ .
\end{aligned}$$

Proof. Starting with Eq. (8) we have

$$\begin{aligned}
Zg_2 &= \sum_{uv\in\mathbf{E}} \lim_{p\to\infty} [M_p(d_u,d_v)\cdot M_{-p}(d_u,d_v)] \\
&= \sum_{uv\in\mathbf{E}} \left[\lim_{p\to\infty} M_p(d_u,d_v)\right]\cdot\left[\lim_{p\to\infty} M_{-p}(d_u,d_v)\right] \\
&= \sum_{uv\in\mathbf{E}} \left[\lim_{p\to\infty} M_p(d_u,d_v)\right]\cdot\left[\lim_{p\to-\infty} M_p(d_u,d_v)\right] .
\end{aligned}$$

Then, by the Jensen inequality,

$$Zg_2 \le \sum_{uv\in\mathbf{E}} \left[\lim_{p\to\infty} M_p(d_u,d_v)\right]\cdot\sum_{uv\in\mathbf{E}}\left[\lim_{p\to-\infty} M_p(d_u,d_v)\right] \tag{9}$$

which implies the first part of Theorem 3.

Denote the expression

$$\sum_{uv\in\mathbf{E}} \left[\lim_{p\to\infty} M_p(d_u,d_v)\right]\cdot\left[\lim_{p\to-\infty} M_p(d_u,d_v)\right]$$

by X. Then by the Cauchy inequality,

$$\begin{aligned}
X &\le \sqrt{\sum_{uv\in\mathbf{E}} \left[\lim_{p\to\infty} M_p(d_u,d_v)\right]^2}\cdot\sqrt{\sum_{uv\in\mathbf{E}}\left[\lim_{p\to-\infty} M_p(d_u,d_v)\right]^2} \\
&= \sqrt{\sum_{uv\in\mathbf{E}} [\max\{d_u,d_v\}]^2}\cdot\sqrt{\sum_{uv\in\mathbf{E}} [\min\{d_u,d_v\}]^2} \\
&\le \sqrt{\sum_{uv\in\mathbf{E}} [\Delta\cdot\max\{d_u,d_v\}]}\cdot\sqrt{\sum_{uv\in\mathbf{E}} [\Delta\cdot\min\{d_u,d_v\}]} \\
&\le \Delta\sqrt{\sum_{uv\in\mathbf{E}} \max\{d_u,d_v\}}\cdot\sqrt{\sum_{uv\in\mathbf{E}} \min\{d_u,d_v\}}
\end{aligned}$$

which combined with (9) implies the second part of Theorem 3. ■

Corollary 4.

$$Zg_2 \le \min\left\{Zg_{1a}\,Zg_{1b}\;,\;\Delta\sqrt{Zg_{1a}\,Zg_{1b}}\right\}.$$

For regular graphs $Zg_{1a} = Zg_{1b}$. Therefore, the difference $Zg_{1a} - Zg_{1b}$ might be viewed as a measure of non-regularity of a (molecular) graph. Otherwise, the meaning and possible chemical applicability of Zg_{1a} and Zg_{1b} are obscure.

One should observe that

$$Zg_{1a} - Zg_{1b} = \sum_{uv \in \mathbf{E}} |d_u - d_v| \ . \tag{10}$$

The expression on the right–hand side of Eq. (10) was recently considered by Fath–Tabar [29], who proposed that this be the *third Zagreb index*. Among other results, he showed that

$$\sum_{uv \in \mathbf{E}} |d_u - d_v| \leq \sqrt{m\ [(n-1)\, Zg_1 - 2\, Zg_2]}$$

with equality holding if and only if the underlying graph is complete [29].

Several other measures of non-regularity of a graph have been studied in the literature (see [31] and the references quoted therein). Of these the *variance of the vertex degrees* might be the simplest. It is easy to show [32, 33] that this variance is equal to $Zg_1/n - (2m/n)^2$.

4. On geometric–arithmetic index

The geometric–arithmetic index GA is a recently invented structure descriptor [8] (see also [13, 34–44]), defined as

$$GA = GA(G) = \sum_{uv \in \mathbf{E}} \frac{\sqrt{d_u\, d_v}}{(d_u + d_v)/2} \ .$$

In the notation introduced above, we may write GA as

$$GA(G) = \sum_{uv \in \mathbf{E}} \frac{M_0(d_u, d_v)}{M_1(d_u, d_v)} \ . \tag{11}$$

What has not been observed so far is that because of the identity

$$\frac{\sqrt{d_u\, d_v}}{d_u + d_v} = \frac{\sqrt{\frac{1}{d_u}\,\frac{1}{d_v}}}{\frac{1}{d_u} + \frac{1}{d_v}}$$

the geometric–arithmetic index can be expressed also in an alternative way as

$$GA(G) = \sum_{uv \in \mathbf{E}} \frac{M_0\left(\frac{1}{d_u}, \frac{1}{d_v}\right)}{M_1\left(\frac{1}{d_u}, \frac{1}{d_v}\right)} \ . \tag{12}$$

At this point it is worth noting that the equality

$$\frac{M_0(d_u, d_v)}{M_p(d_u, d_v)} = \frac{M_0\left(\frac{1}{d_u}, \frac{1}{d_v}\right)}{M_p\left(\frac{1}{d_u}, \frac{1}{d_v}\right)}$$

holds for any value of the parameter p.

Formula (12) indicates that instead of vertex degrees one could use their reciprocal values. That this idea is not completely strange, is seen from the fact that

$$\sum_{uv \in \mathbf{E}} M_0 \left(\frac{1}{d_u}, \frac{1}{d_v} \right)$$

is just the famous Randić connectivity index, whereas by (5), for molecular graphs

$$\sum_{uv \in \mathbf{E}} M_1 \left(\frac{1}{d_u}, \frac{1}{d_v} \right)$$

is simply equal to the number of vertices.

5. Why geometric–arithmetic ?

It may be that the GA index was defined, as given by Eq. (11), because the geometric and arithmetic means are the best known means. Bearing in mind that there are numerous other means (not only those specified via Eqs. (1) and (2)), we may wonder whether it is necessary to use just M_0 and M_1.

Define, therefore, a more general class of indices as

$$Z_{p,q} = Z_{p,q}(G) = \sum_{uv \in \mathbf{E}} \frac{M_p(d_u, d_v)}{M_q(d_u, d_v)}$$

where $GA \equiv Z_{0,1}$.

What first needs to be observed is that GA coincides also with $Z_{-1,0}$. This follows from the (above demonstrated) fact that $M_{-1}\, M_1 = (M_0)^2$, i. e.,

$$\frac{M_{-1}(d_u, d_v)}{M_0(d_u, d_v)} = \frac{M_0(d_u, d_v)}{M_1(d_u, d_v)} \, .$$

More generally, $Z_{p,q} = Z_{-q,-p}$ for all values of the parameters p, q.

We have examined the correlations of the indices $Z_{p,q}$ for $-2 \leq p, q \leq +2$, with $GA = Z_{0,1}$ for several sets of (molecular) graphs. It was found that in all studied cases, the $Z_{p,q}$ index is well correlated with GA; in most cases these correlations are linear or almost linear. A few characteristic examples are found in Figs. 2–5.

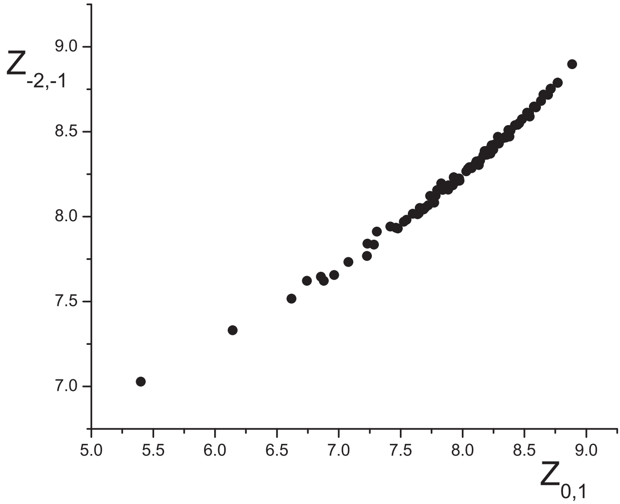

Fig. 2. Correlation between the $Z_{p,q}$ index, $p = -2$, $q = -1$, and the geometric–arithmetic index $GA = Z_{0,1}$ for 10-vertex trees.

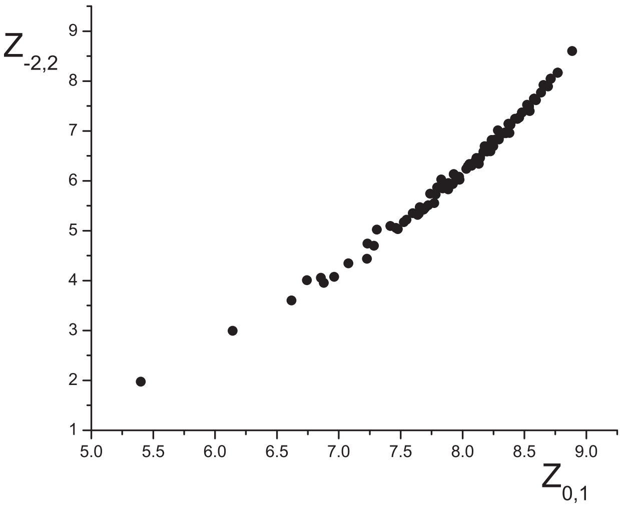

Fig. 3. Same data as in Fig. 2 for $p = -2$, $q = 2$.

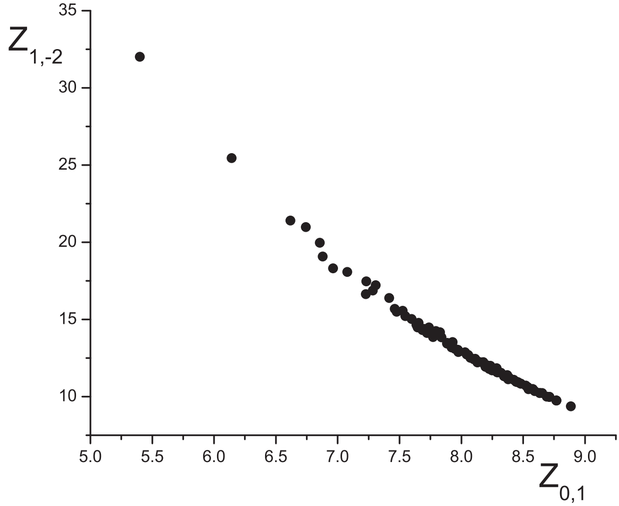

Fig. 4. Same data as in Fig. 2 for $p = 1$, $q = -2$.

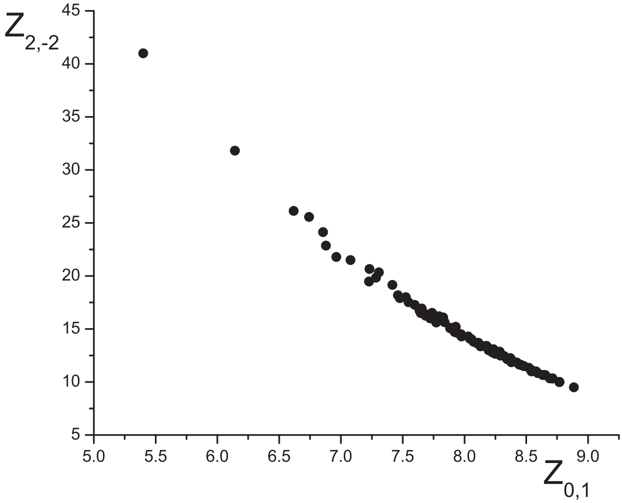

Fig. 5. Same data as in Fig. 2 for $p = 2$, $q = -2$.

These results clearly suggest the following:

(a) The usage of geometric and arithmetic means in the GA index was not a necessary choice. Other $Z_{p,q}$ indices would be equally useful for any chemical (QSPR and QSAR) applications.

(b) There is no (scientific) justification to introduce any further structure descriptor of this kind, i. e., a single $Z_{p,q}$ index (that is GA) is sufficient, and more such indices would be superfluous.

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