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Comparing Degree-Ratio Sombor and Sombor Indices

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Abstract

The Sombor index is a much investigated vertex-degree-based graph invariant defined as $SO = \sum_{uv} \sqrt{d(u)^2 + d(v)^2}$, where $d(u)$ denotes the degree of the vertex u of the underlying graph. Recently, in [10], a new "degree-ratio" variant of the Sombor index is conceived, defined as $DRSO = \sum_{uv} \sqrt{[d(u)/d(v)]^2 + [d(v)/d(u)]^2}$. In this paper, we establish the structural features determining the details of the relations between $DRSO$ and SO.

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1 Introduction

Let G be a simple graph with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. The number of vertices of G is $|\mathbf{V}(G)| = n$. Denote by uv the edge of G, connecting the vertices u and v. Let $d(u)$ be the degree (= number of first neighbors) of the vertex $u \in \mathbf{V}(G)$. Then the *Sombor index* is defined as

$$SO = SO(G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{d(u)^2 + d(v)^2}\,. \tag{1}$$

This vertex-degree-based topological index was introduced in 2021 [3]. Since then, it attracted much attention of both chemists and mathematicians, see the reviews [5, 8, 11]. Recently, Nyauli and Buragohain put forward the *degree-ratio Sombor index*, defined as

$$DRSO = DRSO(G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{\left[\frac{d(u)}{d(v)}\right]^2 + \left[\frac{d(v)}{d(u)}\right]^2}\,. \tag{2}$$

It is worth noting that both SO and $DRSO$ were conceived using (different) geometric arguments.

In the considerations that follow, we will need two other, well known and much studied, vertex-degree-based topological indices: the first Zagreb index (M_1), [6,7,9], and the symmetric division deg index (SDD), [1,2,12]. These are defined as

$$M_1 = M_1(G) = \sum_{u \in \mathbf{V}(G)} d(u)^2 = \sum_{uv \in \mathbf{E}(G)} \big[d(u) + d(v)\big] \tag{3}$$

and

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

The formal algebraic differences between SO and $DRSO$ are seen from Eqs. (1) and (2). There are also some more subtle differences in the geometric ideas lying behind SO (see [3]) and behind $DRSO$ (see [10]). How different SO and $DRSO$ are is best seen from the fact that the

complete graph K_n has maximal SO-value, which is not the case with $DRSO$. At the present moment, the graph with maximal $DRSO$-value is not known, but it certainly is not K_n, since $DRSO(S_n) > DRSO(K_n)$ for $n \geq 4$, where S_n is the star tree.

Therefore, it seems to be worth examining the relations that exist between $DRSO$ and SO. That these relations are far from being simple is seen from Figs. 1 and 2.

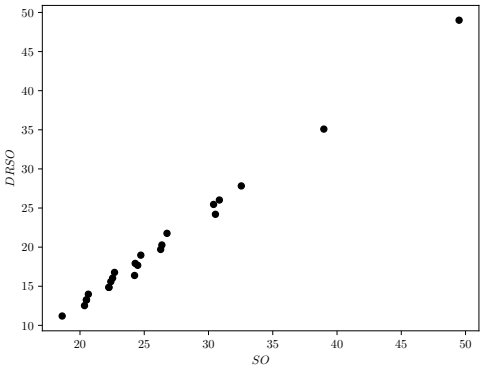

Figure 1. The degree-ratio Sombor indices of 8-vertex trees plotted versus the respective Sombor indices.

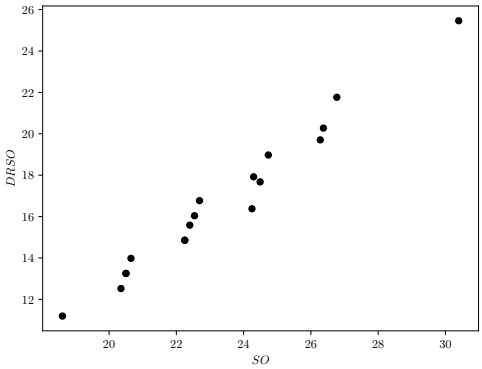

Figure 2. The degree-ratio Sombor indices of 8-vertex molecular trees plotted versus the respective Sombor indices.

2 Analyzing the $DRSO/SO$ correlation

The results displayed in Figs. 1 and 2 correspond to trees with $n = 8$ vertices. Analogous are also the correlations for other values of n, as well as for the (few) examined correlations for cycle-connecting graphs.

The data points in Figs. 1 and 2 are grouped in several clusters. In particular, in Fig. 1 there are 8 such clusters, of which the left-hand one and the two right-hand ones consist of a single element. This clustering is much better seen in Fig. 2, with six clusters, of which the most left and most right are single-element.

Numerical testing (for each value of n) revealed that all data points belonging to a particular cluster pertain to trees with mutually equal first Zagreb index (M_1). Data points belonging to different clusters, pertain to trees with different M_1-values. In fact, each value of M_1 that the considered trees may have, corresponds to a particular cluster. In other words, the number of clusters is equal to the number of different M_1-values.

The data points within a cluster are arranged in a linearly increasing manner, although significant deviations from the line occur in some cases. All such lines have (nearly) equal slopes.

3 Explaining the $DRSO/SO$ correlation

The fact that the first Zagreb index plays a decisive role in the correlation between the Sombor and degree-ratio Sombor indices is no surprise whatsoever. Namely, it has long been known that SO is bounded by M_1 both by below and by above, that is [4]

$$\frac{1}{\sqrt{2}}\, M_1(G) \leq SO(G) < M_1(G)\,.$$

Indeed, a nearly perfect linear correlation exists between SO and M_1, as illustrated in Fig. 3.

In an analogous manner, $DRSO$ is bounded by SDD, namely [10]

$$\frac{1}{\sqrt{2}}\, SDD(G) \leq DRSO(G) < SDD(G)\,.$$

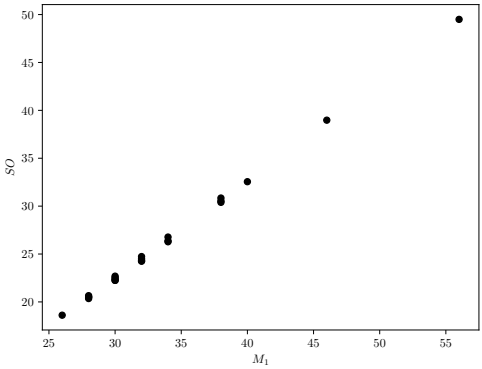

Figure 3. Sombor indices of 8-vertex trees plotted versus the respective first Zagreb indices.

resulting in an equally good linear correlation between $DRSO$ and SDD, cf. Fig. 4.

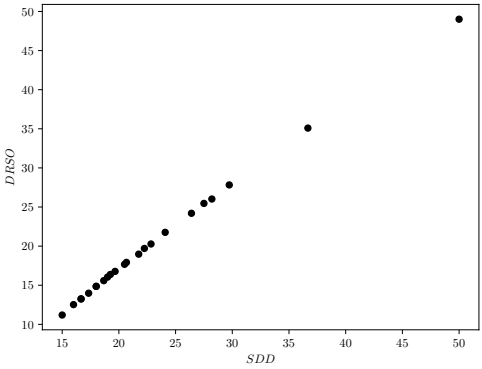

Figure 4. Degree-ratio Sombor indices of 8-vertex trees plotted versus the respective symmetric division deg indices.

On the other hand, the correlation between M_1 and SDD is far from significant, as seen from Fig. 5.

From Fig. 5 we see that trees having the same M_1-value, may possess several mutually different SDD-values. Then, bearing in mind the linearity of the SO/M_1 and $DRSO/SDD$ correlations, cf. Figs. 3 and 4, this property of the SDD/M_1 correlation implies that the data points

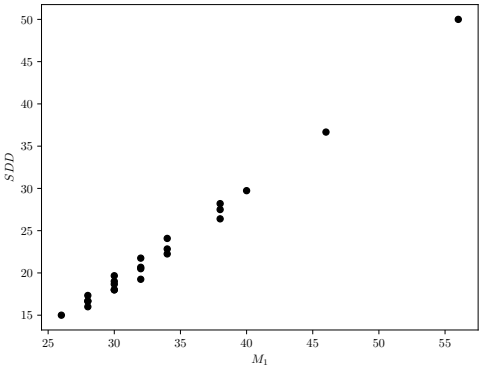

Figure 5. Symmetric division deg indices of 8-vertex trees plotted versus the respective first Zagreb indices. Note that several different SDD-values are associated with a particular M_1-value.

in the $DRSO/SO$ plots are grouped into M_1-dependent clusters. Within each such cluster, the respective trees have mutually equal M_1-values, but different SDD-values.

4 Fine details of the $DRSO/SO$ correlation

In Fig. 6, we show the plot of $DRSO$ versus SO for molecular trees with $n = 10$ vertices. Of course, the grouping of the data points is equivalent to that in Fig. 2.

In Fig. 6, there are 8 clusters, of which only the most-left one has a single element. We number the clusters (from left to right) by 1, 2, ..., 8. In Fig. 6, some fine details of this grouping are seen more clearly. Namely, in cluster No. 4, the data points form two nearly-lying lines, whereas in cluster No. 5 an outlier from the line is seen. In clusters 2, 3, 6, 7, and 8, the data points form a single (straight) line.

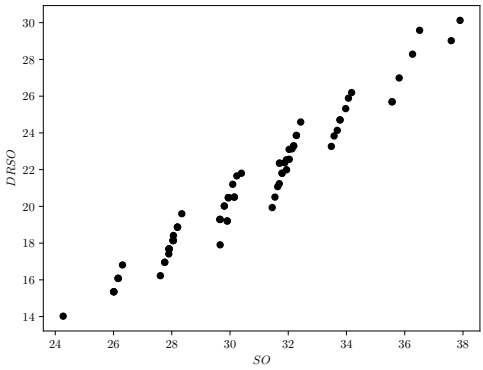

Figure 6. The degree-ratio Sombor indices of 10-vertex molecular trees plotted versus the respective Sombor indices.

In order to understand the reason of this phenomenon, we need a simple theorem.

Theorem 1. *If T is an n-vertex molecular tree with n_3 vertices of degree 3 and n_4 vertices of degree 4, then*

$$M_1(T) = 4n - 6 + 2(n_3 + 3\,n_4)\,. \tag{4}$$

Proof. Molecular graphs have only vertices of degree 1, 2, 3, and 4. Let their number be denoted by n_1 , n_2 , n_3, and n_4, respectively. A molecular tree of order n has $n - 1$ edge. Then

$$\begin{aligned} n &= n_1 + n_2 + n_3 + n_4 && (5)\\ 2(n-1) &= n_1 + 2n_2 + 3n_3 + 4n_4 && (6)\\ M_1(T) &= n_1 + 4n_2 + 9n_3 + 16n_4 && (7) \end{aligned}$$

where (7) is a direct consequence of the definition of the first Zagreb index, Eq. (3). Combining (5) and (6) we get

$$\begin{aligned} n_1 &= n_3 + 2n_4 + 2\\ n_2 &= n - 2 - 2n_3 - 3n_4 \end{aligned}$$

which substituted back into (7) yields

$$M_1(T) = (2n_4 + 2) + 4(n - 2 - 2n_3 - 3n_4) + 9n_3 + 16n_4$$

resulting in Eq. (4). ■

Corollary 2. *Let T_1 and T_2 be two molecular trees of equal order. If both have equal $(n_3 + 3n_4)$-values, then $M_1(T_1) = M_1(T_2)$.*

In particular, if $n_3 = 5$, $n_4 = 0$ in T_1, whereas $n_3 = 2$, $n_4 = 1$ in T_2, then $M_1(T_1) = M_1(T_2)$.

Corollary 3. *If there exist trees T_1 and T_2 specified in Corollary 2, then in the DRSO/SO plot their data points belong to the same cluster, but lie on two distinct close-lying lines.*

In order to illustrate Corollary 3, we first consider the correlation depicted in Fig. 2.

In the case $n = 8$, there exist four molecular trees with $M_1 = 32$, resulting in a 4-membered cluster (cluster No. 4 in Fig. 2). Three of these, trees (pertaining to 2,2-dimethylhexane, 3,3-dimethylhexane, and 3-methyl,3-ethylepentane) have $n_3 = 0$, $n_4 = 1$, whereas one tree (pertaining to 2,3,4-trimethylpentane) has $n_3 = 3$, $n_4 = 0$. The latter becomes the outlier data point in the cluster No. 4. According to Corollary 3, this outlier can be viewed as a single-point line.

Next we consider the case $n = 10$ depicted in Fig. 6. In its cluster No. 4 are the data points of molecular trees with $M_1 = 40$. There exist several molecular trees with this value of first Zagreb index. Some of these trees (one of which pertaining to 2,2-dimethyloctane) have $n_3 = 0$, $n_4 = 1$, whereas some other (one of which pertaining to 2,3,4-trimethylheptane) have $n_3 = 3$, $n_4 = 0$. These two types of molecular trees, having equal M_1-values but a different branching pattern, induce the splitting of the data points of the $DRSO/SO$ correlation into two near-lying (almost parallel) straight lines.

In the cluster No. 5 on Fig. 5 are the data points with $M_1 = 42$. According to Eq. (4), for these molecular trees, $n_3 + 3n_4 = 4$, which will happen is either $n_3 = 4$, $n_4 = 0$ or $n_3 = 1$, $n_4 = 1$. In the considered

cluster, there is an outlier from the line formed by the other data points. Its analysis is analogous to that of cluster No. 4 in Fig. 2: The outlier corresponds to the case $n_3 = 4$, $n_4 = 0$. In fact, there are two molecular trees with $n_3 = 4$ and $n_4 = 0$, both having same $DRSO$– and same SO-values and thus forming a single data point. These are the molecular graphs of 2,3,4,5-tetramethylhexane and 2,4-dimethyl,3-isopropylpentane.

In any other molecular tree of order 10, the above multiple choice of the $(n_3 + 3n_4)$-value cannot happen. Therefore, in the clusters Nos. 2, 3, 6, 7, and 8 in Fig. 6, the data points form (and must form) a single line.

5 Concluding remarks

By means of the present analysis, the main features of the correlation between the degree-ratio and the ordinary Sombor indices have been described, and to a reasonable extent explained and made understandable.

In this work, we reported the $DRSO/SP$ plots for molecular trees up to $n = 10$. In the case of larger values of n, splitting of data points into two (and in case of very large n, into three and more) lines happens more frequently. For instance, the pair $(n_3 = 0\,,\, n_4 = 2)$ and $(n_3 = 3\,,\, n_4 = 1)$ will first time occur at $n = 11$.

In the present work we did not pay much attention to cycle-containing (molecular) graphs. Their study may thus remain a task for the future. To this end, we state here the generalized version of Theorem 1:

Theorem 4. *If G is an n-vertex c-cyclic molecular graph, with n_3 vertices of degree 3 and n_4 vertices of degree 4, then*

$$M_1(T) = 4n + 6(c - 1) + 2(n_3 + 3\,n_4)\,. \tag{8}$$

By Theorem 4, Corollaries 2 and 3 are applicable also in the case of cycle-containing molecular graphs.

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