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Geometric Approach to Degree–Based Topological Indices: Sombor Indices

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Abstract

An alternative interpretation of vertex–degree–based topological indices is proposed. Based on it, a class of novel graph invariants is considered, of which the simplest is the Sombor index SO, defined via the term $\sqrt{\deg(u)^2 + \deg(v)^2}$. Basic properties of SO are established.

1 Introduction

In this paper we are concerned with simple graphs, that is graphs without directed, weighted or multiple edges, and without self loops. Let G be such a graph with n vertices and m edges. Its vertex set is $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$ and its edge set $\mathbf{E}(G)$. The degree (= number of first neighbors) of the vertex v_i is denoted by $\deg(v_i)$. If the vertices v_i and v_j are adjacent, then the edge connecting them is labeled by e_{ij}.

In the mathematical and chemical literature, several dozens of vertex–degree–based graph invariants (usually referred to as “topological indices”) have been introduced and extensively studied [4, 6]. Their general formula is

$$TI = TI(G) = \sum_{e_{ij} \in \mathbf{E}(G)} F\big(\deg(v_i), \deg(v_j)\big) \tag{1}$$

where $F(x, y)$ is some function with the property $F(x, y) = F(y, x)$.

A not necessarily complete list of these topological indices is given in Table 1; for details see [4, 6] and the references cited therein.

$F(x,y)$	name
$x+y$	first Zagreb index
xy	second Zagreb index
$(x+y)^2$	first hyper-Zagreb index
$(xy)^2$	second hyper-Zagreb index
$x^{-3}+y^{-3}$	modified first Zagreb index
$\|x-y\|$	Albertson index
$(x/y+y/x)/2$	extended index
$(x-y)^2$	sigma index
$1/\sqrt{xy}$	Randić index
$\sqrt{xy}$	reciprocal Randić index
$1/\sqrt{x+y}$	sum-connectivity index
$\sqrt{x+y}$	reciprocal sum-connectivity index
$2/(x+y)$	harmonic index
$\sqrt{(x+y-2)/(xy)}$	atom-bond-connectivity (ABC) index
$[xy/(x+y-2)]^3$	augmented Zagreb index
x^2+y^2	forgotten index
$x^{-2}+y^{-2}$	inverse degree
$2\sqrt{xy}/(x+y)$	geometric-arithmetic index
$(x+y)/(2\sqrt{xy})$	arithmetic-geometric index
$xy/(x+y)$	inverse sum indeg index
$x+y+xy$	first Gourava index
$(x+y)xy$	second Gourava index
$(x+y+xy)^2$	first hyper-Gourava index
$[(x+y)xy]^2$	second hyper-Gourava index
$1/\sqrt{x+y+xy}$	sum-connectivity Gourava index
$\sqrt{(x+y)xy}$	product-connectivity Gourava index

Table 1. The main vertex–degree–based topological indices of the form (1).

Note that because of the identity [3]

$$\sum_{e_{ij}\in\mathbf{E}(G)}\left[\deg(v_i)^\alpha+\deg(v_j)^\alpha\right]=\sum_{v_i\in\mathbf{V}(G)}\deg(v_i)^{\alpha+1}$$

the first Zagreb, modified first Zagreb, forgotten, and inverse degree indices are equal to

$$\sum_{v_i\in\mathbf{V}(G)}\deg(v_i)^2\quad,\quad\sum_{v_i\in\mathbf{V}(G)}\frac{1}{\deg(v_i)^2}\quad,\quad\sum_{v_i\in\mathbf{V}(G)}\deg(v_i)^3\quad,\quad\sum_{v_i\in\mathbf{V}(G)}\frac{1}{\deg(v_i)}$$

respectively.

To each of the indices listed in Table 1, it is possible to associate a "reduced" index, replacing x and y by $x-1$ and $y-1$. For formal reasons, we do not mention indices based on vertex degrees of the graph and of its complement (Dakshayani, Lanzhou indices and similar [4]).

In this paper we present a novel approach to the vertex–degree–based topological indices of (molecular) graphs.

2 An alternative interpretation of Eq. (1)

The term $\sum_{e_{ij}\in\mathbf{E}(G)}$ in Eq. (1) is traditionally interpreted as summation over all pairs of adjacent vertices of the graph G. Equally plausible would be to consider it as summation over all edges of the graph G. If so, then the contribution of an edge e_{ij} would depend on the pair (x, y) where $x = \deg(v_i)$ and $y = \deg(v_j)$. In what follows, we shall always assume that $x \leq y$.

Definition 1. The ordered pair (x, y), where $x = \deg(v_i)$, $y = \deg(v_j)$, $x \leq y$, is the *degree-coordinate* (or *d-coordinate*) of the edge $e_{ij} \in \mathbf{E}(G)$. For brevity, this edge will be referred to as an (x, y)-edge. In the (2-dimensional) coordinate system, it pertains to a point called the *degree-point* (or *d-point*) of the edge e_{ij}.

Definition 2. The point with coordinates (y, x) is the *dual-degree-point* (or *dd-point*) of the edge e_{ij}.

Definition 3. The distance between the d-point (x, y) and the origin of the coordinate system is the *degree-radius* (or *d-radius*) of the edge e_{ij}, denoted by $r(x, y)$.

Based on elementary geometry (using Euclidean metrics), we have

$$r(x,y) = \sqrt{x^2 + y^2}\,. \tag{2}$$

From Eq. (2), we immediately see that a d-point and and the corresponding dd-point have equal degree-radii. For the geometric interpretation of degree–based topological indices, the following property would be of great value.

Property 4. *Two degree-points have equal degree-radii if and only if they coincide, i.e., if and only if both have the same degree-coordinates.*

Unfortunately, Property 4 is not generally valid. The smallest counterexample is provided by the points with coordinates $(1, 7)$ and $(5, 5)$, both with radius $r = \sqrt{50}$. Fortunately, however, Property 4 holds for all molecular graphs (in which $\deg(v) \leq 4$), and can thus be used in chemical applications.

It is remarkable that the function $F(x, y) = \sqrt{x^2 + y^2}$ has not been used is the theory of vertex–degree–based topological indices, cf. Table 1. The above considerations motivate us to introduce a new such index. defined as

$$SO = SO(G) = \sum_{e_{ij}\in\mathbf{E}(G)} \sqrt{\deg(v_i)^2 + \deg(v_j)^2} \tag{3}$$

which we propose to be named *Sombor index*.*

In the subsequent section we establish some basic properties of the Sombor index.

3 Mathematical properties of the Sombor index

From the definition of the Sombor index, Eq. (3), we straightforwardly obtain:

Theorem 1. *Let K_n be the complete graph of order n, and $\overline{K_n}$ its complement, the edgeless graph. Then for any graph G of order n,*

$$SO(\overline{K_n}) \leq SO(G) \leq SO(K_n)\,.$$

Equality holds if and only if $G \cong \overline{K_n}$ or $G \cong K_n$. Recall that $SO(\overline{K_n}) = 0$ and $SO(K_n) = n(n-1)^2/\sqrt{2}$.

Theorem 2. *Let P_n be the path of order n. Then for any connected graph G of order n,*

$$SO(P_n) \leq SO(G) \leq SO(K_n)\,.$$

Equality holds if and only if $G \cong P_n$ or $G \cong K_n$. Recall that $SO(P_2) = \sqrt{2}$ whereas $SO(P_n) = 2\sqrt{5} + 2(n-3)\sqrt{2}$ for $n \geq 3$.

Proof. The upper bound in Theorem 2 follows from Theorem 1.

In order to deduce the lower bound, first note that by deleting an edge from the graph G, its SO-index necessarily decreases. Therefore, the connected graph with minimum SO must be a tree.

The cases $n = 2$ and $n = 3$ are trivial. Therefore, we assume that $n \geq 4$.

By direct checking it is easy to verify that among edges that can occur in trees, the $(1,2)$-edge has minimal degree-radius $r(1,2) = \sqrt{5}$, and the next-minimal is $r(2,2) = 2\sqrt{2}$.

The path P_n possesses two $(1,2)$- and $n-3$ $(2,2)$-edges. The tree Q_n possessing three $(1,2)$-edges and as many as possible $(2,2)$-edges, must also posses three $(2,3)$-edges, for which $r(2,3) = \sqrt{13}$. Because

$$3r(1,2) + 3r(2,3) + (n-7)r(2,2) > 2r(1,2) + (n-3)r(2,2)$$

it follows that $SO(Q_n) > SO(P_n)$ holds. By an analogous argument, trees possessing more than three $(1,2)$-edges also have greater SO-value than P_n. The SO-indices of trees with a single $(1,2)$-edge or without such edges evidently exceed $SO(P_n)$. ■

*The ideas outlined in this paper emerged in Sombor, in the Summer of 2020, mainly during the time that the author was spending on chemodialysis.

Theorem 3. *Let S_n be the star of order n. Then for any tree T of order n,*

$$SO(P_n) \leq SO(T) \leq SO(S_n)\,.$$

Equality holds if and only if $T \cong P_n$ or $T \cong S_n$. Recall that $SO(S_n) = (n{-}1)\sqrt{n^2{-}2n{+}2}$.

Proof. The lower bound in Theorem 3 follows from Theorem 2.

In order to deduce the upper bound, observe that the degree-coordinate (x, y) of any edge of an n-vertex tree satisfies $x + y \leq n$. Therefore, the greatest values of $r(x, y)$ will be achieved if $x + y = n$.

By an easy calculation, it can be verified that

$$r(1, n-1) > r(2, n-2) > \cdots > r(\lfloor n/2 \rfloor, \lceil n/2 \rceil)\,.$$

All edges of the star S_n are of $(1, n-1)$ type. Thus, all edges of the star have maximal possible degree-radii. Therefore, the star has maximal SO-value. ∎

4 Applications

Considering the edges of a graph as points in the two-dimensional coordinate system, we can establish distances between them.

1° The distance between a d-point (x, y) and its dual (y, x) is equal to

$$\sqrt{(x-y)^2 + (y-x)^2} = \sqrt{2}\,|x-y|$$

which implies that the respective Sombor index is just the Albertson index [2]

$$Alb(G) = \sum_{e_{ij} \in \mathbf{E}(G)} \big|\deg(v_i) - \deg(v_j)\big|$$

multiplied by $\sqrt{2}$. Thus, the earlier much studied Albertson index, used for quantifying graph irregularity [1, 5], can now be interpreted as the sum of the distances between the d- and dd-points of the underlying graph.

2° The d-point of an isolated edge has coordinates $(1, 1)$. The distances between the degree-points of a graph and of isolated edges leads to

$$SO_{red} = SO_{red}(G) = \sum_{e_{ij} \in \mathbf{E}(G)} \sqrt{\big(\deg(v_i) - 1\big)^2 + \big(\deg(v_j) - 1\big)^2} \tag{4}$$

which is just the reduced version of the Sombor index.

3° For a graph with n vertices and m edges, the average vertex degree is $2m/n$. The respective d-point has coordinates $(2m/n, 2m/n)$. The distances between the degree-points of a graph and of this average point leads to

$$SO_{avr} = SO_{avr}(G) = \sum_{e_{ij} \in \mathbf{E}(G)} \sqrt{\left(\deg(v_i) - \frac{2m}{n}\right)^2 + \left(\deg(v_j) - \frac{2m}{n}\right)^2} \qquad (5)$$

This degree-based graph invariant is equal to zero for regular graphs and is positive-valued for non-regular graphs. Thus, the average Sombor index, Eq. (5), may be considered as a measure of graph irregularity [1,5].

The reduced Sombor index, Eq. (4), and the average Sombor index, Eq. (5), are two new structure-descriptors whose properties await to be examined.

4° Assuming that Property 4 is satisfied (which is the case with all molecular graphs), the edges of the graph G can be, in a consistent manner, ordered by increasing degree-radii. This makes it possible to compare two graphs with equal n and m (that is, two isomeric molecular graphs) edge-by-edge. In particular, if for $i = 1, 2, \ldots, m$, the d-radius of the i-th edge of a graph G is greater than or equal to the respective d-radius of another (isomeric) graph G^*, then G *degree-dominates* G^*. If the i-th d-radii of G and G^* are equal for all $i = 1, 2, \ldots, m$, then G and G^* are *degree-equivalent*. Degree domination is a sufficient, but not necessary condition for the relation $SO(G) \geq SO(G^*)$. If the graphs G and G^* are degree-equivalent, then, of course, $SO(G) = SO(G^*)$.

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