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Sombor Index of Kragujevac Trees

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Abstract: The paper is concerned with the Sombor index (SO) of Kragujevac trees (Kg). A slightly more general definition of Kg is offered. SO is a recently introduced degree-based topological index. A general combinatorial expression for $SO(Kg)$ is established. The species with minimum and maximum $SO(Kg)$-values are determined.

Keywords: Sombor index, Kragujevac tree, Zagreb index.

1 Introduction

In this paper we use the following (standard) graph-theoretical notation and terminology. Let G be a simple graph, with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. Then $|\mathbf{V}(G)|$ and $|\mathbf{E}(G)|$ are the number of vertices and edges of G. By $uv \in \mathbf{E}(G)$ we denote the edge of G, connecting the vertices u and v. The degree (= number of first neighbors) of a vertex $u \in \mathbf{V}(G)$ is denoted by $d(u)$. For other graph-theoretical notions, the readers are referred to textbooks [4, 15, 23].

In the mathematical and chemical literature, some fifty or more different vertex-degree-based graph invariants have been defined and examined. The oldest such invariant, conceived as early as in the 1970s, is the *first Zagreb index*, Zg [13]. One of the newest such invariant is the *Sombor index*, SO [11, 12]. They are defined as

$$Zg = Zg(G) = \sum_{u \in \mathbf{V}(G)} d(u)^2 \tag{1.1}$$

$$SO = SO(G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{d(u)^2 + d(v)^2}\,. \tag{1.2}$$

Recently the Sombor index attracted much attention and numerous of its mathematical properties have already been established (see, for instance, [6, 7, 9, 16, 17, 20]). For chemical applications of SO see [2, 21].

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In this paper we are concerned with a class of trees, called *Kragujevac trees*, defined below. Kragujevac trees emerged within the study of the atom-bond-connectivity (*ABC*) index. It was conjectured that the graph with minimal *ABC*-index is a Kragujevac tree [14]. Later it was found that the conjecture is violated for graphs with larger number of vertices [8]. For more details on this matter see the recent survey [1] and the references cited therein. Nevertheless, Kragujevac trees were studied in numerous papers (see, for instance, [3, 5, 10, 18, 19, 22]). In the present article we focus our attention to the Sombor index of Kragujevac trees.

2 Preliminaries

Definition 2.1. *Let n be a positive integer. For $k = 0, 1, \ldots, n$, we denote by B_k the rooted tree with $2k+1$ vertices, constructed by attaching k two-vertex branches to the root.*

In Fig. 1 a few examples are depicted, illustrating Definition 2.1.

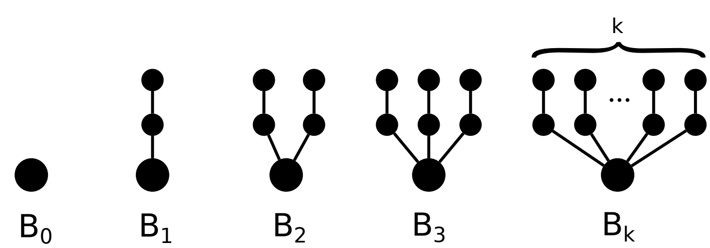

Fig. 1. The rooted trees B_0, B_1, B_2, B_3, and B_k. Their roots are indicated by large dots.

Let k_i, $i = 1, 2, \ldots, n$, be non-negative integers, such that

$$0 \leq k_1 \leq k_2 \leq \cdots \leq k_n . \tag{2.1}$$

Definition 2.2. *Let the parameters $k_1, k_2, \ldots, k_n$ satisfy the condition (2.1). Then the Kragujevac tree $Kg(k_1, k_2, \ldots, k_n)$ is the tree obtained from B_{k_1}, B_{k_2}, $\ldots B_{k_n}$, by connecting their roots to a new vertex.*

In Fig. 2 an example is depicted, illustrating Definition 2.2.

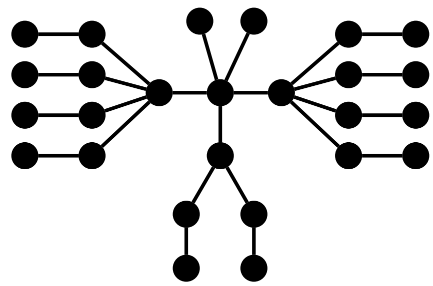

Fig. 2. The Kragujevac tree $Kg(0,0,2,4,4)$, for which $n = 5$ and $K = 10$. Note that there exist 30 mutually non-isomorphic Kragujevac trees with parameters $n = 5$ and $K = 10$.

In the original definition of Kragujevac trees [14], because of their expected relation to the minimum-*ABC* graphs, it was required that $k_1 \geq 2$. Since we now know that such a relation does not exist, in this paper we decided to use the mathematically more appropriate choice of parameters, Eq. (2.1).

According to Definition 2.2, the Kragujevac tree with parameters $k_1, k_2, \ldots, k_n$ has

$$1 + \sum_{i=1}^{n} (2\,k_i + 1) = 2K + n + 1$$

vertices, where

$$\sum_{i=1}^{n} k_i = K\,. \tag{2.2}$$

Throughout this paper, both n and K are considered to have fixed values.

Directly from Definitions 2.1 and 2.2 we obtain:

Proposition 2.1. *Let $Kg(k_1, k_2, \ldots, k_n)$ be a Kragujevac tree. Then it has K vertices of degree 1, K vertices of degree 2, a vertex of degree $k_i + 1$ for each $i = 1, 2, \ldots, n$, and a vertex of degree n.*

An edge connecting a vertex of degree i and a vertex of degree j will be referred to as an (i, j)-edge.

Proposition 2.2. *Let $Kg(k_1, k_2, \ldots, k_n)$ be a Kragujevac tree. Then it has K $(1,2)$-edges, k_i $(k_i + 1, 2)$-edges for each $i = 1, 2, \ldots, n$, and a $(k_i + 1, n)$-edge for each $i = 1, 2, \ldots, n$.*

Applying Proposition 2.1 to Eq. (1.1) we arrive at:

Lemma 2.1. *Let $Kg = Kg(k_1, k_2, \ldots, k_n)$ be the Kragujevac tree whose parameters satisfy Eqs. (2.1) and (2.2). Then*

$$\begin{aligned} Zg(Kg) &= K \cdot 1^2 + K \cdot 2^2 + \sum_{i=1}^{n} (k_i+1)^2 + n^2 \\ &= 7K + n(n+1) + \sum_{i=1}^{n} k_i^2 \,. \end{aligned} \tag{2.3}$$

In an analogous manner, from Proposition 2.2 and Eq. (1.2) we obtain:

Lemma 2.2. *With the same notation as in Lemma 2.1,*

$$\begin{aligned} SO(Kg) &= K\sqrt{1^2+2^2} + \sum_{i=1}^{n} k_i \sqrt{(k_i+1)^2+2^2} + \sum_{i=1}^{n} \sqrt{(k_i+1)^2+n^2} \\ &= \sqrt{5}K + n(n+1) + \sum_{i=1}^{n} \left[k_i \sqrt{k_i^2+2k_i+5} + \sqrt{k_i^2+2k_i+n^2+1} \right] . \end{aligned} \tag{2.4}$$

3 Main Results

In this section we determine the Kragujevac trees that are extremal (minimal and maximal) with respect to the Sombor index. In order to achieve this goal, we first need to do the same for the first Zagreb index. We start with the following Lemma 3.1. Its proof is based on elementary arithmetic and will be skipped.

Lemma 3.1. *Let k_i, $i = 1, 2, \ldots, n$, be integers satisfying Eqs. (2.1) and (2.2). Let $S = \sum_{i=1}^{n} k_i^2$.*

(a) The sum S assumes its minimal value if and only if

$$k_i \in \left\{ \left\lfloor \frac{K}{n} \right\rfloor , \left\lceil \frac{K}{n} \right\rceil \right\} . \tag{3.1}$$

More precisely, if $K \equiv p \pmod{n}$, then $k_i = \lfloor K/n \rfloor$ $(n-p)$ times, whereas $k_i = \lceil K/n \rceil$ p times.

(b) The sum S assumes its maximal value if and only if

$$k_1 = k_2 = \cdots = k_{n-1} = 0 \qquad \text{and} \qquad k_n = K \,. \tag{3.2}$$

Lemma 3.2. *Using the same notation as in Lemma 3.1,*

$$K \leq S \leq K^2 .$$

Proof. From Lemma 3.1(b), it is evident that

$$\max \left\{ \sum_{i=1}^{n} k_i^2 \right\} = K^2 .$$

We now show that

$$\min \left\{ \sum_{i=1}^{n} k_i^2 \right\} = K \tag{3.3}$$

If $p = 0$, then $\lfloor K/n \rfloor = \lceil K/n \rceil = K/n$, and relation (3.3) evidently holds.

Let $p \neq 0$ and $K = qn + p$ for some integers q and $p < n$. Then by Lemma 3.1(a),

$$\begin{aligned} \min \left\{ \sum_{i=1}^{n} k_i^2 \right\} &= (n-p) \left\lfloor \frac{K}{n} \right\rfloor + p \left\lceil \frac{K}{n} \right\rceil = (n-p) \left\lfloor \frac{K}{n} \right\rfloor + p \left(\left\lfloor \frac{K}{n} \right\rfloor + 1 \right) = n \left\lfloor \frac{K}{n} \right\rfloor + p \\ &= n \left\lfloor \frac{qn+p}{n} \right\rfloor + p = nq + p = K . \end{aligned}$$

□

Based on Lemma 3.1, using formula (2.3) and recalling that the parameters n and K are assumed to be constant, we can straightforwardly determine the Kragujevac trees extremal with respect to the first Zagreb index.

Theorem 3.1. *Let $Kg = Kg(k_1, k_2, \ldots, k_n)$ be the Kragujevac tree whose parameters satisfy Eqs. (2.1) and (2.2). Then $Zg(Kg)$ is minimal if and only if the condition (3.1) holds. $Zg(Kg)$ is maximal if and only if the condition (3.2) holds.*

By Lemma 3.2, from Eq. (2.3), we get:

Corollary 3.1. *If Kg is a Kragujevac tree with parameters n and K, then*

$$8K + n(n+1) \leq Zg(Kg) \leq 7K + K^2 + n(n+1) .$$

One should note that a results analogous to Theorem 3.1 was earlier communicated in [5, 19], but for the special case when $k_1 \geq 2$. Then the minimality condition would be same as in Theorem 3.1, whereas the maximality conditions is

$$k_1 = k_2 = \cdots = k_{n-1} \qquad \text{and} \qquad k_n = K - (n-1)k_1\,.$$

For such Kragujevac trees, instead of Corollary 3.1, we have

$$11K + K^2 - 4nK + 5n^2 - 3n \leq Zg(Kg) \leq 7K + K^2 + n(n+1)\,.$$

Bearing in mind formula (2.4), Lemmas 3.1 and 3.2 are insufficient for finding the extremal values of $SO(Kg)$. In order to achieve this goal, we need to use a different approach.

For any graph G, the Sombor index and the first Zagreb index are related as [17]

$$\frac{Zg(G)}{\sqrt{2}} \leq SO(G) \leq Zg(G)\,.$$

These inequalities indicate that the two indices should be linearly correlated. Indeed, in the case of trees (with a fixed number of vertices) this correlation was found to be remarkably good, see Figs. 3 and 4, and Table 1.

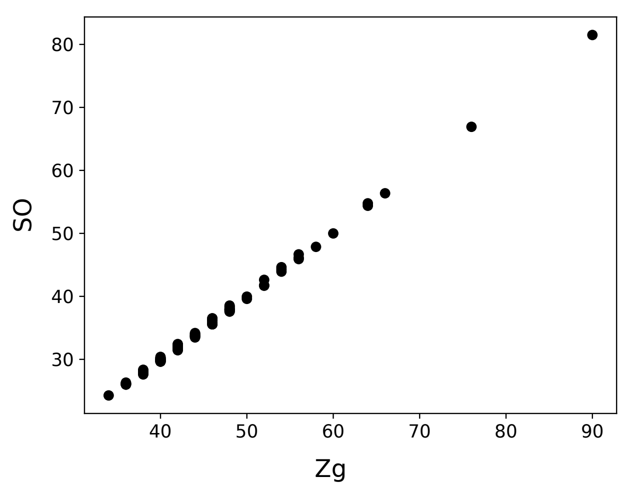

Fig. 3. Sombor indices (SO) of 10-vertex trees, plotted versus the respective first Zagreb indices (Zg), cf. Table 1.

N	a	b	R
10	1.019 ± 0.003	-10.81 ± 0.15	0.9994
11	1.015 ± 0.002	-11.99 ± 0.12	0.9993
12	1.011 ± 0.002	-13.13 ± 0.09	0.9993
13	1.008 ± 0.001	-14.29 ± 0.07	0.9992
14	1.005 ± 0.001	-15.43 ± 0.05	0.9991
15	1.003 ± 0.001	-16.59 ± 0.04	0.9990

Table 1. The parameters of the regression line $SO = a\,Zg + b$ for N-vertex trees; R = correlation coefficient.

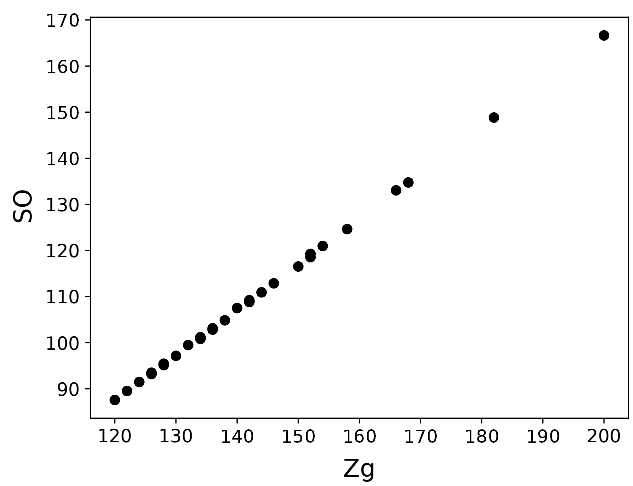

Fig. 4. Sombor indices (SO) of Kragujevac trees with parameters $n = 5$ and $K = 10$, plotted versus the respective first Zagreb indices (Zg); cf. caption of Fig. 2.

Bearing these numerical results in mind, we state the following replica of Theorem 3.1:

Claim 3.1. *Let $Kg = Kg(k_1, k_2, \ldots, k_n)$ be the Kragujevac tree whose parameters satisfy Eqs. (2.1) and (2.2). Then $SO(Kg)$ is minimal if and only if the condition (3.1) holds. $SO(Kg)$ is maximal if and only if the condition (3.2) holds.*

Assuming that Claim 3.1 is valid, we have the following results, paralleling Corollary 3.1:

Corollary 3.2. *If Kg is a Kragujevac tree with parameters n and K, then the maximum value of $SO(Kg)$ is*

$$n(n+1)+(n-1)\sqrt{n^2+1}+\sqrt{5}K+K\sqrt{K^2+2K+5}+\sqrt{K^2+2K+1+n^2}\,.$$

The minimum value of $SO(Kg)$ depends on the parameter p, defined via $K \equiv p \pmod{n}$. For $p=0$, this minimum value is

$$\sqrt{5}K+n(n+1)+n\left[\frac{K}{n}\sqrt{\left(\frac{K}{n}+1\right)^2+4}+\sqrt{\left(\frac{K}{n}+1\right)^2+n^2}\right]$$

whereas for $p>0$,

$$\sqrt{5}K+n(n+1)+(n-p)\left[\left(\frac{K-p}{n}+1\right)\sqrt{\left(\frac{K-p}{n}+1\right)^2+4}+\sqrt{\left(\frac{K-p}{n}+1\right)^2+n^2}\right]$$

$$+p\left[\left(\frac{K-p}{n}+2\right)\sqrt{\left(\frac{K-p}{n}+2\right)^2+4}+\sqrt{\left(\frac{K-p}{n}+2\right)^2+n^2}\right].$$

Although Claim 3.1 could be viewed as a conjecture, there should be almost no doubt in its correctness. It, nevertheless, remains a task for the future to construct a formal proof of this Claim.

4 Concluding Remarks

In this paper, a generalized definition of the Kragujevac trees is offered, and a combinatorial expression established for their Sombor indices, Eq. (2.4). Because of the perplexed form of formula (2.4), the study of the minimum and maximum values of $SO(Kg)$ had to relay on the existence of an excellent linear correlation between the Sombor and first Zagreb indices (both for general trees and for Kragujevac trees, see Figs. 3 and 4). The extremal cases are determined in Claim 3.1, whose rigorous mathematical proof remains a challenge for the future.

Extending the same argument, especially bearing in mind the numerical results presented in Fig. 4, we could conjecture a stronger relation:

Conjecture 4.1. *Let Kg_a and Kg_b be two Kragujevac trees with equal n and K values. Then*

$$Zg(Kg_a) > Zg(Kg_b) \;\Leftrightarrow\; SO(Kg_a) > SO(Kg_b)\,.$$

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