

Nirmala Index of Kragujevac Trees

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Abstract: The paper is concerned with the Nirmala index (N) of Kragujevac trees (Kg). The Kragujevac trees are a class of graphs that emerged within the study of the atom-bond connectivity index. The Nirmala index is a recently introduced degree-based structure descriptor. A general combinatorial expression for $N(Kg)$ is established. The trees with minimum and maximum $N(Kg)$ -values are determined.

Keywords: Nirmala index, Kragujevac tree, Zagreb index.

Mathematics Subject Classification: 05C05, 05C07, 05C09, 05C90

I. Introduction

In this paper we are concerned with the Nirmala index (N), a recently conceived vertex-degree-based graph invariant [1,2], and with the Kragujevac trees (Kg), a class of trees introduced in 2014 [3,4] within the search for the graphs with minimal atom-bond connectivity (ABC) index (for details see the recent review [5]). We establish a general combinatorial expression for the Nirmala index of Kragujevac trees and then study the extremal cases (the Kg -trees with minimal and maximal N -values).

We use standard graph-theoretical notation and terminology. By G we denote a graph with vertex set $V(G)$ and edge set $E(G)$. If $u, v \in V(G)$ are adjacent vertices of the graph G , then uv is an edge of G . The degree of a vertex u is denoted by $d(u)$. For other graph-theoretical notions see the textbooks [6,7].

At least fifty different vertex-degree-based graph invariants have been considered in the mathematical and chemical literature [8,9], the Nirmala index being one on them. It is defined as [1,2]

$$N = N(G) = \sum_{uv \in E(G)} \sqrt{d(u) + d(v)}. \quad (1)$$

For reasons that will become clear below, we shall need the classical first Zagreb index, that could be defined as [10]

$$Zg = Zg(G) = \sum_{uv \in E(G)} [d(u) + d(v)]. \quad (2)$$

We now provide the definition of the Kragujevac trees. Note that this definition (first put forward in [11]) slightly differs from what was used in earlier works on this topic [3,4,12,13].

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



In Figure 1 a few examples are depicted, illustrating Definition 1.

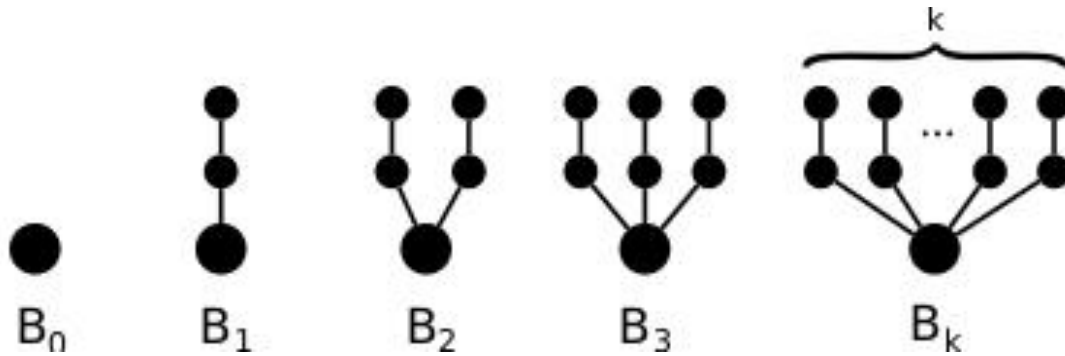


Figure 1. The rooted trees B_0, B_1, B_2, B_3 , and B_k . Their roots are indicated by large dots.

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

$$0 \leq k_1 \leq k_2 \leq \dots \leq k_n. \tag{3}$$

Let an auxiliary parameter K be defined as

$$\sum_{i=1}^n k_i = K. \tag{4}$$

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

Definition 2. Let the parameters k_1, k_2, \dots, k_n satisfy the condition (3). Then the Kragujevac tree $Kg(k_1, k_2, \dots, k_n)$ is the tree obtained from $B_{k_1}, B_{k_2}, \dots, B_{k_n}$ by connecting their roots to a new vertex.

In Figure 2 an example is depicted, illustrating Definition 2.

As a simple check of Definition 2, note that the number of vertices of the Kragujevac tree $Kg(k_1, k_2, \dots, k_n)$ is equal to

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

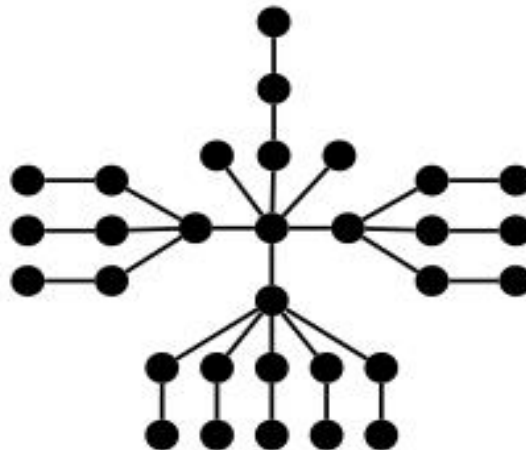


Figure 2. The Kragujevac tree $Kg(0,0,1,3,3,5)$ for which $n=6$ and $K=12$.

In the present article we focus our attention to the Nirmala index of Kragujevac trees.

II. General expression for the Nirmala index of Kragujevac trees

We say that an edge connecting a vertex of degree i and a vertex of degree j is an (i,j) -edge. Then directly from Definitions 1 and 2 we conclude that the Kragujevac tree $Kg(k_1, k_2, \dots, k_n)$ has:

- (a) K copies of $(1,2)$ -edges,
- (b) k_i copies of $(k_i + 1, 2)$ -edges for each $i = 1, 2, \dots, n$, and
- (c) a $(k_i + 1, n)$ -edge for each $i = 1, 2, \dots, n$.

Combining this with Eq. (1) we arrive at:

Lemma 1. Let $Kg = Kg(k_1, k_2, \dots, k_n)$ be the Kragujevac tree whose parameters satisfy Eqs. (3) and (4). Then

$$Zg(Kg) = K \times (1+2) + \sum_{i=1}^n [k_i(k_i + 1 + 2)] + \sum_{i=1}^n (k_i + 1 + n)$$

which implies

$$Zg(Kg) = 7K + n(n+1) + \sum_{i=1}^n (k_i)^2. \tag{5}$$

In an analogous manner, using Eq. (2) we obtain:

Lemma 2. Let $Kg = Kg(k_1, k_2, \dots, k_n)$ be the Kragujevac tree whose parameters satisfy Eqs. (3) and (4). Then

$$N(Kg) = K \times \sqrt{1+2} + \sum_{i=1}^n [k_i \times \sqrt{k_i + 1 + 2}] + \sum_{i=1}^n \sqrt{k_i + 1 + n}$$

which implies

$$N(Kg) = \sqrt{3}K + \sum_{i=1}^n [k_i \sqrt{k_i + 3} + \sqrt{k_i + n + 1}]. \tag{6}$$

III. Extremal values for the Nirmala index of Kragujevac trees

In this section we determine the Kragujevac trees that are extremal (minimal and maximal) with respect to the Nirmala index. In order to achieve this goal, we first turn to the first Zagreb index. Namely, below we show that in the case of both general trees and Kragujevac trees, N and Kg are strongly correlated, and (surprisingly!) this correlation is linear.

Bearing in mind Eq. (5) and assuming that n and K are constants, we see that the extremal values of $Zg(Kg)$ are determined by the extremal values of the sum of squares of k_i , $i = 1, 2, \dots, n$. In [11] the following elementary results were established.

Lemma 3. Let k_1, k_2, \dots, k_n be integers satisfying Eqs. (3) and (4). Then $K \leq \sum_{i=1}^n (k_i)^2 \leq K^2$. In addition,

$\sum_{i=1}^n (k_i)^2$ is minimal if and only if $k_i \in \left\{ \left\lfloor \frac{K}{n} \right\rfloor, \left\lceil \frac{K}{n} \right\rceil \right\}$. If $K \equiv q \pmod{n}$, then $k_i = \lfloor K/n \rfloor (n-q)$ times, and $k_i = \lceil K/n \rceil q$ times.

Lemma 4. Let k_1, k_2, \dots, k_n be integers satisfying Eqs. (3) and (4). Then,

$\sum_{i=1}^n (k_i)^2$ is maximal if and only if $k_1 = k_2 = \dots = k_{n-1} = 0$ and $k_n = K$.

Combining Lemmas 3 and 4 with Eq. (5) we directly determine the extremal values of $Zg(Kg)$.

Theorem 1. Let $Kg = Kg(k_1, k_2, \dots, k_n)$ be the Kragujevac tree whose parameters satisfy Eqs. (3) and (4). Then $Zg(Kg)$ is minimal if and only if the conditions of Lemma 3 hold. $Zg(Kg)$ is maximal if and only if the conditions of Lemma 4 hold.

One should note that results equivalent to Theorem 1 were earlier communicated in [12,13], but for the special case when $k_1 \geq 2$ (which was of relevance for using Kragujevac trees in connection with the minimal-ABC problem).

By examining formula (6) and comparing it with formula (5), we must conclude that Lemmas 3 and 4 are insufficient for finding extremal values of $N(Kg)$. The way out of this difficulty may be an almost perfect and nearly linear correlation between the first Zagreb and the Nirmala indices. In the case of trees (with a fixed number of vertices), the quality of this correlation is illustrated in Figures 3 and 4, and in Table 1.

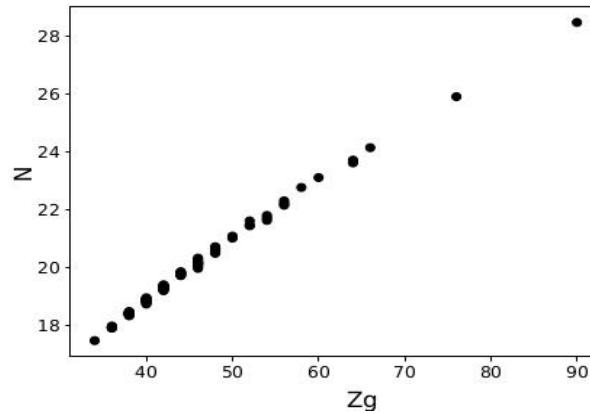


Figure 3. Nirmala indices (N) of 10-vertex trees, plotted versus the respective first Zagreb indices (Zg), cf. Table 1.

r	a	b	R
10	0.203	10.77	0.9977
11	0.200	12.12	0.9971
12	0.198	13.42	0.9967
13	0.197	14.72	0.9964
14	0.196	15.99	0.9962
15	0.196	17.26	0.9961

Table 1, The parameters of the regression line $N = aZg + b$ for r -vertex trees; R = correlation coefficient.

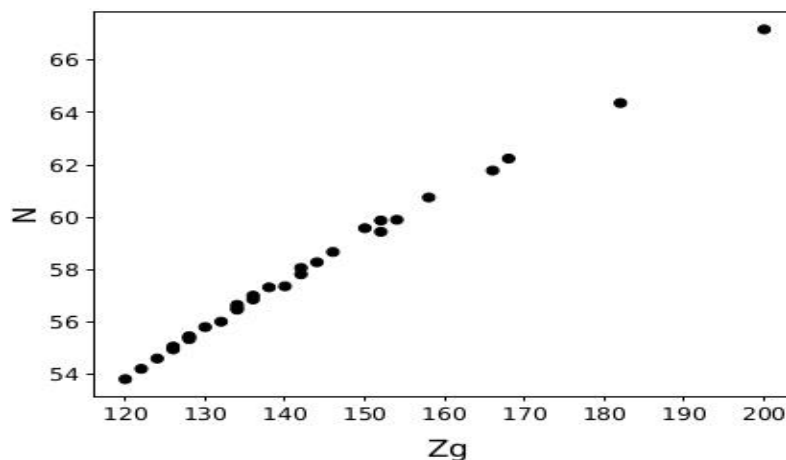


Figure 4. Nirmala indices (N) of Kragujevac trees with parameters $n=5$ and $K=10$, plotted versus the respective first Zagreb indices (Zg).

Bearing these numerical results in mind, we state the following parallel to Theorem 1:

Theorem 2. Let $Kg = Kg(k_1, k_2, \dots, k_n)$ be the Kragujevac tree whose parameters satisfy Eqs. (3) and (4). Then $N(Kg)$ is minimal if and only if the conditions of Lemma 3 hold. $N(Kg)$ is maximal if and only if the conditions of Lemma 4 hold.

Corollary 2.1. If Kg is a Kragujevac tree with parameters n and K , then the minimum value of $N(Kg)$ depends on the parameter q , defined via $K \equiv q \pmod{n}$.

For $q=0$, this minimum value is

$$N(Kg)_{\min} = \sqrt{3}K + \frac{1}{\sqrt{n}} \left[K\sqrt{K+3n} + \sqrt{K+n(n+1)} \right]$$

whereas for $q>0$,

$$N(Kg)_{\min} = \sqrt{3}K + (n-p) \left[\frac{K-p}{n} \sqrt{\frac{K-p}{n} + 3} + \sqrt{\frac{K-p}{n} + n+1} \right] + p \left[\left(\frac{K-p}{n} + 1 \right) \sqrt{\frac{K-p}{n} + 4} + \sqrt{\frac{K-p}{n} + n+2} \right].$$

Corollary 2.2. If Kg is a Kragujevac tree with parameters n and K , then the maximum value of $N(Kg)$ is

$$N(Kg)_{\max} = (n-1)\sqrt{n+1} + \sqrt{3}K + K\sqrt{K+3} + \sqrt{K+n+1}.$$

IV. Concluding remarks

In this section, we give some concluding remarks and indicate some possible directions for future work. The Sombor index is defined as [14]

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

Recently, the p -Sombor index of a graph was defined as [15]

$$SO_p = SO_p(G) = \sum_{uv \in E(G)} [d(u)^p + d(v)^p]^{1/p}$$

where $p \neq 0$. We easily see that SO_1 is the first Zagreb index and SO_2 is the Sombor index. In addition, SO_{-1} is the inverse sum indeg index [16].

Future works may be directed towards

- (a) establishing a general combinatorial expression for $SO_{-1}(Kg)$;
- (b) obtaining the minimal and maximal SO_{-1} of Kragujevac trees.

One of the present authors proposed the first (a, b) -KA index [17] and defined it as

$$KA_{a,b}^1(G) = \sum_{uv \in E(G)} [d_G(u)^a + d_G(v)^a]^b$$

where a and b are real numbers. The first (a, b) -KA indices are of interest for properly selected values of a and b . Clearly $KA_{1,1}^1(G)$ is the first Zagreb index, whereas $KA_{2, \frac{1}{2}}^1(G)$ is the Sombor index. The Nirmala index [1] is defined via $a=1$,

$b=1/2$. Therefore, it would be challenging

- (c) to study $KA_{a,b}^1(Kg)$ and its extremal values.

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