Communications in Combinatorics and Optimization
Vol. 9, No. 1 (2024), pp. 177-183
https://doi.org/10.22049/cco.2023.28058.1430

CCO
Commun. Comb. Optim.

Research Article

Extremal Kragujevac trees with respect to Sombor indices

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Received: 29 October 2022; Accepted: 3 January 2023
Published Online: 6 January 2023

Abstract: The concept of the Sombor indices of a graph was introduced by Gutman. A vertex-edge variant of the Sombor index of graphs is called the KG-Sombor index. Recently, the Sombor and KG-Sombor indices of Kragujevac trees were studied, and the extremal Kragujevac trees with respect to these indices were empirically determined. Here we give analytical proof of the results.

Keywords: Sombor index, KG-Sombor index, Kragujevac tree

AMS Subject classification: 05C35, 05C09, 05C90, 05C92

1. Introduction

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex v of G is the number of edges incident with v, and it is denoted by $d(v)$. By $e = uv \in E(G)$, we denote the edge of G connecting the vertices u and v. The degree of an edge e is the number of edges that are incident to e, and it is denoted by $d(e)$.

Gutman [6] introduced a vertex-degree-based graph invariant, named "Sombor index" of a graph G, denoted by $SO(G)$ and is defined by

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

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Although SO hasn't been long after being introduced, numerous of its mathematical properties and chemical applications have been established. Moreover, the various variants of SO index and their properties can be found in [1–5, 7, 10–14].
Recently, Kuli and Gutman introduced a vertex-edge variant of the Sombor index and it is defined as

$$KG(G) = \sum_{ue} \sqrt{d(u)^2 + d(e)^2},$$

where the summation goes over pairs of vertex u and edge e, such that u is an endvertex of e.
Let n be a positive integer. Denote by T_k is the rooted tree with $2k+1$ vertices for $k = 0, 1, \ldots, n$ such that k number of two-vertex branches diverging from a root. Let $k_1, k_2, \ldots, k_n$ be a non-decreasing non-negative integer sequence. The Kragujevac tree $Kg(k_1, k_2, \ldots, k_n)$ is the tree obtained $T_{k_1}, T_{k_2}, \ldots, T_{k_n}$ rooted trees, by connecting their roots to new vertex.
Gutman et al. studied Sombor index [8] and KG-Sombor index [9] of Kragujevac trees and empirically determined the extremal Kragujevac trees with respect to SO and KG indices as follows:

Theorem 1. [8, 9] *Let $Kg = Kg(k_1, k_2, \ldots, k_n)$ be the Kragujevac tree with $k_1 + k_2 + \cdots + k_n = K$. Then $KG(Kg)$ (or $SO(Kg)$) is minimal if and only if*

$$k_i \in \left\{ \left\lfloor \frac{K}{n} \right\rfloor, \left\lceil \frac{K}{n} \right\rceil \right\} \quad \text{for} \quad 1 \leq i \leq n$$

and $KG(Kg)$ (or $SO(Kg)$) is maximal if and only if $k_1 = k_2 = \cdots = k_{n-1} = 0$ and $k_n = K$.

In the conclusion of [8] and [9], the authors mentioned that finding rigorous analytical proof of our results remains a challenge for the future. In this paper, we give analytical proof of Theorem 1 and give support for a conjecture in [8].

2. Main results

Let $(m_1, m_2, \ldots, m_n)$ and $(k_1, k_2, \ldots, k_n)$ be two non-decreasing sequences of real numbers. Then it is said that the sequence $(m_1, m_2, \ldots, m_n)$ is majorized by the sequence $(k_1, k_2, \ldots, k_n)$ if the following two conditions are satisfied. (i) $m_{i+1} + m_{i+2} + \cdots + m_n \leq k_{i+1} + k_{i+2} + \cdots + k_n$ for all $1 \leq i < n$ (ii) $m_1 + m_2 + \cdots + m_n = k_1 + k_2 + \cdots + k_n$.

Now, we give a well known inequality due to Karamata.

Lemma 1. *Let $f\colon I \to \mathbb{R}$ be a convex function. If m_i and k_i, $1 \leq i \leq n$ are numbers in I such that $(m_1, m_2, \ldots, m_n)$ is majorized by $(k_1, k_2, \ldots, k_n)$, then*

$$f(m_1) + f(m_2) + \cdots + f(m_n) \leq f(k_1) + f(k_2) + \cdots + f(k_n).$$

If f is strictly convex, then the above inequality holds with equality if and only if $m_i = k_i$, $1 \leq i \leq n$.

Gutman et al. gave the explicit formulas of KG-Sombor [9] and Sombor [8] indices for a Kragujevac tree which depends on its structural parameters.

Lemma 2. [9] *Let $Kg(k_1, k_2, \ldots, k_n)$ be a Kragujevac tree with $k_1 + k_2 + \cdots + k_n = K$. Then*

$$\begin{aligned} KG(Kg) &= (\sqrt{5}+\sqrt{2})K + \sum_{i=1}^{n} k_i \left[\sqrt{2}(k_i+1) + \sqrt{(k_i+1)^2+4}\right] \\ &+ \sum_{i=1}^{n} \left[\sqrt{(k_i+1)^2+(n+k_i-1)^2} + \sqrt{n^2+(n+k_i-1)^2}\right]. \end{aligned} \tag{1}$$

Lemma 3. [8] *Let $Kg(k_1, k_2, \ldots, k_n)$ be a Kragujevac tree with $k_1 + k_2 + \cdots + k_n = K$. Then*

$$SO(Kg) = \sqrt{5}K + \sum_{i=1}^{n} \left[k_i\sqrt{(k_i+1)^2+4} + \sqrt{(k_i+1)^2+n^2}\right].$$

Lemma 4. *Let $f \colon \mathbb{R}^+ \to \mathbb{R}$ be a function defined by*

$$f(x) = x\left(\sqrt{2}(x+1) + \sqrt{(x+1)^2+4}\right) + \sqrt{(x+1)^2+(a+x-1)^2} + \sqrt{a^2+(a+x-1)^2}$$

where a is a positive real number. Then f is strictly convex.

Proof. For the convenience, we denote $z = x + 1$. Then f can be rewritten as a function of z as follows:

$$F(z) = (z-1)\left(\sqrt{2}z + \sqrt{z^2+4}\right) + \sqrt{z^2+(a-2+z)^2} + \sqrt{a^2+(a-2+z)^2}$$

where $z \geq 1$. Now, we calculate the second derivative of F. Then

$$F'(z) = \sqrt{2}z + \sqrt{z^2+4} + (z-1)\left(\sqrt{2} + \frac{z}{\sqrt{z^2+4}}\right) + \frac{2z+a-2}{\sqrt{z^2+(a-2+z)^2}} + \frac{z+a-2}{\sqrt{a^2+(a-2+z)^2}}$$

and

$$F''(z) = 2\sqrt{2} + \frac{3z-1}{\sqrt{z^2+4}} - \frac{z^2(z-1)}{(\sqrt{z^2+4})^3} + \frac{(a-2)^2}{(\sqrt{z^2+(a-2+z)^2})^3} + \frac{a^2}{(\sqrt{a^2+(a-2+z)^2})^3}.$$

Therefore, since

$$2\sqrt{2} + \frac{3z-1}{\sqrt{z^2+4}} - \frac{z^2(z-1)}{(\sqrt{z^2+4})^3} = 2\sqrt{2} + \frac{2z^3+12z-4}{(\sqrt{z^2+4})^3} > 0$$

for all $z \geq 1$, we have $F''(z) > 0$ for all $z \geq 1$ and it follows that f is strictly convex. □

The proof of Theorem 1. For K and n, there are non-negative integers q and r such that $K = nq + r$ with $0 \leq r < n$. Since $k_1 + k_2 + \cdots + k_n = K$, there exists a positive integer t such that

$$k_1 \leq k_2 \leq \cdots \leq k_t \leq q < q + 1 \leq k_{t+1} \leq \cdots \leq k_n. \tag{2}$$

We now consider the sequence $(m_1, m_2, \dots, m_n)$ with

$$m_1 = \cdots = m_{n-r} = q \quad \text{and} \quad m_{n-r+1} = \cdots = m_n = q + 1, \tag{3}$$

and prove that it is majorized by the sequence $(k_1, k_2, \dots, k_n)$. Clearly, we have $m_{i+1} + m_{i+2} + \cdots + m_n \leq k_{i+1} + k_{i+2} + \cdots + k_n$ for all $t \leq i \leq n$.
Suppose that

$$m_{j+1} + m_{j+2} + \cdots + m_n > k_{j+1} + k_{j+2} + \cdots + k_n \quad \text{for some} \quad 1 \leq j < t. \tag{4}$$

From (2) and (3), we get

$$m_1 + m_2 + \cdots + m_j \geq qj \geq k_1 + k_2 + \cdots + k_j. \tag{5}$$

Then, we get a contradiction from (4) and (5). Therefore $(m_1, m_2, \dots, m_n)$ is majorized by $(k_1, k_2, \dots, k_n)$.
First, to prove the theorem (for the KG-Sombor index), we consider the function

$$f(x) = x\left(\sqrt{2}(x+1) + \sqrt{(x+1)^2 + 4}\right) + \sqrt{(x+1)^2 + (n+x-1)^2} + \sqrt{n^2 + (n+x-1)^2}$$

where $x \in \mathbb{R}^+$. By Lemma 4, this function is strictly convex over $\mathbb{R}^+$. Then, by Lemma 1, we have

$$f(m_1) + f(m_2) + \cdots + f(m_n) \leq f(k_1) + f(k_2) + \cdots + f(k_n) \tag{6}$$

with equality if and only if $m_i = k_i$ for all $1 \leq i \leq n$. Thus, by Lemma 2 and (6), we obtain

$$KG(Kg(m_1, m_2, \dots, m_n)) \leq KG(Kg(k_1, k_2, \dots, k_n))$$

with equality if and only if $m_i = k_i$ for all $1 \leq i \leq n$. Hence, the proof of the first part of the theorem is done. Because $q = \left\lfloor \frac{K}{n} \right\rfloor$ and $q + 1 = \left\lceil \frac{K}{n} \right\rceil$.

On the other hand, we easily see that the given sequence $(k_1, k_2, \dots, k_n)$ is majorized by $(0, \dots, 0, K)$. Therefore, similarly to the first part of the proof, we get

$$KG(Kg(k_1, k_2, \dots, k_n)) \leq KG(Kg(0, \dots, 0, K))$$

with equality if and only if $k_i = 0$ for all $1 \leq i \leq n - 1$ and $k_n = K$. Hence, the proof of the second part of the theorem is finished (for the KG-Sombor index).

Now, to prove the theorem (for the Sombor index), we consider the function

$$g(x) = x\sqrt{(x+1)^2+4} + \sqrt{(x+1)^2+a^2}.$$

Set $z = x+1$. Then g can be rewritten as $G(z) = (z-1)\sqrt{z^2+4} + \sqrt{z^2+a^2}$ where $z \geq 1$. Hence

$$\left((z-1)\sqrt{z^2+4}\right)'' = \frac{2z^3+12z-4}{(\sqrt{z^2+4})^3}$$

and

$$\left(\sqrt{z^2+a^2}\right)'' = \frac{a^2}{(\sqrt{z^2+4})^3}.$$

Therefore, from the above $G''(z) > 0$ and it follows that g is strictly convex. Similarly to the above proof, we easily prove the theorem (for the Sombor index), by using Karamata's inequality and Lemma 3.

3. Conclusion

Gutman et al. gave the following conjecture.

Conjecture 1. [8] Let Kg_a and Kg_b be the Kragujevac trees with equal n and K. Then

$$Zg(Kg_a) > Zg(Kg_b) \text{ if and only if } SO(Kg_a) > SO(Kg_b),$$

where Zg is the first Zagreb index.

Proposition 1. *Let $Kg_a = K(a_1, a_2, \ldots, a_n)$ and $Kg_b = K(b_1, b_2, \ldots, b_n)$ be the Kragujevac trees with equal K. If $(b_1, b_2, \ldots, b_n)$ is majorized by $(a_1, a_2, \ldots, a_n)$ then $SO(Kg_a) > SO(Kg_b)$ and $Zg(Kg_a) > Zg(Kg_b)$.*

Proof. One can easily calculate that $Zg_a = 7K+n(n+1)+\sum_{i=1}^{n} a_i^2$. Therefore, since $(b_1, b_2, \ldots, b_n)$ is majorized by $(a_1, a_2, \ldots, a_n)$ and the function x^2 is strictly convex, we have $Zg(Kg_a) > Zg(Kg_b)$ by Lemma 1. Also, since $(b_1, b_2, \ldots, b_n)$ is majorized by $(a_1, a_2, \ldots, a_n)$ and $g(x)$ is strictly convex, we get $SO(Kg_a) > SO(Kg_b)$ by Lemma 3 and Lemma 1. □

Proposition 1 tells us the Conjecture 1 is true for the Kragujevac trees $Kg_a = K(a_1, a_2, \ldots, a_n)$ and $Kg_b = K(b_1, b_2, \ldots, b_n)$ when $(b_1, b_2, \ldots, b_n)$ is majorized by $(a_1, a_2, \ldots, a_n)$. We believe that Conjecture 1 is true. However, currently, we do not have its complete proof.

Acknowledgment.
The authors thank the anonymous reviewers for their helpful suggestions. This

work is supported by Mongolian Foundation for Science and Technology (Grant No. SHUTBIKHKHZG-2022/162).

Conflict of interest. The authors declare that they have no conflict of interest.

Data Availability. Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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