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The Schultz and the Modified Schultz Indices of Kragujevac Trees

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Abstract Let G be simple connected graph with the vertex and edge sets $V(G)$ and $E(G)$, respectively. The Schultz and the Modified Schultz indices of G are defined as $Sc(G) = \frac{1}{2}\sum_{u,v\in V(G)}(d_u+d_v)d(u,v)$, $Sc^*(G) = \frac{1}{2}\sum_{u,v\in V(G)}$ $(d_u \times d_v)d(u,v)$, where $d(u,v)$ is the topological distance between vertices u and v, d_v is the degree of vertex v of G. In this paper, computation of the Schultz and the Modified Schultz indices of the Kragujevac trees is proposed. As an application, we obtain an upper bound and a lower bound for the Schultz and the modified Schultz indices of these trees.

Keywords Schultz index · Modified Schultz index · Kragujevac tree

Mathematics Subject Classification (2010) 05C12 · 05C05

1 Introduction

Let G be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. For vertices u and v in V(G), we denote by $d(u,v)$ the topological distance i.e., the number of edges on the shortest path, joining the two vertices of G. A topological index is a numerical quantity derived in an unambiguous manner from the structure graph of a molecule. As a graph structural invariant, i.e. it does not depend on the labelling or the pictorial representation of a graph. Various topological indices usually reflect molecular size and shape [1]-[2].

The Schultz index of a molecular graph G was introduced by Schultz [3] in 1989 for characterizing alkanes by an integer as follows:

$$Sc(G) = \frac{1}{2}\sum_{u,v\in V(G)}(d_u + d_v)d(u,v). \tag{1}$$

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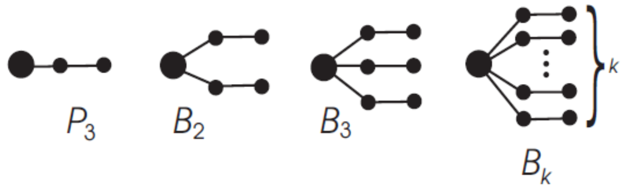

Fig. 1 The branches of Kragujevac trees

The Modified Schultz index of a graph G was introduced by S. Klavžar and I. Gutman in 1996 as follows [4]:

$$Sc^*(G) = \frac{1}{2} \sum_{u,v \in V(G)} (d_u \times d_v) d(u, v). \tag{2}$$

A connected acyclic graph is called a tree. The number of vertices of a tree T is its order. A rooted tree is a tree in which one particular vertex is distinguished, this vertex is referred to as the root (of the rooted tree). The class of Kragujevac trees emerged in several studies addressed to solve the problem of characterizing the tree with minimal atom-bond connectivity index [5]-[7]. In order to define the Kragujevac trees, we first explain the structure of its branches [8].

Definition 1 Let P_3 be the 3-vertex tree, rooted at one of its terminal vertices. For $k = 2, 3, \ldots,$ construct the rooted tree B_k by identifying the roots of k copies of P_3 . The vertex obtained by identifying the roots of P_3-trees is the root of B_k. Examples illustrating the structure of the rooted tree B_k are depicted in Fig. 1.

Definition 2 Let $d \geq 2$ be an integer. Let $B_1, B_2, \ldots, B_d$ be rooted trees specified in Definition 1. A Kragujevac tree T is a tree possessing a vertex of degree d, adjacent to the roots of $B_1, B_2, \ldots, B_d$. This vertex is said to be the central vertex of T, whereas d is the degree of T. The subgraphs $B_1, B_2, \ldots, B_d$ are the branches of T (Fig. 2). Recall that some (or all) branches of T may be mutually isomorphic. If all branches of T are isomorphic, then T is called regular Kragujevac tree.

In this paper, we compute the Schultz and modified Schultz indices of the Kragujevac tree. Also, we obtain a lower bound and an upper bound for this tree in term of d and the degree of the roots of $B_1, B_2, \ldots, B_d$.

2 Schultz index

In this section, we denote a Kragujevac tree by $T(k_1, k_2, \ldots, k_d)$, if $B_1, B_2, \ldots, B_d$ are its branches and k_i is the degree of the rooted vertex of B_i for $1 \leq i \leq d$.

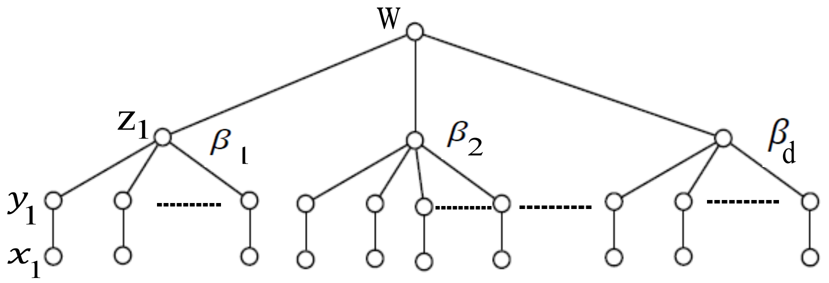

Fig. 2 A Kragujevac tree with d branches.

To compute the Schultz index of $T = T(k_1, k_2, \ldots, k_d)$, the distance between all vertices of tree must be calculated. For this purpose we consider four various types for vertices of this tree and compute the distance between each of four types of vertices and other vertices of T as follow.

At first we denote by x_i, a pendant vertex of B_i for $1 \leq i \leq d$ (see Fig. 2). The sum of the distance between x_i for $1 \leq i \leq d$, and each other vertex of T as v with coefficients $(d_v + d_{x_i})$ is computed as follow:

$$\begin{aligned}
d(x) &= \sum_{i=1}^{d} \sum_{v \in V(T)} k_i d(x_i, v)(d_{x_i} + d_v) \\
&= \sum_{i=1}^{d} k_i \Big((d_{x_i} + d_{y_i}) + 2(d_{x_i} + d_{z_i}) + 3((d_{x_i} + d_w) + (k_i - 1)(d_{x_i} + d_{y_i})) + \\
&\quad 4((k_i - 1)(d_{x_i} + d_{x_i}) + \sum_{j \neq i = 1}^{d} (d_{x_i}, d_{z_j})) + 5 \sum_{j \neq i = 1}^{d} k_j (d_{x_i} + d_{y_j}) \\
&\quad + 6 \sum_{j \neq i = 1}^{d} k_j (d_{x_i} + d_{x_j}) \Big) \\
&= \sum_{i=1}^{d} k_i \Big(3 + 2(k_i + 2) + 3(d + 1 + 3(k_i - 1)) \\
&\quad + 4(2(k_i - 1) + 2 \sum_{j \neq i = 1}^{d} (k_j + 2)) + 5 \sum_{j \neq i = 1}^{d} 3k_j + 6 \sum_{j \neq i = 1}^{d} 2k_j \Big) \\
&= \sum_{i=1}^{d} k_i \Big(11d - 12k_i - 15 + 31 \sum_{j=1}^{d} k_j \Big). \qquad (3)
\end{aligned}$$

Now let y_i denote the adjacent vertex of x_i in B_i for $1 \leq i \leq d$. The sum of the distance between vertices y_i for $1 \leq i \leq d$, and each other vertex v of T with coefficients $(d_v + d_{y_i})$ is computed as follow:

$$
\begin{aligned}
d(y) &= \sum_{i=1}^{d} \sum_{v \in V(T)} k_i d(y_i, v)(d_{y_i} + d_v) \\
&= \sum_{i=1}^{d} k_i \Bigg((d_{y_i} + d_{x_i}) + (d_{y_i} + d_{z_i}) + 2((d_{y_i} + d_w) + (k_i - 1)(d_{y_i} + d_{y_i})) + \\
&\quad 3((k_i - 1)(d_{y_i} + d_{x_i}) + \sum_{j \neq i=1}^{d} (d_{y_i}, d_{z_j})) + 4 \sum_{j \neq i=1}^{d} k_j (d_{y_i} + d_{y_j}) \\
&\quad +5 \sum_{j \neq i=1}^{d} k_j (d_{y_i} + d_{x_j}) \Bigg) \\
&= \sum_{i=1}^{d} k_i \Bigg(3 + (k_i + 3) + 2(d + 2 + 4(k_i - 1)) + 3(3(k_i - 1) + \sum_{j \neq i=1}^{d} (k_j + 3)) \\
&\quad +4 \sum_{j \neq i=1}^{d} 4k_j + 5 \sum_{j \neq i=1}^{d} 3k_j \Bigg) \\
&= \sum_{i=1}^{d} \Bigg(11d - 16k_i - 16 + 34 \sum_{j=1}^{d} k_j \Bigg). \qquad (4)
\end{aligned}
$$

If z_i denotes the rooted vertex of B_i for $1 \leq i \leq d$, then the sum of the distance between vertices z_i for $1 \leq i \leq d$, and each other vertex v of T with coefficients $(d_v + d_{z_i})$ is given:

$$
\begin{aligned}
d(z) &= \sum_{i=1}^{d} \sum_{v \in V(T)} k_i d(z_i, v)(d_{z_i} + d_v) \\
&= \sum_{i=1}^{d} k_i \Bigg((d_{z_i} + d_{y_i}) + (d_{z_i} + d_w) + 2(k_i(d_{z_i} + d_{x_i}) + \sum_{j \neq i=1}^{d} (d_{z_i} + d_{z_j})) + \\
&\quad 3 \sum_{j \neq i=1}^{k_i} k_j (d_{z_i} + d_{y_j}) + 4 \sum_{j \neq i=1}^{d} k_j (d_{z_i} + d_{x_j}) \Bigg) \\
&= \sum_{i=1}^{d} k_i \Bigg((k_i + 3) + k_i + d + 1 + 2(k_i(k_i + 2) + \sum_{j \neq i=1}^{d} (k_i + k_j + 2) \\
&\quad +3 \sum_{j \neq i=1}^{d} k_j (k_i + 3) + 4 \sum_{j \neq i=1}^{d} k_j (k_i + 2) \Bigg) \\
&= 5d^2 - 3d + \sum_{i=1}^{d} \Bigg(k_i(2d - 4k_i - 13 + 7 \sum_{j=1}^{d} k_j) + 19 \sum_{j=1}^{d} k_j \Bigg). \qquad (5)
\end{aligned}
$$

Finally, if w is the central vertex of T, then the sum of the distance between w and each other vertex v of T with coefficients (d_v+d_w) is computed as follow:

$$\begin{aligned} d(w) &= \sum_{v\in V(T)} d(w,v)(d_w+d_v) \\ &= \sum_{i=1}^{d}\Big((d_w+d_{z_i})+2k_i(d_w+d_{y_i})+3k_i(d_w+d_{x_i})\Big) \\ &= \sum_{i=1}^{d}\Big(d+k_i+1+2\sum_{i=1}^{d}k_i(d+2)+3\sum_{i=1}^{d}k_i(d+1)\Big) \\ &= d^2+d+\sum_{i=1}^{d}k_i(5d+8). \end{aligned} \tag{6}$$

Theorem 1 *Let $d,k\geq 2$ and $T=T(k_1,k_2,\ldots,k_d)$ be a Kragujevac tree. The Schultz index of T is computed as :*

$$Sc(T)=3d^2-d+\frac{1}{2}\sum_{i=1}^{d}\Big((29d-32k_i-36)k_i+(19k_i+72)\sum_{j=1}^{d}k_j\Big).$$

Proof By use of (1)*, the Schultz index of T can be computed by summing the distance between all vertices of T with its appropriate coefficients that there exist in the formula of computation of the Schultz index. By use of equations* $(3)-(6)$*, we get*

$$\begin{aligned} Sc(T) &= \frac{1}{2}(d(x)+d(y)+d(z)+d(w)) \\ &= 3d^2-d+\frac{1}{2}\sum_{i=1}^{d}\Big((29d-32k_i-36)k_i+(19k_i+72)\sum_{j=1}^{d}k_j\Big). \end{aligned}$$

In the following corollary we compute the Schultz index of the regular Kragujevac trees.

Corollary 1 *Let $d,k\geq 2$ and $T_{d,k}$ be a regular Kragujevac tree. Then*

$$Sc(T_{d,k})=4k^2d(9d-4)+2kd(12d-9)+3d^2-d.$$

Proof If $k_i=k$ for $1\leq i\leq d$, then $T(k_1,k_2,\ldots,k_d)=T_{d,k}$ and $\sum_{j=1}^{d}k_j=dk$. Thus by use of Theorem 1*, we have*

$$\begin{aligned} Sc(T_{d,k}) &= 3d^2-d+\frac{1}{2}\sum_{i=1}^{d}\Big(k(29d-32k-36)kd+(19k+72)kd\Big) \\ &= 4k^2d(9d-4)+2kd(12d-9)+3d^2-d. \end{aligned}$$

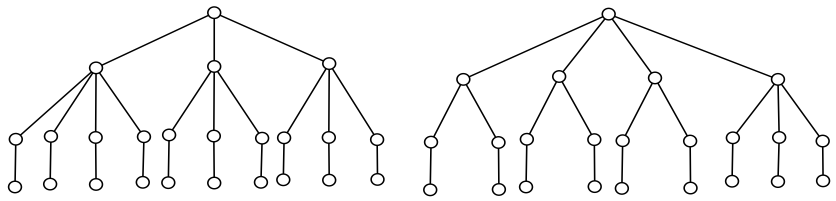

Fig. 3 Two types of Kragujevac trees.

Let $d \geq 2$ and $T = T(k_1, k_2, \ldots, k_d)$ be a Kragujevac tree of order n and degree d. If $k_i = 2$ for $1 \leq i \leq d-1$ and $k_d = k$ (hence $k = \frac{n-5d+3}{2}$), then we denote T by $K(2, d, n)$. Now let $r = \lfloor \frac{n-d-1}{2} \rfloor$ and $b = 1 + \lfloor \frac{r}{d} \rfloor$. If $k_i = b > 2$ for $1 \leq i \leq r - d(b-1) < d$ and $k_i = b - 1$ for $r - d(b-1) + 1 \leq i \leq d$, we denote T by $K(b, d, n)$ (see Fig. 3).

Theorem 2 *Among Kragujevac trees with fixed order n and degree d, $T(b, d, n)$ ($T(2, d, n)$) has maximal (respectively minimal) value of the Schultz index.*

Proof *Let $T = T(k_1, k_2, \ldots, k_d)$ be a Kragujevac tree of order n and degree d where $k_j > k_l + 1$ for some $1 \leq j, l \leq d$. If T^1 is the Kragujevac tree obtained from T by deleting a pendant path (P_3) of B_{k_j} and adding this pendant path to B_{k_l}, then*

$$Sc(T^1) - Sc(T) = \frac{1}{2}(d(x_j) + d(y_j) - d(x_l) - d(y_l)) = 32(k_j - k_l - 1) > 0.$$

Thus $Sc(T^1) > Sc(T)$.

Now let T be a Kragujevac tree of order n and degree d. If the degree of rooted vertex of B_{k_i} for $1 \leq i \leq d$ is largest among the branches of T, we can construct another Kragujevac tree which its Schultz index is more than $Sc(T)$, by deleting a pendant path (P_3) from B_{k_i} and adding a pendant path to another branch of T with less degree than k_i, hence $T(2, d, n)$ has minimum value of the Schultz index and $T(b, d, n)$ has maximum value of the Schultz index Among Kragujevac trees with fixed order n and degree d.

Corollary 2 *If T is a Kragujevac tree of order n and degree d, then*

$$Sc(T) \geq n(5n - 34d - 51) - 10d(10d - 7) + 46.$$

Proof *By use of Theorem 2, $Sc(T) \geq Sc(T(2, d, n))$. If $k_i = 2$ for $1 \leq i \leq d-1$ and $k_d = k$, then by using Theorem 1, we have*

$$Sc(T(2, d, n)) = 2k(10k + 84d - 81) + d(195d - 437) + 244.$$

Since $k = \frac{n-5d+3}{2}$, thus

$$Sc(T(2, d, n)) = n(5n - 34d - 51) - 10d(10d - 7) + 46.$$

Corollary 3 *let T be a Kragujevac tree of order n and degree d. If $r = \lfloor \frac{n-d-1}{2} \rfloor$ and $b = 1 + \lfloor \frac{r}{d} \rfloor$, then*

$$Sc(T) \leq 36r^2 + (24d - 32b - 2)r + 16db(b-1) + 3d^2 - d.$$

Proof Since $T = T(\underbrace{B_b, \ldots, B_b}_{r-d(b-1)}, \underbrace{B_{b-1}, \ldots, B_{b-1}}_{bd-r})$, *hence by use of Theorem* 1, *we get*

$$Sc(T(b,d,n)) = 36r^2 + (24d - 32b - 2)r + 16db(b-1) + 3d^2 - d.$$

Therefore the corollary is proved by use of Theorem 2.

3 Modified Schultz index

In this section, we compute the modified Schultz index of $T = T(k_1, k_2, \ldots, k_d)$. For this purpose we will use of a method similar to the used method for computation of the Schultz index of this tree.

Let $d^*(x)$ denote the sum of the distance between x_i (pendant vertices of B_i) for $1 \leq i \leq d$, and each other vertex v of T with coefficients $(d_{x_i} \times d_v)$. By using calculation technique of $d(x)$, we get:

$$\begin{aligned} d^*(x) &= \sum_{i=1}^{d} k_i \Bigg(2 + 2(k_i+1) + 3(2(k_i-1)+d) + 4(k_i-1) + \sum_{j \neq i=1}^{d} (k_j+1)) \\ &\quad +5 \sum_{j \neq i=1}^{d} 2k_j + 6 \sum_{j \neq i=1}^{d} k_j \Bigg) \\ &= \sum_{i=1}^{d} k_i \left(7d - 8k_i - 10 + 20 \sum_{j=1}^{d} k_j \right). \end{aligned} \tag{7}$$

Now let $d^*(y)$ denote the sum of the distance between vertices y_i of branch B_i for $1 \leq i \leq d$, and each other vertex v of T with coefficients $(d_{y_i} \times d_v)$. Then

$$\begin{aligned} d^*(y) &= \sum_{i=1}^{d} k_i \Bigg(2 + (2k_i+2) + 2(4(k_i-1)+2d) + 3(2(k_i-1) + \sum_{j \neq i=1}^{d} 2(k_j+1)) \\ &\quad +4 \sum_{j \neq i=1}^{d} 4k_j + 5 \sum_{j \neq i=1}^{d} 2k_j \Bigg) \\ &= \sum_{i=1}^{d} \left(10d - 16k_i - 16 + 32 \sum_{j=1}^{d} k_j \right). \end{aligned} \tag{8}$$

If $d^*(z)$ denotes the sum of the distance between vertices z_i for $1 \leq i \leq d$, and each other vertex v of T with coefficients $(d_{z_i} \times d_v)$, then

$$\begin{aligned} d^*(z) &= \sum_{i=1}^{d} k_i \Bigg(2(k_i+1) + (k_i+1)d + 2(k_i(k_i+1) + \sum_{j \neq i=1}^{d} (k_i+1)(k_j+1)) \\ &\quad +3 \sum_{j \neq i=1}^{d} 2(k_i+1)k_j + 4 \sum_{j \neq i=1}^{d} (k_i+1)k_j \Bigg) \\ &= 3d^2 - 2d + \sum_{i=1}^{d} \Bigg(k_i(3d - 8k_i - 10) + 12 \sum_{j=1}^{d} (k_i+1)k_j \Bigg). \qquad (9) \end{aligned}$$

Finally, if $d^*(w)$ denote the sum of the distance between the central vertex of T and each other vertex v of T with coefficients $(d_w \times d_v)$, then

$$\begin{aligned} d^*(w) &= \sum_{i=1}^{d} \Bigg(d(k_i+1) + 4dk_i + 3dk_i \Bigg) \\ &= d^2 + 8 \sum_{i=1}^{d} dk_i. \qquad (10) \end{aligned}$$

Theorem 3 *Let $k, d \geq 2$ and $T = T(k_1, k_2, \ldots, k_d)$ be a Kragujevac tree. The modified Schultz index of T is computed as :*

$$Sc^*(T) = 2d^2 - d + \frac{1}{2} \sum_{i=1}^{d} \Bigg(k_i(28d - 32k_i - 36 + 52 \sum_{j=1}^{d} k_j) + 12 \sum_{j=1}^{d} k_j(k_i+1) \Bigg).$$

Proof The modified Schultz index of T can be computed by summing the distance between all vertices of T with its appropriate coefficients (see (2)). By use of equations (7) – (10), we get

$$\begin{aligned} Sc^*(T) &= \frac{1}{2}[d^*(x) + d^*(y) + d^*(z) + d^*(w)] \\ &= 2d^2 - d + \frac{1}{2} \sum_{i=1}^{d} \Bigg(k_i(28d - 32k_i - 36 + 52 \sum_{j=1}^{d} k_j) + 12 \sum_{j=1}^{d} k_j(k_i+1) \Bigg). \end{aligned}$$

In the following corollary we compute the modified Schultz index of the regular Kragujevac trees.

Corollary 4 *Let $d, k \geq 2$ and $T_{d,k}$ be a regular Kragujevac tree. Then*

$$Sc^*(T_{d,k}) = 16k^2 d(2d-1) + 2kd(10d-9) + 2d^2 - d.$$

Proof *If* $k_i = k$ *for* $1 \leq i \leq d$, *then* $T(k_1, k_2, \ldots, k_d) = T_{d,k}$ *and* $\sum_{j=1}^{d} k_j = dk$. *Therefore by use of Theorem* 3, *we have*

$$\begin{aligned} Sc^*(T_{d,k}) &= 2d^2 - d + \frac{1}{2}\sum_{i=1}^{d}\Big(k(28d - 32k - 36 + 52dk) + 12dk(k+1)\Big) \\ &= 16k^2 d(2d-1) + 2kd(10d-9) + 2d^2 - d. \end{aligned}$$

Theorem 4 *Among Kragujevac trees of order* n *and degree* d, $T(b, d, n)$ $(T(2, d, n))$ *has maximal (respectively minimal) value of the modified Schultz index.*

Proof The proof of this theorem is similar to the proof of Theorem 2.

Corollary 5 *If* T *is a Kragujevac tree of order* n *and degree* d, *then*

$$Sc^*(T) \geq n(34d + 4n - 49) - 10d(10d - 7) + 45.$$

Proof *If* $k_i = 2$ *for* $1 \leq i \leq d - 1$ *and* $k_d = k$, *then by using Theorem* 3, *we have*

$$Sc^*(T(2, d, n)) = d(170d - 397) + 2k(74d + 8k - 73) + 228.$$

Since $k = \frac{n-5d+3}{2}$, *by use of Theorem* 4, *we have*

$$Sc^*(T) \geq n(34d + 4n - 49) - 10d(10d - 7) + 45.$$

Corollary 6 *Let* T *be a Kragujevac tree of order* n *and degree* d. *If* $r = \lfloor \frac{n-d-1}{2} \rfloor$ *and* $b = 1 + \lfloor \frac{r}{d} \rfloor$, *then*

$$Sc^*(T) \leq 32r^2 + (20d - 32b - 2)r + 16db(b-1) + 2d^2 - d.$$

Proof *Since* $T = T(\underbrace{B_b, \ldots, B_b}_{r-d(b-1)}, \underbrace{B_{b-1}, \ldots, B_{b-1}}_{bd-r})$, *by use of Theorem* 3, *we have*

$$Sc^*(T(b, d, n)) = 32r^2 + (20d - 32b - 2)r + 16db(b-1) + 2d^2 - d.$$

Therefore the corollary is proved by use of Theorem 4.

4 Conclusion

In this manuscript, the authors obtain exact formulas for computation the Schultz index and the modified Schultz index of a Kragujevac tree in term of the vertex degree of central vertex of its branches. Also an upper bound and a lower bound for these topological indices of a Kragujevac tree in term of its order and degree are computed. These results can be used to calculation some topological indices of molecular graphs which have similar structure to a Kragujevac tree.

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