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On the Wiener index and the hyper-Wiener index of the Kragujevac trees

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Abstract

In this paper, the Wiener index and the hyper-Wiener index of the Kragujevac trees is computed in term of its vertex degrees. As application, we obtain an upper bond and a lower bound for the Wiener index and the hyper-Wiener index of these trees.

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1. Introduction

Let G be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. For vertices $v_1, v_2 \in V(G)$, we denote by $d(v_1, v_2)$ the topological distance (i.e., the number of edges on the shortest path) joining the two vertices of G. The Wiener index of graph G is the half sum of distances over all its vertex pairs (i, j):

$$W(G) = \frac{1}{2} \sum_{i,j \in V(G)} d(i, j).$$

The hyper-Wiener index of acyclic graphs was introduced by Randic in 1993 [1]. Then Klein et al. [2] extended the definition for all connected graphs, as a generalization of the Wiener index. Similar to the symbol for the Wiener index, the hyper-Wiener index is traditionally denoted by $WW(G)$. The hyper-Wiener index of G is defined as follows:

$$WW(G) = \frac{1}{2}\left(\sum_{i,j \in V(G)} d(i, j) + \sum_{i,j \in V(G)} d^2(i, j) \right).$$

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). In order to define the Kragujevac trees, we first explain the structure of its branches [3].

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.*

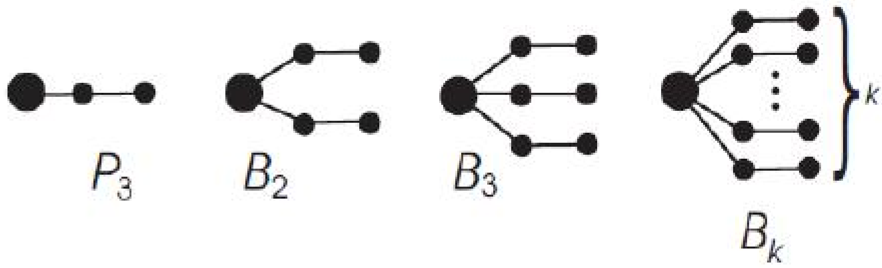

Figure 1: The branches of Kragujevac trees

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.*

The class of Kragujevac trees emerged in several studies addressed to solve the problem of characterizing the tree with minimal atom-bond connectivity index [4]-[6].In this paper, we compute the Wiener and hyper-Wiener indices of the Kragujevac trees. Also, we obtain lower and upper bounds for these trees in term of d and the degree of roots of $B_1, B_2, \ldots, B_d$.

2. Wiener 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 root vertex of B_i for $1 \leq i \leq d$.

At first we compute the Wiener index of $T(k_1, k_2, \ldots, k_d)$. For this purpose the sum of the distance between each vertex of this tree and other vertices of the tree must be calculated. Let v be a arbitrary vertex of $T(k_1, k_2, \ldots, k_d)$, we denote by $V_j(v)$ the set of vertices of the tree which are at distance j from v.

If x_i is a pendant vertex of B_i for $1 \leq i \leq d$ (see Fig. 2), then the sum of the distance between x_i and other vertices of the tree is $d(x_i) =$

$\sum_{j=1}^{6} j|V_j(x_i)|$. Thus the sum of the distance between pendant vertices and other vertices of the tree is given as follows:

$$
\begin{aligned}
d(x) &= \sum_{i=1}^{d}\left(k_i d(x_i)\right) \\
&= \sum_{i=1}^{d}\left(k_i \sum_{j=1}^{6} j|V_j(x_i)|\right) \\
&= \sum_{i=1}^{d}\left(k_i + 2k_i + 3k_i^2 + 4k_i(k_i+d-2) + 5k_i \sum_{j=1, j\neq i}^{d} k_j + 6k_i \sum_{j=1, j\neq i}^{d} k_j\right) \\
&= \sum_{i=1}^{d} k_i\left(4d-5-4k_i+11\sum_{j=1}^{d} k_j\right).
\end{aligned}
$$

Now let y_i be the adjacent vertex of x_i in B_i for $1 \leq i \leq d$. The sum of the distance between y_i and other vertices of the tree is $d(y_i) = \sum_{j=1}^{5} j|V_j(y_i)|$. Thus the sum of the distance between all adjacent pendant vertices of $T(k_1, k_2, \ldots, k_d)$ and other vertices of the tree is given as follows:

$$
\begin{aligned}
d(y) &= \sum_{i=1}^{d}\left(k_i d(y_i)\right) \\
&= \sum_{i=1}^{d}\left(k_i \sum_{j=1}^{5} j|V_j(x_i)|\right) \\
&= \sum_{i=1}^{d}\left(2k_i + 2k_i^2 + 3k_i(k_i+d-2) + 4k_i \sum_{j=1, j\neq i}^{d} k_j + 5k_i \sum_{j=1, j\neq i}^{d} k_j\right) \\
&= \sum_{i=1}^{d} k_i\left(3d-4-4k_i+9\sum_{j=1}^{d} k_j\right).
\end{aligned}
$$

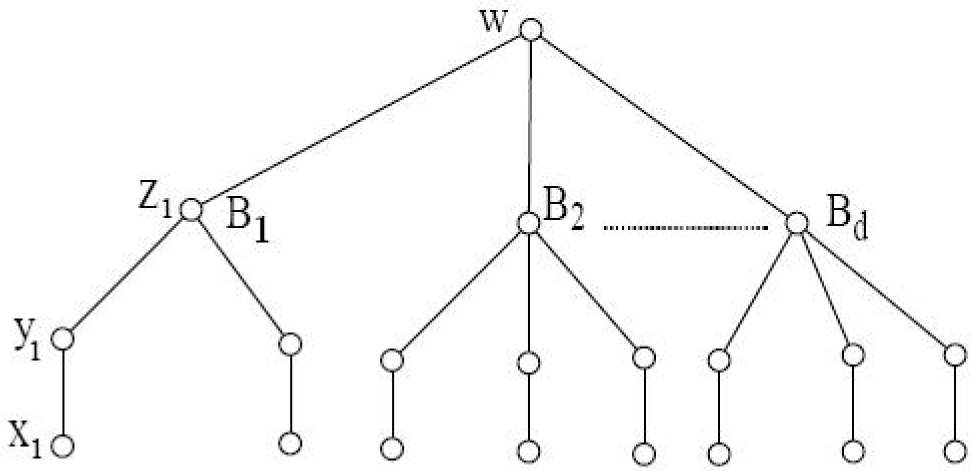

Figure 2: A Kragujevac tree with d branches.

If z_i is the rooted vertex of B_i for $1 \leq i \leq d$, then sum of the distance between z_i and other vertices of the tree is $d(z_i) = \sum_{j=1}^{4} j|V_j(z_i)|$. Thus the sum of the distance between all rooted vertices of B_i for $1 \leq i \leq d$ and other vertices of the tree is given as follows:

$$\begin{aligned} d(z) &= \sum_{i=1}^{d} d(z_i) \\ &= \sum_{i=1}^{d} \left(\sum_{j=1}^{4} j|V_j(z_i)| \right) \\ &= \sum_{i=1}^{d} \left(1 + k_i + 2(k_i + d - 1) + 3 \sum_{j=1, j\neq i}^{d} k_j + 4 \sum_{j=1, j\neq i}^{d} k_j \right) \\ &= \sum_{i=1}^{d} \left(2d - 1 - 4k_i + 7 \sum_{j=1}^{d} k_j \right). \end{aligned}$$

Finally, if w is the central vertex of $T(k_1, k_2, \ldots, k_d)$, then sum of the distance between w and other vertices of the tree is given as follows:

$$d(w) = d + 2 \sum_{j=1}^{d} k_j + 3 \sum_{j=1}^{d} k_j$$

$$= \quad d + 5\sum_{j=1}^{d} k_j.$$

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

$$W(T) = d^2 + \frac{1}{2}\sum_{i=1}^{d}\left((7d - 8k_i - 8)k_i + (20k_i + 7)\sum_{j=1}^{d} k_j\right).$$

Proof. *The Wiener index of T can be computed by summing the distance between all vertices of T. By use of previous results, we have*

$$\begin{aligned} W(T) &= \frac{1}{2}[d(x) + d(y) + d(z) + d(w)] \\ &= d^2 + \frac{1}{2}\sum_{i=1}^{d}\left((7d - 8k_i - 8)k_i + (20k_i + 7)\sum_{j=1}^{d} k_j\right). \end{aligned}$$

□

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

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

$$W(T_{d,k}) = d^2 + dk(10kd + 7d - 4k - 4).$$

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*

$$\begin{aligned} W(T_{d,k}) &= d^2 + \frac{1}{2}\sum_{i=1}^{d}\left((7d - 8(k+1))k + (20k + 7)\sum_{j=1}^{d} k\right) \\ &= d^2 + dk(10kd + 7d - 4k - 4). \end{aligned}$$

□

Let $d \geq 2$ and $T = T(k_1, k_2, \ldots, k_d)$ be a Kragujevac tree of order n. If $k_i = 2$ for $1 \leq i \leq d-1$ and $k_d = \frac{n-5d+3}{2}$, 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 and 4).

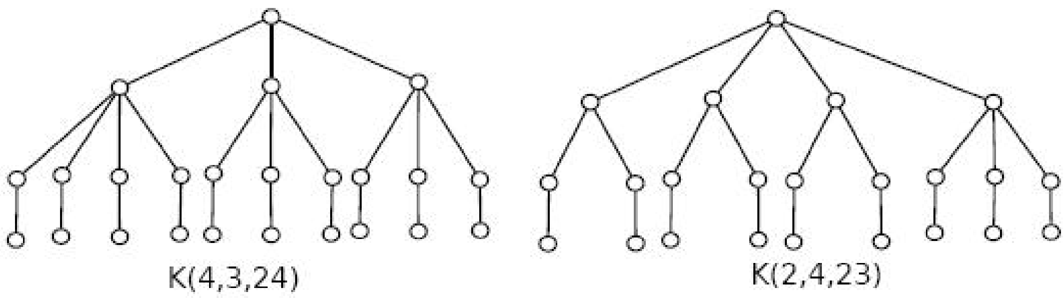

Figure 3: Two types of Kragujevac trees.

Theorem 2. *[3] Among Kragujevac trees of order n and degree d, $K(b, d, n)$ ($K(2, d, n)$) has maximal (respectively minimal) value of the Wiener index.*

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

$$W(T) \geq \frac{n}{2}(3n + 17d - 26) - \frac{5d}{2}(10d - 7) + \frac{23}{2}.$$

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

$$W(K(2, d, n)) = k(6k + 47d - 44) + d(55d - 118) + 64.$$

By use of Theorem 2, $W(T) \geq W(K(2, d, n))$. Since $k = \frac{n-5d+3}{2}$, thus

$$W(T) \geq \frac{n}{2}(3n + 17d - 26) - \frac{5d}{2}(10d - 7) + \frac{23}{2}.$$

$\square$

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*

$$W(T) \leq d(4b(b-1) + 7r + d) + 2r(5r - 4b).$$

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

$$W\Bigg(K(b,d,n)\Bigg) = d(4b(b-1) + 7r + d) + 2r(5r - 4b).$$

Therefore the corollary is proved by use of Theorem 2. □

3. Hyper-Wiener index

In this section, we compute the hyper-Wiener index of $T = T(k_1, k_2, \ldots, k_d)$. For this purpose, the sum of the square distance between each vertex of this tree and other vertices of the tree must be computed.

Let $d^2(x_i)$ denote the sum of the square distance between x_i, and other vertices of T. The sum of the square distance between the pendant vertices of T and all vertices of the tree is given as:

$$\begin{aligned} d^2(x) &= \sum_{i=1}^{d}\Bigg(k_i d^2(x_i)\Bigg) \\ &= \sum_{i=1}^{d}\Bigg(k_i + 4k_i + 9k_i^2 + 16k_i(k_i + d - 2) + 25k_i \sum_{j=1, j\neq i}^{d} k_j \\ &\quad +36k_i \sum_{j=1, j\neq i}^{d} k_j\Bigg) \\ &= \sum_{i=1}^{d} k_i\Bigg(16d - 36k_i - 27 + 61\sum_{j=1}^{d} k_j\Bigg). \end{aligned}$$

Now let $d^2(y_i)$ denote the sum of the square distance between y_i, and other vertices of T. Hence the sum of the square distance between the adjacent pendant vertices of T and all vertices of the tree is given as:

$$\begin{aligned}
d^2(y) &= \sum_{i=1}^{d}\left(k_i d^2(y_i)\right) \\
&= \sum_{i=1}^{d}\left(2k_i + 4k_i^2 + 9k_i(k_i+d-2) + 16k_i \sum_{j=1, j\neq i}^{d} k_j + 25k_i \sum_{j=1, j\neq i}^{d} k_j\right) \\
&= \sum_{i=1}^{d} k_i\left(9d - 28k_i - 16 + 41\sum_{j=1}^{d} k_j\right).
\end{aligned}$$

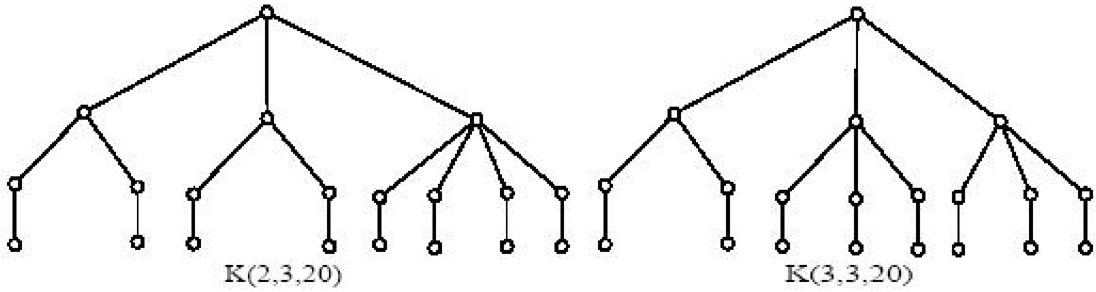

Figure 4: The graphs of two Kragujevac trees with extremal Wiener and hyper-Wiener indices.

If $d^2(z_i)$ denotes the sum of the square distance between z_i, and other vertices of T, then the sum of the square distance between the rooted vertices of B_i for $1 \leq i \leq d$ and all vertices of the tree is given as:

$$\begin{aligned}
d^2(z) &= \sum_{i=1}^{d}\left(d^2(z_i)\right) \\
&= \sum_{i=1}^{d}\left(1 + k_i + 4(k_i+d-1) + 9\sum_{j=1, j\neq i}^{d} k_j + 16\sum_{j=1, j\neq i}^{d} k_j\right) \\
&= \sum_{i=1}^{d}\left(4d - 3 - 20k_i + 25\sum_{j=1}^{d} k_j\right).
\end{aligned}$$

Finally, if $d^2(w)$ denotes the sum of the square distance between the central vertex and other vertices of the tree, then

$$\begin{aligned} d^2(w) &= d + 4\sum_{j=1}^{d} k_j + 9\sum_{j=1}^{d} k_j \\ &= d + 13\sum_{j=1}^{d} k_j. \end{aligned}$$

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

$$WW(T) = 3d^2 - d + \frac{1}{2}\sum_{i=1}^{d}\left((32d - 72k_i - 58)k_i + (122k_i + 32)\sum_{j=1}^{d} k_j\right).$$

Proof. *The hyper-Wiener index of T can be computed by summing the distance and the square distance between all vertex of T. By use of previous results and Theorem 1, we have*

$$\begin{aligned} WW(T) &= \frac{1}{2}[d^2(x) + d^2(y) + d^2(z) + d^2(w)] + W(T) \\ &= 3d^2 - d + \frac{1}{2}\sum_{i=1}^{d}\left((32d - 72k_i - 58)k_i + (122k_i + 32)\sum_{j=1}^{d} k_j\right). \end{aligned}$$

□

In the following corollary we compute the hyper-Wiener index of the regular Kragujevac trees by using Theorem 3.

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

$$WW(T_{d,k}) = k^2d(61d - 36) + dk(32d - 29) + 3d^2 - d.$$

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 3, we have*

$$\begin{aligned} WW(T_{d,k}) &= 3d^2 - d + \frac{1}{2}\sum_{i=1}^{d}\Bigg((32d - 72k - 58)k + (122k + 32)dk\Bigg) \\ &= k^2 d(61d - 36) + dk(32d - 29) + 3d^2 - d. \end{aligned}$$

□

In continue we obtain an upper bound and a lower bound for hyper-Wiener index of Kragujevac trees.

Theorem 2. *Among Kragujevac trees of order n and degree d, $K(b,d,n)$ ($K(2,d,n)$) has maximal (respectively minimal) value of the hyper-Wiener index.*

Proof. *Let $T = T(k_1, k_2, \ldots, k_d)$ be a Kragujevac tree of order n and $k_r > k_s + 1$ for $1 \le r, s \le d$. If T^1 is the Kragujevac tree obtained from T by deleting a pendant path (P_3) of B_{k_r} and adding this pendant path to B_{k_s}, then*

$$\begin{aligned} WW(T^1) - WW(T) &= \frac{1}{2}(d(x_r) + d^2(x_r) - d(x_s) - d^2(x_s)) \\ &= 72(k_r - k_s - 1) > 0, \end{aligned}$$

thus $WW(T^1) > WW(T)$.

Therefore when we have a Kragujevac tree with two branches which the difference between the degree of their rooted vertices is greater than one, we can construct another Kragujevac tree with greater value of the hyper-Wiener index, by reducing this difference and with less value of the hyper-Wiener index, by increasing this difference between the degree of rooted vertex of these branches. Thus $K(2,d,n)$ has minimum value of the hyper-Wiener index and $K(b,d,n)$ has maximum value of the hyper-Wiener index. □

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

$$WW(T) \ge \frac{1}{4}[n(25n + 302d - 396) - d(891d - 616) + 371].$$

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

$$WW\Bigg(K(2,d,n)\Bigg) = k(25k + 276d - 273) + d(311d - 755) + 446.$$

On the other hand $k = \frac{n-5d+3}{2}$, *hence by use of Theorem* 4, *we have*

$$WW(T) \geq \frac{1}{4}[n(25n + 302d - 396) - d(891d - 616) + 371].$$

□

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

$$WW(T) \leq 36bd(b-1) - r(72b - 32d - 61r - 7) + 3d^2 - d.$$

Proof. *For* $K(b,d,n) = T(\underbrace{b,\ldots,b}_{r-d(b-1)}, \underbrace{b-1,\ldots,b-1}_{bd-r})$, *by use of Theorem* 3, *we have*

$$WW\Big(K(b,d,n)\Big) = 36bd(b-1) - r(72b - 32d - 61r - 7) + 3d^2 - d.$$

Therefore the corollary is proved by use of Theorem 4. □

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