ON THE TERMINAL WIENER INDEX AND ZAGREB INDICES OF KRAJUJEVAC TREES

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Abstract: In this paper we find the extremal values of the terminal Wiener index, Zagreb indices and Zagreb coindices of Kragujevac trees. Further, we find the terminal Wiener index of line graphs of Kragujevac trees.

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1. Introduction

Let \( G = (V, E) \) be a graph. The number of vertices of \( G \) we denote by \( n \) and the
number of edges we denote by \( m \), thus \( |V(G)| = n \) and \( |E(G)| = m \). The degree of a vertex \( v \), denoted by \( \deg_G(v) \). If \( \deg_G(v) = 1 \) then \( v \) is called a pendent vertex. An edge \( e = uv \) of a graph \( G \) is called a pendent edge if \( \deg_G(u) = 1 \) or \( \deg_G(v) = 1 \). The distance between the vertices \( v_i \) and \( v_j \), \( v_i, v_j \in V(G) \), is equal to the length (= number of edges) of the shortest path starting at \( v_i \) and ending at \( v_j \) (or vice versa) and will be denoted by \( d(v_i, v_j \setminus G) \). The line graph \( L(G) \) of a graph is the graph derived from \( G \) in such a way that the edges in \( G \) are replaced by vertices in \( L(G) \) and two vertices in \( L(G) \) are connected whenever the corresponding edges in \( G \) are adjacent [16].

The oldest molecular structure is the one put forward in 1947 by H. Wiener [34], nowadays referred to as the Wiener index and denoted by \( W \). It is defined as the sum of distance between all pairs of vertices of a graph.

\[
W(G) = \sum_{\{u,v\subseteq V(G)\}} d(u, v \setminus G) = \sum_{1 \leq i < j \leq n} d(u, v \setminus G) \tag{1}
\]

For details on its chemical applications and mathematical properties one may refer to [7, 8, 9, 12, 22, 28] and the references cited therein.

If \( G \) has \( k \)-pendent vertices labeled by \( v_1, v_2 \cdots v_k \), then its terminal distance matrix is the square matrix of order \( k \) whose \((i, j)\)-th entry is \( d(v_i, v_j \setminus G) \). Terminal distance matrices were used for modeling amino acid sequences of proteins and of the genetic code [18, 26, 27].

The terminal Wiener index \( TW(G) \) of a connected graph \( G \) is defined as the sum of the distances between all pairs of its pendent vertices. Thus if \( V_T = \{v_1, v_2, \cdots, v_k\} \) is the set of all pendent vertices of \( G \), then

\[
TW(G) = \sum_{\{u,v\subseteq V_T(G)\}} d(u, v \setminus G) = \sum_{1 \leq i < j \leq k} d(u, v \setminus G) \tag{2}
\]

This distance-based molecular structure descriptor was recently put forward by Gutman et.al.,[11]. For more details on terminal wiener index refer to [17, 18, 25, 35].

The Zagreb indices were first introduced by Gutman and Trinajstić [13]. They are important molecular descriptors and have been closely correlated with many chemical properties [29]. There was a vast research concerning the mathematical properties and bounds for Zagreb indices and their various variants [3, 5, 6, 15, 19, 21, 23, 24, 30, 31, 32, 33, 36].

\[
M_1(G) = \sum_{u \in V(G)} \deg_G(u)^2 \quad \text{and} \quad \tag{3}
\]
\[ M_2(G) = \sum_{uv \in E(G)} \deg_G(u) \deg_G(v). \quad (4) \]

Noticing that contribution of nonadjacent vertex pairs should be taken into account when computing the weighted Wiener polynomials of certain composite graphs (see [7]) defined first Zagreb coindex and second Zagreb coindex as

\[ M_1(G) = \sum_{uv \notin E(G)} \left[ \deg_G(u) + \deg_G(v) \right] \quad (5) \]

and

\[ M_2(G) = \sum_{uv \notin E(G)} \deg_G(u) \deg_G(v). \quad (6) \]

For more information on Zagreb coindices see [1, 2].

**Kragujevac trees**

The formal definition of a Kragujevac tree was introduced in [10].

**Definition 1.** [10] Let \( P_3 \) be the 3-vertex tree, rooted at one of its terminal vertices. For \( k = 2, 3, \cdots \), construct the rooted tree \( B_k \) by identifying the roots of \( k \) copies of \( P_3 \). The vertex obtained by identifying the roots \( P_3 \)-trees is the root of \( B_k \).

Examples illustrating the structure of the rooted tree \( B_k \) are depicted in Figure 1.

![Figure 1](image)

**Definition 2.** [10] Let \( d \geq 2 \) be an integer. Let \( \beta_1, \beta_2, \cdots, \beta_d \) be rooted trees specified in Definition 1, i.e., \( \beta_1, \beta_2, \cdots, \beta_d \in \{ B_2, B_3, \cdots \} \). A Kragujevac tree \( T \) is a tree possessing a vertex of degree \( d \), adjacent to the roots of \( \beta_1, \beta_2, \cdots, \beta_d \). This vertex is said to be the central vertex of \( T \), whereas \( d \) is the degree of \( T \). The subgraphs \( \beta_1, \beta_2, \cdots, \beta_d \) are the branches of \( T \). Recall that some (or all) branches of \( T \) may be mutually isomorphic.

A typical Kragujevac tree is depicted in Figure 2.
Recent information on Kragujevac trees can be found in [4].

2. Terminal Wiener Index of Kragujevac Trees

By the definition 1, the branch $B_{k_i}$ contains $k_i$ pendant vertices and the vertex set of $B_{k_i} = 2k_i + 1$.

Theorem 1. Let $T$ be the Kragujevac tree of degree $d \geq 2$ with branches $B_{k_i}$, $i = 1, 2, \ldots$, then

$$TW(T) = 4 \sum_{i=1}^{n} \frac{k_i(k_i - 1)}{2} + 6 \sum_{1 \leq i < j \leq n} k_i k_j$$  \hspace{1cm} (7)

Proof. By the definition of Kragujevac tree of degree $d \geq 2$ contains branches $B_{k_i}$, $i = 1, 2, \ldots$. Consider first the branch $B_{k_i}$ which contains $k_i$ pendant vertices. Each of these are at distance 4, and therefore their contribution to $TW(T)$ is $\frac{k_i(k_i - 1)}{2} \times 4$. This lead to the first term on the right-hand side of (3).

Consider the branches $B_{k_i}$ and $B_{k_j}$, $i \neq j$ with $k_i$ and $k_j$ pendant vertices. Each of these are at distance 6. Since there are $k_j \times k_j$ pairs of pendant vertices of this kind, their contribution to $TW(T)$ is equal to $6k_i k_j$. This leads to the second term on the right-hand side of (3).

Before going to prove our next results, we have the following observations.

Observation 2. The order and size of the Kragujevac tree are $n = 1 + \sum_{i=1}^{d} (2k_i + 1)$ and $m = \sum_{i=1}^{d} (2k_i + 1)$ respectively.
Observation 3. Let $e = uv$ be an edge of Kragujevac tree such that $\deg_T(u) = 1$ and $\deg_T(v) = 2$. Then $\deg_{L(T)}(e) = \deg_T(u) + \deg_T(v) - 2 = 1$. Therefore, $e$ is a pendant vertex of $L(T)$.

We define $D_2(T)$ as

$$D_2(T) = \{v \mid \deg_T(v) = 2 \text{and one neighbour of } v \text{ is pendent}\}$$

Now we are at a position to establish our next result.

**Theorem 4.** Let $T$ be a Kragujevac tree with $d \geq 2$ and let $D_2(T) = \{v_1, v_2, \ldots, v_k\}$. Then

$$TW(L(T)) = \sum_{1 \leq i < j \leq m} d(v_i, v_j \setminus T) + \frac{m(m-1)}{2}. \quad (8)$$

**Proof.** Bearing in mind Observation 2 and 3. The proof of (8) follows from the same lines of the proof of Theorem 2.1 in [25]. \qed

### 3. Zagreb Indices of Kragujevac Trees

We begin with the following straightforward, previously known, auxiliary result.

**Lemma 1.** [1] Let $G$ be any nontrivial graph of order $n$ and size $m$. Then

$$M_1(G) + \overline{M_1}(G) = 2m(n-1).$$

**Lemma 2.** [1] Let $G$ be any nontrivial graph of order $n$ and size $m$. Then

$$\overline{M_2}(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G).$$

**Theorem 5.** Let $T$ be the Kragujevac tree of degree $d \geq 2$ with branches $B_{k_i}, i = 1, 2, \ldots$, then

$$M_1(T) = d^2 + \sum_{i=1}^{n} [(k_i + 1)^2 + 5k_i]. \quad (9)$$

**Proof.** We obtain formula (9) by applying Eq. (3). First consider the branch $B_k$, by Definition 1, it is clear that the degree of a root $u$ is $k$ and the
degree of vertices which are adjacent to \( u \) is 2 i.e., \( \text{deg}_B(N(u)) = 2 \), finally, the degree of remaining vertices are one. Hence,

\[
M_1(B_k) = \sum_{i=1}^{n} \text{deg}_B(v_i)^2 = k^2 + k4 + k = k^2 + 5k.
\]

Note that, \( \text{deg}_T(u_i) = (k_i + 1), i = 1, 2, \cdots \). With this background by employing Eq. (3) to the Kragujevac tree \( T \), we have

\[
M_1(T) = \sum_{i=1}^{n} \text{deg}_T(v_i)^2 = d^2 + \sum_{i=1}^{n} [(k_i + 1)^2 + 5k_i].
\]

This leads to the right-hand side of (9).

**Corollary 6.** Let \( T \) be the Kragujevac tree of degree \( d \geq 2 \) with branches \( B_{k_i}, i = 1, 2, \cdots \), then

\[
\overline{M}_1(T) = 2 \sum_{i=1}^{n} (2k_i + 1)^2 - d^2 - \sum_{i=1}^{n} [(k_i + 1)^2 + 5k_i]. \quad (10)
\]

**Proof.** Apply Lemma 1 and Theorem 5, bearing in mind that \( n = 1 + \sum_{i=1}^{d} (2k_i + 1) \) and \( m = \sum_{i=1}^{d} (2k_i + 1) \).

**Theorem 7.** Let \( T \) be the Kragujevac tree of degree \( d \geq 2 \) with branches \( B_{k_i}, i = 1, 2, \cdots \), then

\[
M_2(T) = d^2 \sum_{i=1}^{n} (k_i + 1) + 2 \sum_{i=1}^{n} k_i(k_i + 2). \quad (11)
\]

**Proof.** We obtain formula (11) by applying Eq. (4). First consider the branch \( B_k \), by Definition 1, it is clear that the degree of a root \( u \) is \( k \) and the degree of vertices which are adjacent to \( u \) is 2 i.e., \( \text{deg}_B(N(u)) = 2 \), finally, the degree of remaining vertices are one. Hence,

\[
M_2(B_k) = \sum_{v_i, v_j \in E(B_k)} \text{deg}_B(v_i)\text{deg}_B(v_j).
\]
Note that, $\deg_T(u_i) = (k_i + 1), i = 1, 2, \cdots$. With this background by employing Eq. (4) to the Krugujevac tree $T$, we have

$$M_2(T) = \sum_{i=1}^{n} \deg_T(v_i)^2$$

$$= d^2 + \sum_{v_i, v_j \in E(T)} d \sum_{i=1}^{n} (k_i + 1)d + \sum_{i=1}^{n} 2k_i(k_i + 2)$$

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

This leads to the right-hand side of (11).

Corollary 8. Let $T$ be the Krugujevac tree of degree $d \geq 2$ with branches $B_{k_i}, i = 1, 2, \cdots$, then

$$\overline{M_2(T)} = 2 \sum_{i=1}^{n} (2k_i + 1)^2 - d^2 \sum_{i=1}^{n} (k_i + 1) - 2 \sum_{i=1}^{n} k_i(k_i + 2)$$

$$- \frac{1}{2} [d^2 + \sum_{i=1}^{n} [(k_i + 1)^2 + 5k_i]].$$

Proof. Apply Lemma 2 and Theorem 7, bearing in mind that $n = 1 + \sum_{i=1}^{d} (2k_i + 1)$ and $m = \sum_{i=1}^{d} (2k_i + 1)$.

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