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WIENER INDEX OF SUBDIVISIONS OF A TREE

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ABSTRACT. The Wiener index $W(T)$ of a tree T is defined as the sum of distances between all vertices of T . The edge k -subdivision T_e is constructed from a tree T by replacing its edge e with the path on $k + 2$ vertices. Edge k -subdivisions of each of edges $e_1, e_2, \dots, e_{n-1}$ of a tree with n vertices generate a family containing $n - 1$ trees. A relation between quantities $W(T_{e_1}) + W(T_{e_2}) + \dots + W(T_{e_{n-1}})$ and $W(T)$ is established.

Keywords: tree, graph invariant, Wiener index.

1. INTRODUCTION

In this paper we are concerned with finite undirected connected graphs G with vertex set $V(G)$ and edge set $E(G)$. Degree of a vertex v is denoted by $\deg(v)$. If u and v are vertices of G , then the number of edges in a shortest path connecting them is said to be their distance and is denoted by $d_G(u, v)$. Distance of a vertex v is the sum of distances from v to all vertices of a graph, $d_G(v) = \sum_{u \in V(G)} d(v, u)$. The Wiener index is a graph invariant based on distances between all vertices of G :

$$W(G) = \sum_{u, v \in V(G)} d(u, v) = \frac{1}{2} \sum_{v \in V(G)} d_G(v).$$

It was introduced as a structural descriptor for tree-like molecular graphs [17] and found numerous applications in organic chemistry. Details on the mathematical properties and chemical applications of the Wiener index can be found in books [1, 7, 8, 9, 14, 15] and reviews [2, 3, 12, 13]. One of the directions in the research of the Wiener index is comparing the index of a graph and its derived graphs such

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FIG. 1. k -subdivision of edge e in a tree T .

as the line graph, the total graph, thorny and subdivision graphs of various kinds [4, 5, 6, 11, 16].

Denote by P_n the path with n vertices. The edge k -subdivision T_e is constructed from a tree T by replacing its edge e with path P_{k+2} as shown in Fig. 1. Vertices $v_1, v_2, \dots, v_k$ are called the subdivision vertices. The k -subdivision S is constructed from n -vertex tree T by replacing of each of edges $e_1, e_2, \dots, e_{n-1}$ of T with path P_{k+2} . All edge k -subdivisions form a family containing $n-1$ trees T_e , $e \in E(T)$. In this paper, relations between Wiener indices of subdivisions of a tree are presented.

2. MAIN RESULT

Let tree T_e be an edge k -subdivision of n -vertex tree T (see Fig. 1). Define two vertex sets with respect to endvertices of edge $e = (x, y)$: $V_x = \{w \in V(T) \mid d(w, x) < d(w, y)\}$ and $V_y = \{w \in V(T) \mid d(w, y) < d(w, x)\}$ with cardinality $n_x = |V_x|$ and $n_y = |V_y|$, $n_x + n_y = n$. Edge k -subdivisions of T are $(n+k)$ -vertex trees. Wiener indices of a tree and its edge k -subdivisions are connected by the following relation.

Theorem 1. *Let $T_{e_1}, T_{e_2}, \dots, T_{e_{n-1}}$ be edge k -subdivisions of a tree T with edges $e_1, e_2, \dots, e_{n-1}$. Then*

$$\begin{aligned} W(T_{e_1}) + W(T_{e_2}) + \dots + W(T_{e_{n-1}}) = \\ = (3k + n - 1)W(T) + (n - 1) \binom{k+1}{3} + 2 \binom{k}{2} \binom{n}{2}. \end{aligned}$$

Note that $\binom{k+1}{3}$ is the Wiener index of path P_k . We will use the same numbering of subdivision vertices for all edges. The sum of distances between vertices from T in new trees can be also expressed through the Wiener index of T .

Corollary 1. *Let $T_{e_1}, T_{e_2}, \dots, T_{e_{n-1}}$ be edge k -subdivisions of a tree T with subdivision vertices $v_1, v_2, \dots, v_k$. Then*

$$\begin{aligned} W(T_{e_1}) + W(T_{e_2}) + \dots + W(T_{e_{n-1}}) - \sum_{i=1}^{n-1} (d_{T_{e_i}}(v_1) + \dots + d_{T_{e_i}}(v_k)) = \\ = (k + n - 1)W(T) - (n - 1) \binom{k+1}{3}. \end{aligned}$$

It is known that for Wiener indices of an n -vertex tree T and its k -subdivision S with $n' = k(n-1) + n$ vertices the following equality is valid [2]:

$$W(S) = (k+1)^3 W(T) + \binom{n'+1}{3} - (k+1)^3 \binom{n+1}{3}.$$

This implies a relation between S and edge subdivisions of T .

Corollary 2. For k -subdivision S of an n -vertex tree T with edges $e_1, e_2, \dots, e_{n-1}$,

$$W(S) = \frac{(k+1)^3}{3k+n-1} (W(T_{e_1}) + W(T_{e_2}) + \dots + W(T_{e_{n-1}})) - \\ - \frac{1}{6} k(k+1)(n-1) \left(\frac{(k-1)(k+1)^2(k+3n+1)}{3k+n-1} + (k+1)(3n-1) + 2 \right).$$

The simplest edge subdivisions correspond to the case $k = 1$.

Corollary 3. For edge 1-subdivisions of a tree T ,

$$W(T_{e_1}) + W(T_{e_2}) + \dots + W(T_{e_{n-1}}) = (n+2)W(T).$$

From the above results it follows that the sum of the distances of subdivision vertices is twice the Wiener index, $d_{T_{e_1}}(v_1) + d_{T_{e_2}}(v_1) + \dots + d_{T_{e_{n-1}}}(v_1) = 2W(T)$. Then $W(T)$ is close to the average value of Wiener indices of 1-subdivisions without distances of v_1 .

Corollary 4. For Wiener indices of edge 1-subdivisions of a tree T ,

$$W(T) = \frac{1}{n} (W(T_{e_1}) + W(T_{e_2}) + \dots + W(T_{e_{n-1}}) \\ - d_{T_{e_1}}(v_1) - d_{T_{e_2}}(v_1) - \dots - d_{T_{e_{n-1}}}(v_1)).$$

As an illustration, consider tree T with 10 vertices and its 2-subdivisions shown in Fig. 2. Wiener indices are indicated near diagrams of the corresponding trees, $W(T_{e_1}) + W(T_{e_2}) + \dots + W(T_{e_9}) = 3 \cdot 230 + 2 \cdot 222 + 234 + 214 + 2 \cdot 226 = 2034$ and $W(S) = 2682$. By Theorem 1,

$$W(T_{e_1}) + W(T_{e_2}) + \dots + W(T_{e_9}) = 15 \cdot 129 + 9 \cdot 1 + 2 \cdot 1 \cdot 45 = 2034,$$

and by Corollary 2,

$$W(S) = \frac{9}{15} 2034 - \frac{2 \cdot 3 \cdot 9}{6} \left(\frac{1 \cdot 9 \cdot 33}{15} + 3 \cdot 29 + 2 \right) = 2682.$$

3. PROOF OF THEOREM 1

The distance between two subsets $X, Y \subseteq V(G)$ of a graph G is defined as $d_G(X, Y) = \sum_{x \in X} \sum_{y \in Y} d_G(x, y)$. Let T be an n -vertex tree and $e \in E(T)$. Then the Wiener index of T_e can be presented as follows

$$(1) \quad W(T_e) = \sum_{u \in V_x} \sum_{w \in V_y} d_{T_e}(u, w) + \sum_{u, w \in V_x} d_{T_e}(u, w) + \sum_{u, w \in V_y} d_{T_e}(u, w) \\ + \sum_{i=1}^k d_{T_e}(v_i) - \frac{1}{2} \sum_{i,j=1}^k d_{T_e}(v_i, v_j) \\ = \sum_{u \in V_x} \sum_{w \in V_y} (d_T(u, w) + k) + \sum_{u, w \in V_x} d_T(u, w) + \sum_{u, w \in V_y} d_T(u, w) \\ + \sum_{i=1}^k d_{T_e}(v_i) - W(P_k) \\ = W(T) + k n_x n_y + \sum_{i=1}^k d_{T_e}(v_i) - W(P_k).$$

FIG. 2. 2-subdivision S and edge 2-subdivisions of a tree T .

For subdivision vertex $v_i \in T_e$,

$$\begin{aligned}
 d_{T_e}(v_i) &= \sum_{w \in V_x} d_{T_e}(v_i, w) + \sum_{w \in V_y} d_{T_e}(v_i, w) + \sum_{j=1}^k d_{T_e}(v_i, v_j) \\
 &= \sum_{w \in V_x} (d_{T_e}(v_i, x) + d_T(x, w)) + \sum_{w \in V_y} (d_{T_e}(v_i, y) + d_T(y, w)) + d_{P_k}(v_i) \\
 &= d_T(x, V_x) + d_T(y, V_y) + n_x i + n_y (k - i + 1) + d_{P_k}(v_i).
 \end{aligned}$$

Summing the later equation for all subdivision vertices v_i , we get

$$\begin{aligned}
 \sum_{i=1}^k d_{T_e}(v_i) &= k(d_T(x, V_x) + d_T(y, V_y)) + k(k+1)(n_x + n_y)/2 + 2W(P_k) \\
 &= k(d_T(x, V_x) + d_T(y, V_y)) + n k(k+1)/2 + 2W(P_k).
 \end{aligned}$$

Express $d_T(x, V_x) + d_T(y, V_y)$ through distances of vertices x and y . We have

$$\begin{aligned} d_T(x) &= d_T(x, V_x) + \sum_{w \in V_y} (d_T(x, y) + d_T(y, w)) \\ &= d_T(x, V_x) + n_y + d_T(y, V_y), \end{aligned}$$

$$\begin{aligned} d_T(y) &= d_T(y, V_y) + \sum_{w \in V_x} (d_T(y, x) + d_T(x, w)) \\ &= d_T(y, V_y) + n_x + d_T(x, V_x). \end{aligned}$$

Then $d_T(x, V_x) + d_T(y, V_y) = (d_T(x) + d_T(y) - n)/2$ and

$$(2) \quad \sum_{i=1}^k d_{T_e}(v_i) = k(d_T(x) + d_T(y) - n)/2 + n k(k+1)/2 + 2W(P_k).$$

Inserting (2) back into equation (1), we obtain

$$(3) \quad W(T_e) = W(T) + k n_x n_y + k(d_T(x) + d_T(y) - n)/2 + n k(k+1)/2 + W(P_k).$$

Wiener's formula for a tree T states that [17]

$$W(T) = \sum_{(x,y) \in E(T)} n_x n_y.$$

Then, summing equations (3) for all edges of T , we can write

$$\begin{aligned} \sum_{e \in E(T)} W(T_e) &= (n-1)W(T) + k \sum_{(x,y) \in E(T)} n_x n_y + \frac{1}{2} k \sum_{(x,y) \in E(T)} (d_T(x) + d_T(y)) \\ &\quad - (n-1)nk/2 + (n-1)nk(k+1)/2 + (n-1)W(P_k) \\ &= (k+n-1)W(T) + \frac{1}{2} k \sum_{v \in V(T)} \deg(v) d_T(v) \\ (4) \quad &+ (n-1)W(P_k) + k^2 n(n-1)/2. \end{aligned}$$

The Wiener index of path P_k is equal to $\binom{k+1}{3}$. Klein et al. proved that [10]

$$(5) \quad \sum_{v \in V(T)} \deg(v) d_T(v) = 4W(T) - n(n-1).$$

Substitution this sum into equation (4) completes the proof. $\square$

Equalities (2) and (5) lead to a relation for distances of subdivision vertices $v_1, v_2, \dots, v_k$ in k -subdivisions of an n -vertex tree T :

$$\sum_{i=1}^{n-1} (d_{T_{e_i}}(v_1) + \dots + d_{T_{e_i}}(v_k)) = 2k W(T) + \frac{1}{6} k(k-1)(n-1)(2k+3n+2).$$

Corollary 1 follows from this equation and Theorem 1.

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