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On the Wiener Index of the Forest Induced by Contraction of Edges in 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. For an edge $e = (u, v)$ of a tree T, the edge contraction is an operation which removes e from T and then identifies vertices u and v. The resulting tree T_e has one less edge than T. Contraction of every edge $e_1, e_2, \dots, e_{n-1}$ of a tree T with n vertices generates the forest $F = \{T_{e_1}, T_{e_2}, \dots, T_{e_{n-1}}\}$. A relation between quantities $W(F) = W(T_{e_1}) + W(T_{e_2}) + \cdots + W(T_{e_{n-1}})$ and $W(T)$ is established.

1 Introduction

In this paper we are concerned with finite undirected graphs G with vertex set $V(G)$ and edge set $E(G)$. The *order* of a graph is its number of vertices. 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 $d_G(u, v)$. The distance between two subsets $X, Y \subseteq V(G)$ of a graph G is defined as $d_G(X, Y) = \sum_{x \in X} \sum_{y \in Y} d_G(x, y)$. *Vertex distance*, $d_G(v)$, is the sum of distances from a vertex v to all vertices of a graph, $d_G(v) = d_G(v, V(G))$. 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 [21] and found numerous applications in organic chemistry. Details on the mathematical properties and chemical applications of the Wiener index can be found in books [2, 11–13, 17, 18, 20] and reviews [5,6,15,16]. Denote by S_n and P_n the star and the path of order n, respectively. It is known that S_n and P_n have the minimal and the maximal Wiener indices among all trees of order n, where $W(S_n) = (n-1)^2$ and $W(P_n) = n(n-1)(n+1)/6$ [9].

One of the directions in the research of the Wiener index is the comparison of the index of a graph and its derived graphs such as the line graph, the total graph, thorny and subdivision graphs of various kinds [7,8,10,14,19]. In a tree T, the *contraction of an edge* $e = (x, y)$ is the replacement of vertices x and y with a new vertex z such that edges incident to z are the edges other than e that were incident with x or y. The resulting tree T_e has one less edge than T (see Fig. 1ab). Contraction of every edge $e_1, e_2, \ldots, e_{n-1}$ of a tree T with n vertices generates the forest $F = \{T_{e_1}, T_{e_2}, \ldots, T_{e_{n-1}}\}$. The Wiener index of a forest F is defined as the sum of the Wiener indices of its components,

$$W(F) = W(T_{e_1}) + W(T_{e_2}) + \cdots + W(T_{e_{n-1}}).$$

The *subdivision of an edge* e in a tree T is the replacement of e with a new path of order 3 as shown in Fig. 1c. Vertex w_e is called the *subdivision vertex* of e.

In this paper, a relation between the Wiener indices of a tree and the forest generated by edge contractions is presented. The obtained result may be useful for estimating how the Wiener index changes on average under such structural transformations of a tree.

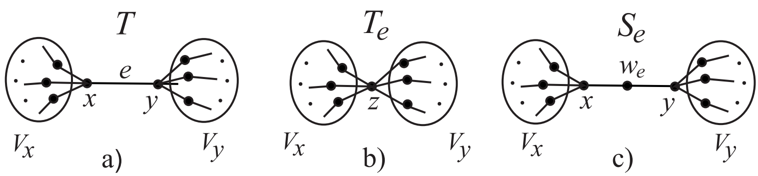

Figure 1. Contraction T_e and subdivision S_e of an edge e in a tree T.

2 Main result

Let tree T_e be a tree obtained by contraction of an edge e of n-vertex tree T. Define two vertex sets with respect to the endvertices of edge $e = (x, y)$: $V_x = \{w \in V(T) \,|\, d(w, x) < d(w, y)\} \setminus \{x\}$ and $V_y = \{w \in V(T) \,|\, d(w, y) < d(w, x)\} \setminus \{y\}$ with cardinality $n_x = |V_x|$ and $n_y = |V_y|$, $n_x + n_y = n - 2$ (see Fig. 1a).

The following result establishes a relation between the Wiener indices of a tree and the corresponding forest.

Proposition 1. *Let T be a tree with $n \geq 2$ vertices and edges $e_1, e_2, \ldots, e_{n-1}$. For the forest $F = \{T_{e_1}, T_{e_2}, \ldots, T_{e_{n-1}}\}$ obtained by contractions of edges in T,*

$$W(F) = (n-4)W(T) + n(n-1).$$

As an illustration, consider the tree T with 7 vertices and the induced forest $F(T) = \{T_{e_1}, T_{e_2}, \ldots, T_{e_6}\}$ shown in Fig. 2. Wiener indices are indicated below the diagrams of the corresponding trees. Computer calculations give $W(T) = 46$ and $W(F) = 2 \cdot 31 + 28 + 32 + 2 \cdot 29 = 180$. By Proposition 1, we have $W(F) = (7-4)46 + 7 \cdot 6 = 180$.

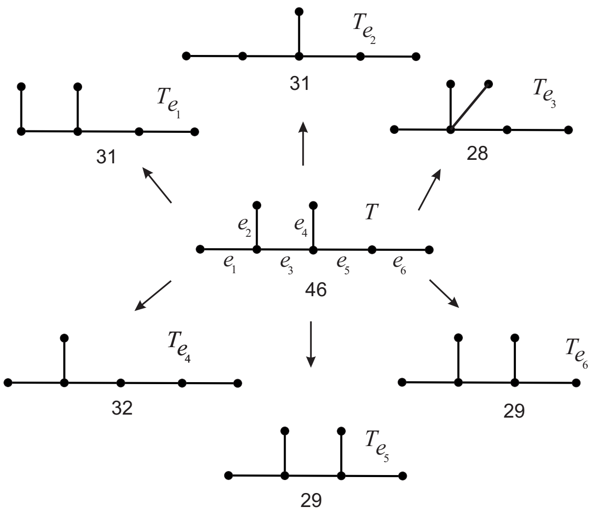

Figure 2. Tree T and forest $F = \{T_{e_1}, T_{e_2}, \ldots, T_{e_6}\}$ induced by edge contractions.

Corollary 1. *Let F_1 and F_2 be the forests obtained from trees T_1 and T_2 with the same number of vertices $n \geq 5$ by contractions of edges. Then $W(F_1) = W(F_2)$ if and only if $W(T_1) = W(T_2)$.*

Note that the path P_4 and the star S_4 generate the same forest $\{P_3, P_3, P_3\}$ and have distinct Wiener indices. It is known that the Wiener indices of trees with odd number of vertices are even [1].

Corollary 2. *The Wiener index of the forest induced by contraction of edges of a tree is always even.*

By Corollary 2, the forest F always contains an even number of components with odd Wiener indices.

Since each tree of order $n \geq 3$ has either a vertex of degree 2 or a vertex with two neighbors of degree 1, any forest F induced by contraction contains components with the same Wiener indices.

Let $W_{\rm avr}(F)$ be the average value of the Wiener indices of trees in a forest F, $W_{\rm avr}(F) = W(F)/(n-1)$. It is clear that if $W(T)$ is a prime number, then $W_{\rm avr}(F)$ is fractional. For some trees, the corresponding forest has integer $W_{\rm avr}(F)$. For example, $W_{\rm avr}(F) = 30$ for the forest in Fig. 2. Since contractions of edges of the path P_n or the star S_n produce isomorphic trees, $W_{\rm avr}(F)$ is obviously integer for P_n and S_n (note that $W(P_n)$ may not be divisible by $n-1$). Trees of order $n = 16$ (total 19320 trees) generate 3872 forests F with integer $W_{\rm avr}(F)$. Among them, Wiener indices of 1316 trees are divisible by $n-1$.

3 Proof of Proposition 1

Let $e = (x, y)$ be an edge of an n-vertex tree T. Consider contraction of the edge e and the corresponding tree T_e. Denote by z a new vertex in T_e obtained by identifying vertices x and y (see Fig. 1b). Then Wiener indices of T and T_e can be represented as the sum of several parts:

$$\begin{aligned} W(T) &= d_T(x,V_x) + d_T(x,V_y) + d_T(x,y) + d_T(y,V_y) + d_T(y,V_x) + d_T(V_x,V_y), \\ W(T_e) &= d_{T_e}(z,V_x) + d_{T_e}(z,V_y) + d_{T_e}(V_x,V_y). \end{aligned}$$

By the construction of the trees, we have $d_T(x,V_x) = d_{T_e}(z,V_x)$, $d_T(y,V_y) = d_{T_e}(z,V_y)$, and $d_T(V_x,V_y) - d_{T_e}(V_x,V_y) = n_x n_y$ (see Fig. 1ab). Then

$$W(T_e) = W(T) - n_x n_y - 1 - [\, d_T(x,V_y) + d_T(y,V_x)\,].$$

Since $n_x n_y = (n_x+1)(n_y+1) - (n_x+n_y) - 1 = (n_x+1)(n_y+1) - n + 1$,

$$W(T_e) = W(T) - (n_x+1)(n_y+1) + n - 2 - [\, d_T(x,V_y) + d_T(y,V_x)\,].$$

Summing the last equation for all edges of T, we have

$$\begin{aligned} W(F) &= (n-1)W(T) - \sum_{(x,y)\in E(T)} (n_x+1)(n_y+1) + (n-1)(n-2) \qquad (1) \\ &- \sum_{(x,y)\in E(T)} [\, d_T(x,V_y) + d_T(y,V_x)\,]. \end{aligned}$$

Wiener's formula for a tree T states that [21]

$$\sum_{(x,y)\in E(T)} (n_x+1)(n_y+1) = W(T).$$

To calculate the last sum of equation (1), we use the subdivision of an edge e in T and the corresponding tree S_e (see Fig. 1c). It is clear that $d_T(x,V_y) = d_{S_e}(w_e,V_y)$ and $d_T(y,V_x) = d_{S_e}(w_e,V_x)$. Then $d_T(x,V_y)+d_T(y,V_x) = d_{S_e}(w_e)-2$ and

$$W(F) = (n-1)W(T) - W(T) + n(n-1) - \sum_{e\in E(T)} d_{S_e}(w_e). \qquad (2)$$

It is known that the sum of distances of subdivision vertices w_{e_i} of S_{e_i} for $i=1,2,\dots n-1$ is twice the Wiener index of the initial tree T [3, 4],

$$d_{S_{e_1}}(w_{e_1}) + d_{S_{e_2}}(w_{e_2}) + \cdots + d_{S_{e_{n-1}}}(w_{e_{n-1}}) = 2W(T).$$

Substituting this sum into equation (2) completes the proof. □

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