Trees with the Greatest Wiener and Edge–Wiener Index

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ABSTRACT

The Wiener index $W$ and the edge-Wiener index $W_e$ of $G$ are defined as the sum of distances between all pairs of vertices in $G$ and the sum of distances between all pairs of edges in $G$, respectively. In this paper, we identify the four trees, with the first through fourth greatest Wiener and edge–Wiener index among all trees of order $n \geq 10$.

1. INTRODUCTION

Throughout this paper we consider undirected graphs without loops and multiple edges. Let $G$ be such a graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. The distance between two vertices $u$ and $v$ in $G$, denoted by $d(u,v|G)$, is defined as the length of a shortest path between $u$ and $v$. Let $f = xy$ and $g = uv$ be two edges of $G$. The distance between $f$ and $g$ is denoted by $d_e(f,g|G)$ and defined as the distance between the vertices of $f$ and $g$ in the line graph of $G$. The degree of a vertex $v$ in $G$, $d_G(v)$, is the number of edges incident to $v$ and $N[v,G]$ denotes the set of vertices adjacent to $v$. A pendent vertex is a vertex with degree one. We use the notations $\Delta = \Delta(G)$ and $n_l = n_l(G)$ to denote the maximum degree and the number of vertices of degree $l$ in $G$, respectively. Obviously, $\sum_{l=1}^{\Delta(G)} n_l = |V(G)|$. Let $S \subseteq V(G)$ be any subset of vertices of $G$. Then the induced subgraph $G[S]$ is the graph whose vertex set is $S$ and whose edge set consists of all of the
edges in $E(G)$ that have both endpoints in $S$. If $W$ is a subset of $V(G)$ then $G - W$ will be the subgraph of $G$ obtained by deleting the vertices of $W$ and similarly, for a subset $F$ of $E(G)$, the subgraph obtained by deleting all edges in $F$ is denoted by $G - F$. In the case that $W = \{v\}$ or $F = \{xy\}$, the subgraphs $G - W$ and $G - F$ will shortly be written as $G - v$ or $G - xy$, respectively. For any two nonadjacent vertices $x$ and $y$ in $G$, let $G + xy$ be the graph obtained from $G$ by adding an edge $xy$.

If $G$ is acyclic and connected graph, then $G$ is a tree. Any tree with at least two vertices has at least two pendant vertices. The set of all $n-$vertex trees is denoted by $\tau(n)$. In chemical graph theory, a topological index is a number invariant under graph automorphisms. These numbers play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations, see [7, 11].

Harold Wiener in [18], introduced Wiener index defined as

$$W(G) = \sum_{\{u, v\} \subseteq V(G)} d(u, v|G),$$

which is the sum of distances between all pairs of vertices of $G$. The edge-Wiener index of $G$, denoted by $W_e(G)$, is defined as

$$W_e(G) = \sum_{\{f, g\} \subseteq E(G)} d_e(f, g|G),$$

which is the sum of distances between all pairs of edges of $G$. This invariant was independently introduced in [10, 13]. Edge-Wiener index is one of the most interesting topological indices. Dankelmann et al. [5], recalled that, $W_e(G) \leq \frac{26}{5}n^5 + O \left( n^{\frac{28}{15}} \right)$, for graphs of order $n$. Dou et al. [6], characterized the polyphenyl chains with minimum and maximum edge-Wiener indices among all the polyphenyl chains with $h$ hexagons. They also characterized the explicit formulas for the edge-Wiener indices of extremal polyphenyl chains. Yousefi-Azari et al. [19], proved that for every tree $T$, $Sz_e(T) = W_e(T)$, $Sz_e(T)$ denotes the edge Szeged index of $T$. Nadjafi-Arani et al. [16], showed that for every connected graph $G$, $Sz_e(G) \geq W_e(G)$ with equality if and only if $G$ is a tree. Alizadeh et al. [1], characterized the edge-Wiener index of suspensions, bottlenecks, and thorny graphs. Knor et al. [12], proved that $W_e(G) \geq \frac{\delta^2 - 1}{4}W(G)$ where $\delta$ denotes the minimum degree in $G$. Kelenc et al. [14], characterized an algorithm developed that, for a given benzenoid system $G$ with $m$ edges, computes the edge-Wiener index of $G$ in $O(m)$ time. Chen et al. [4], studied explicit relation between the Wiener index and the edge-Wiener index of the catacondensed hexagonal systems. We refer the reader to [2, 9] for more information on the edge-Wiener index. Buckley in [3] and Tratnik et al. in [17], for a tree $T$ with $n$ vertices proved that:

$$W_e(T) = W(T) - \frac{n(n - 1)}{2},$$

(1)
Deng [8], the trees with the greatest Wiener index were investigated, where the trees on \( n \) vertices \( (n \geq 9) \) with the first to seventeenth greatest Wiener index were found. However, it turned out that the results in [8] were not correct and therefore, paper [15] was published. In that paper, the trees on \( n \) vertices \( (n \geq 28) \) with the first to fiftieth greatest Wiener index were found. Hence by Equation (1), the trees on \( n \) vertices \( (n \geq 28) \) with the first to fiftieth greatest Wiener index in [15] are the trees on \( n \) vertices \( (n \geq 28) \) with the first to fiftieth greatest edge-Wiener index. In this paper, we identify the four trees, with the first through fourth greatest Wiener and edge-Wiener index among all trees of order \( n \geq 10 \).

2. Main Results

In this section, some graph transformations are presented by which we can increase the edge-Wiener index of trees. By applying these graph operations, we identify the four trees, with the first through fourth greatest edge-Wiener index among all trees of order \( n \geq 10 \).

\[ \begin{array}{c}
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\text{Transformation } \mathcal{A}.
\end{array}
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\begin{equation}
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\text{Suppose } w \text{ is a vertex in a connected graph } G \text{ with at least two vertices and } \mathcal{N}(w, G) = \{x_1, x_2, \ldots, x_{d_G(w)}\}. \text{In addition, we assume that } P: u_k u_{k-1} \ldots u_2 u_1 \text{ and } Q: v_l v_{l-1} \ldots v_2 v_1, \text{are two new paths of lengths } k, l (k \geq l \geq 1), \text{respectively. Let } G_1 \text{ be the graph obtained from } G, P \text{ and } Q \text{ by attaching edges } v_l w, w u_k, \text{ and } G_2 = G_1 - \{wx_i: x_i \in \mathcal{N}(w, G)\} + \{v_ix_i: x_i \in \mathcal{N}[w, G]\}. \text{Such graphs have been illustrated in Figure 1.}
\end{array}
\end{array}
\end{equation}

**Figure 1.** The graphs \( P, Q, G, G_1 \) and \( G_2 \) in Transformation \( \mathcal{A} \).

**Lemma 2.1.** Let \( G_1 \) and \( G_2 \) be two graphs as shown in Figure 1. Then we have 

\[ W_e(G_1) < W_e(G_2). \]

**Proof.** Let \( E^*(G) = E(G) \setminus \{xw|x \in \mathcal{N}(w, G)\} \) and \( \bar{E}(G) = E^*(G) \cup \{xv_i|x \in \mathcal{N}(w, G)\} \). From definition,
\[ W_e(G_1) - W_e(G_2) = \sum_{i=1}^{l-1} \sum_{f \in E(G)} d_e(f, v_i v_{i+1} | G_1) + \sum_{i=1}^{k-1} d_e(f, u_i u_{i+1} | G_1) 
+ \sum_{f \in E(G)} d_e(f, wu_k | G_1) 
- \left[ \sum_{i=1}^{l-1} \sum_{f \in E(G)} d_e(f, v_i v_{i+1} | G_2) + \sum_{i=1}^{k-1} d_e(f, u_i u_{i+1} | G_2) \right] 
+ \sum_{f \in E(G)} d_e(f, wu_k | G_2) 
= \sum_{i=1}^{l-1} \sum_{f \in E(G)} d_e(f, v_i v_{i+1} | G_1) + \sum_{i=1}^{k-1} d_e(f, u_i u_{i+1} | G_1) 
+ \sum_{f \in E(G)} d_e(f, wu_k | G_1) 
- \left[ \sum_{i=1}^{l-1} \sum_{f \in E(G)} (d_e(f, v_i v_{i+1} | G_1) - 1) \right] 
+ \sum_{i=1}^{k-1} \sum_{f \in E(G)} (d_e(f, u_i u_{i+1} | G_1) + 1) 
+ \sum_{f \in E(G)} (d_e(f, wu_k | G_1) + 1) 
= \sum_{i=1}^{l-1} \sum_{f \in E(G)} 1 - \sum_{i=1}^{k-1} \sum_{f \in E(G)} 1 - \sum_{f \in E(G)} 1 < 0 \text{ as } k \geq l \geq 1. \]

which completes the proof. \(\square\)
Transformation B. Suppose \( G_1 \) and \( G_2 \) are two trivial graphs with vertices \( w_1 \) and \( w_2 \), respectively. In addition, we assume that \( P : v_1 v_2 \ldots v_{k-1} v_k \) is a path of length \( k (k \geq 5) \). Let \( T_1 \) be the graph obtained from \( G_1, G_2 \) and \( P \) by attaching edges \( w_1 v_i, w_2 v_j \), and \( T_2 = T_1 - \{w_1 v_i, w_2 v_j\} + \{w_1 v_2, w_2 v_{k-1}\} \), such that at least one of the two \( i \neq 2, j \neq k - 1 \) is true and \( 1 < i < j < k \). Such graphs have been illustrated in Figure 2.

Lemma 2.2. Let \( T_1 \) and \( T_2 \) be two graphs as shown in Figure 2. Then we have \( W_e(T_1) < W_e(T_2) \).

Proof. Let \( S = \{v_1, v_2, \ldots, v_i, v_{i+1}, w_1\} \) and \( R = \{v_{j-1}, v_j, \ldots, v_{k-1}, v_k, w_2\} \). Then from definition \( T_1[S] \cong T_2[S] \) and \( T_1[R] \cong T_2[R] \). Therefore, we have,

\[
W_e(T_1) - W_e(T_2) = \sum_{h=i+1}^{k-1} d_e(w_1 v_i, v_h v_{h+1}|T_1) + \sum_{h=1}^{j-2} d_e(w_2 v_j, v_h v_{h+1}|T_1) + d_e(w_1 v_i, w_2 v_j|T_1)
\]

\[
- \left[ \sum_{h=i+1}^{k-1} d_e(w_1 v_2, v_h v_{h+1}|T_2) + \sum_{h=1}^{j-2} d_e(w_2 v_{k-1}, v_h v_{h+1}|T_2) + d_e(w_1 v_2, w_2 v_{k-1}|T_2) \right]
\]

\[
= \sum_{h=i+1}^{k-1} d_e(w_1 v_i, v_h v_{h+1}|T_1) + \sum_{h=1}^{j-2} d_e(w_2 v_j, v_h v_{h+1}|T_1) + d_e(w_1 v_i, w_2 v_j|T_1)
\]

\[
- \left[ \sum_{h=i+1}^{j-2} (d_e(w_1 v_i, v_h v_{h+1}|T_1) + i - 2) + \sum_{h=1}^{k-j-1} (d_e(w_2 v_j, v_h v_{h+1}|T_1) + k - j - 1) \right]
\]
\[ + (d_e(w_1v_i, w_2v_j)|T_1) + k + i - j - 3] \]
\[ = - \left[ \sum_{h=i+1}^{k-1} (i - 2) + \sum_{h=1}^{j-2} (k - j - 1) + (k + i - j - 3) \right]. \]

Now, suppose that \( i \neq 2 \). So,
\[ W_e(T_1) - W_e(T_2) = - \left[ \sum_{h=i+1}^{k-1} (i - 2) + \sum_{h=1}^{j-2} (k - j - 1) + (k + i - j - 3) \right] \]
\[ \leq - \left[ \sum_{h=i+1}^{k-1} (3 - 2) + \sum_{h=1}^{j-2} [(k - (k - 1) - 1) + 1] \right] < 0. \]

If \( j \neq k - 1 \), then we have,
\[ W_e(T_1) - W_e(T_2) = - \left[ \sum_{h=i+1}^{k-1} (i - 2) + \sum_{h=1}^{j-2} [(k - j - 1) + (k + i - j - 3)] \right] \]
\[ \leq - \left[ \sum_{i=1}^{k-1} (2 - 2) + \sum_{i=1}^{j-2} [(k - (k - 2) - 1) + (k + 2 - (k - 2) - 3)] \right] < 0, \]
which completes the proof. \( \Box \)

Let the vertices of the path \( P_{n-1} \) be numbered consecutively by \( 1, 2, \ldots, n - 1 \). Construct the graph \( P_{n-1}(j) \) by attaching a pendent vertex at position \( j \) of the \( (n - 1) - \)vertex path. For positive integers \( x_1, \ldots, x_m, \) and \( y_1, \ldots, y_m \), let \( T(y_1x_1, \ldots, y_mx^m) \) be the class of trees with \( x_i \) vertices of degree \( y_i, i = 1, \ldots, m \). For some values of \( x_1, \ldots, x_m, \) and \( y_1, \ldots, y_m \), the class \( T(y_1x_1, \ldots, y_mx^m) \) may be empty.

**Lemma 2.3.** Let \( P_{n-1}(2), P_{n-1}(3), P_{n-1}(4), T_1, T_2 \) and \( T_3 \) be six trees with \( n(\geq 10) \) vertices as shown in Figure 3. Then we have
\[ W_e(P_n) > W_e(P_{n-1}(2)) > W_e(P_{n-1}(3)) > W_e(T_1) > \max\{W_e(P_{n-1}(4)), W_e(T_2), W_e(T_3)\}. \]

**Proof.** By Lemma 2.1, we have \( W_e(P_n) > W_e(P_{n-1}(2)) > W_e(P_{n-1}(3)) \). Now, it is easy to see, \( P_{n-1}(3)|\{1, 2, \ldots, n - 2\} \cong P_{n-1}(4)|\{1, 2, \ldots, n - 2\} \cong T_1|\{v_1, v_2, \ldots, v_{n-2}\} \), and
\[ \sum_{i=2}^{n-3} d_e((n - 1)(n - 2), (i)(i + 1)|P_{n-1}(3)) = \sum_{i=2}^{n-3} d_e((n - 1)(n - 2), (i)(i + 1)|P_{n-1}(4)) = \sum_{i=1}^{n-4} d_e(v_{n-1}v_{n-3}, v_1v_{i+1}|T_1). \]
Then for \( n \geq 10 \), we have
\[ W_e(P_{n-1}(3)) - W_e(T_1) = 1 + 2 + n - 3 + \sum_{i=1}^{n-4} i - [1 + 1 + n - 4 + \sum_{i=1}^{n-4} i] > 0 \]
and
\[ W_e(T_1) - W_e(P_{n-1}(4)) = 1 + 1 + n - 4 + \sum_{i=1}^{n-4} i + - [1 + 2 + n - 3 + \sum_{i=1}^{n-5} i]. \]
Theorem 2.4. Let $P_{n-1}(2)$, $P_{n-1}(3)$ and $T_1$ be trees with $n$ vertices as shown in Figure 3. If $n \geq 10$ and $T \in \tau(n) \setminus \{P_n, P_{n-1}(2), P_{n-1}(3), T_1\}$, then

$$W_e(P_n) > W_e(P_{n-1}(2)) > W_e(P_{n-1}(3)) > W_e(T_1) > W_e(T).$$
Proof. From Lemma 2.3, \( W_e(P_n) > W_e(P_{n-1}(2)) > W_e(P_{n-1}(3)) > W_e(T_1) \). Now, suppose that \( \Delta(T) = 3 \) and \( n_3(T) = 1 \). In this case, if \( T \in \{ P_{n-1}(i); i = 4, 5, \ldots, \left\lfloor \frac{n}{2} \right\rfloor \} \) then by Lemma 2.1 and Lemma 2.3, \( W_e(T_1) > W_e(P_{n-1}(4)) \geq W_e(T) \). Otherwise, by Lemma 2.1 and Lemma 2.3, \( W_e(T_1) > W_e(T_2) \geq W_e(T) \). For the case of \( \Delta(T) = 3 \) and \( n_3(T) \geq 2 \), by Lemma 2.1 and Lemma 2.2, \( W_e(T_1) > W_e(T) \). If \( \Delta(T) \geq 4 \), then by Lemma 2.1 and Lemma 2.3, \( W_e(T_1) > W_e(T_3) \geq W_e(T) \). Otherwise, \( T \in \{ P_n, P_{n-1}(2), P_{n-1}(3), T_1 \} \). This proves our theorem. □

Corollary 2.5. Among all trees with \( n(\geq 10) \) vertices, \( P_n, P_{n-1}(2), P_{n-1}(3) \) and \( T_1 \) have the maximum values of first through fourth Wiener index, respectively.

Proof. Equation (1) and Theorem 2.4 give us the result. □

REFERENCES


