Trees with the Greatest Wiener and Edge–Wiener Index

A. GHALAVAND*

Department of Pure Mathematics, Faculty of Mathematical Science, University of Kashan, Kashan 87317–53153, I. R. Iran

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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 $n_i = n_i(G)$ to denote the maximum degree and the number of vertices of degree $i$ in $G$, respectively. Obviously, $\sum_{i=1}^{\Delta(G)} n_i = |V(G)|$. 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

*Corresponding Author (Email address: Ali.ghalavand.kh@gmail.com)
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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 the 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, $W_e(G) \leq \frac{25}{8} n^5 + O\left(n^6\right)$, 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 fift\(eenth\) greatest Wiener index were found. Hence by Equation (1), the trees on \(n\) vertices \((n \geq 28)\) with the first to fift\(eenth\) greatest Wiener index in [15] are the trees on \(n\) vertices \((n \geq 28)\) with the first to fift\(eenth\) 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 \(n \geq 10\).

Transformation A. Suppose \(w\) is a vertex in a connected graph \(G\) with at least two vertices and \(N[w,G] = \{x_1,x_2,\ldots,x_{d_G(w)}\}\). In addition, we assume that \(P: u_ku_{k-1}\ldots u_2u_1\) and \(Q: v_lv_{l-1}\ldots v_2v_1\), are two new paths of lengths \(k,l (k \geq l \geq 1)\), respectively. Let \(G_1\) be the graph obtained from \(G, P\) and \(Q\) by attaching edges \(v_lv_k\) and \(w_{u_k}\), and \(G_2 = G_1 - \{wx_i: x_i \in N[w,G]\}\) + \(\{v_ix_i: x_i \in N[w,G]\}\). Such graphs have been illustrated in Figure 1.

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

which completes the proof. \( \Box \)
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 $P : v_1v_2 \ldots v_{k-1}v_k$ 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 $w_1v_i$, $w_2v_j$, and $T_2 = T_1 - \{w_1v_i, w_2v_j\} + \{w_1v_2, w_2v_{k-1}\}$, 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,

$$W_e(T_1) - W_e(T_2) = \sum_{h=i+1}^{k-1} d_e(w_1v_i, v_hv_{h+1}|T_1) + \sum_{h=1}^{j-2} d_e(w_2v_j, v_hv_{h+1}|T_1)$$

$$+ d_e(w_1v_i, w_2v_j)|T_1|$$

$$- \left[ \sum_{h=i+1}^{k-1} d_e(w_1v_2, v_hv_{h+1}|T_2) + \sum_{h=1}^{j-2} d_e(w_2v_{k-1}, v_hv_{h+1}|T_2) \right]$$

$$+ d_e(w_1v_2, w_2v_{k-1}|T_2)$$

$$= \sum_{h=i+1}^{k-1} d_e(w_1v_i, v_hv_{h+1}|T_1) + \sum_{h=1}^{j-2} d_e(w_2v_j, v_hv_{h+1}|T_1)$$

$$+ d_e(w_1v_i, w_2v_j)|T_1|$$

$$- \left[ \sum_{h=i+1}^{j-2} (d_e(w_1v_i, v_hv_{h+1}|T_1) + i - 2) \right]$$

$$+ \sum_{h=1}^{j-1} (d_e(w_2v_j, v_hv_{h+1}|T_1) + k - j - 1)$$
\[
+ (d_e(w_1v_i,w_2v_j|T_1)+k+i-j-3)
\]
\[
= - \left[ \sum_{h=i+1}^{k-1} (i-2) + \sum_{h=1}^{j-2} (k-j-1) + (k+i-j-3) \right].
\]

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

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
\[
W_e(P_n) > W_e(P_{n-1}(2)) > W_e(P_{n-1}(3)) > W_e(T_1) > \max\left\{ W_e(P_{n-1}(4)), W_e(T_2), W_e(T_3) \right\}.
\]

**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 \( \sum_{i=2}^{n-2} d_e(\{n-1\}(n-2),(i)(i+1)|P_{n-1}(3)) = \sum_{i=2}^{n-2} d_e((n-1)(n-2),(i)(i+1)|P_{n-1}(4)) = \sum_{i=1}^{n-4} d_e(v_{n-1}v_{n-3},v_i|v_i+1|T_1) \). Then for \( n \geq 10 \), we have
\[
W_e(P_{n-1}(3)) - W_e(T_1) = 1 + 2 + n - 3 + \sum_{i=1}^{n-4} i - \left[ 1 + 1 + n - 4 + \sum_{i=1}^{n-4} i \right] > 0
\]
and
\[
W_e(T_1) - W_e(P_{n-1}(4)) = 1 + 1 + n - 4 + \sum_{i=1}^{n-4} i + \left[ 1 + 2 + n - 3 + \sum_{i=1}^{n-5} i \right].
\]
Figure 3. The trees in Lemma 2.3 \((T_1 \in T(3^2, 2^{n-6}, 1^4), T_2 \in T(3^1, 2^{n-4}, 1^3), T_3 \in T(4^1, 2^{n-5}, 1^4))\).

In addition, \(T_1[\{v_1, v_2, \ldots, v_{n-2}\}] \cong T_2[\{u_1, u_2, \ldots, u_{n-2}\}],\) \(\sum_{i=2}^{n-3} d_e(v_n v_2, v_i v_{i+1} | T_1) = \sum_{i=2}^{n-3} d_e(u_n u_{n-1}, u_i u_{i+1} | T_2) + d_e(u_n u_{n-1}, u_{n-1} u_3 | T_2)\) and \(\sum_{i=2}^{n-4} d_e(v_{n-1} v_n - 3, v_i v_{i+1} | T_1) = \sum_{i=2}^{n-4} d_e(u_{n-1} u_3, u_i u_{i+1} | T_2).\) Then we have

\[ W_e(T_1) - W_e(T_2) = 1 + 1 + n - 4 + n - 4 - (2 + 3 + 1 + 2) > 0 \text{ as } n \geq 10. \]

Finally,

\[ T_1[\{v_1, v_2, \ldots, v_{n-2}\}] \cong T_3[\{x_1, x_2, \ldots, x_{n-2}\}], \]
\[ \sum_{i=2}^{n-3} d_e(v_n v_2, v_i v_{i+1} | T_1) = \sum_{i=2}^{n-3} d_e(x_{n-1} x_2, x_i x_{i+1} | T_3), \]
\[ \sum_{i=2}^{n-4} d_e(v_{n-1} v_n - 3, v_i v_{i+1} | T_1) = \sum_{i=2}^{n-4} d_e(x_{n-1} x_2, x_i x_{i+1} | T_3). \]

Then we have,

\[ W_e(T_1) - W_e(T_3) = n - 4 - (1 + 1 + 1) > 0 \text{ as } n \geq 10. \]

which completes the proof. \(\square\)

**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 \( T \in \{ P_{n-1}(i); i = 4, 5, \ldots, \left[ \frac{n}{2} \right] \} \) 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. \( \Box \)

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. \( \Box \)

References