

Wiener index of graphs with fixed number of pendant or cut vertices

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Abstract

The Wiener index of a connected graph is defined as the sum of the distances between all unordered pair of its vertices. In this paper, we characterize the graphs which extremize the Wiener index among all graphs on n vertices with k pendant vertices. We also characterize the graph which minimizes the Wiener index over the graphs on n vertices with s cut vertices.

Key words: Unicyclic graph; Distance; Wiener index; Pendant vertex; Cut vertex

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1 Introduction

Throughout this paper, graphs are finite, simple, connected and undirected. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, $N_G(v)$ denotes the set of all neighbours of v in G . A vertex of degree one is called a *pendant vertex*. A vertex v of G is called a *cut-vertex* if $G \setminus v$ is disconnected. The distance between two vertices $u, v \in V(G)$, denoted by $d_G(u, v)$ or $d(u, v)$ (if the context is clear), is the number of edges in a shortest path joining u and v . The distance of a vertex $v \in V(G)$, denoted by $D_G(v)$, is defined as $D_G(v) = \sum_{u \in V(G)} d_G(u, v)$. We refer to [18] for undefined notations and terminologies.

The *Wiener index* of G , denoted by $W(G)$, is defined as the sum of distances between all unordered pair of its vertices. *i.e.*

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

Different names such as *graph distance* [6], *transmission* [10], *total status* [3] and *sum of all distances* [7, 23] have been used to study the graphical invariant $W(G)$. Apparently, the chemist H. Wiener was the first to point out in 1947 (see [22]) that $W(G)$ is well correlated with certain physio-chemical properties of the organic compound from which G is derived. The *mean distance* [5, 19] or *the average distance* [1, 4] between the vertices is a quantity closely related to $W(G)$. By considering G as an interconnection network connecting many processors, the average distance of G between the nodes of the network is a measure of the average delay for traversing the messages from one node to another.

In Mathematical literature, the Wiener index is first studied by Entringer et al. in [6]. This gave an important direction to the researchers to characterize the graphs with extremal Wiener index in certain classes of graphs. In last 20 years a lot of studies for the optimal graphs in different classes of trees and unicyclic graphs have been done (see [9, 11, 13, 16, 17, 20, 21, 24, 25]).

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Apart from trees and unicyclic graphs, some other classes of graphs are also studied for the characterization of graphs having extremal Wiener index. Wiener index of graphs with fixed maximum degree is studied in [14]. The graphs with maximum and minimum Wiener index among all Eulerian graphs on n vertices are characterized in [8].

Wiener index of unicyclic graphs with fixed number of pendent vertices or cut vertices is studied in [17]. In this paper, we characterize the graphs having maximum and minimum Wiener index over all connected graphs on n vertices with k pendant vertices. We also obtain the graph which minimizes the Wiener index among all connected graphs on n vertices with s cut-vertices.

1.1 Main results

We first construct some classes of graphs. For $g < n$, let $U_{n,g}^p$ be the graph obtained by attaching $n - g$ pendant vertices at one vertex of the cycle C_g and $U_{n,g}^l$ be the graph obtained by joining an edge between a pendant vertex of the path P_{n-g} with a vertex of C_g .

Let $\mathfrak{H}_{n,k}$ denote the class of all connected graphs on n vertices and k pendant vertices. Let $\mathfrak{T}_{n,k}$ be the subclass of $\mathfrak{H}_{n,k}$ containing all the trees on n vertices and k pendant vertices.

The path $[v_1 v_2 \dots v_n]$ on n vertices is denoted by P_n . For positive integers k, l, d with $n = k + l + d$, let $T(k, l, d)$ be the tree obtained by taking the path P_d and adding k pendant vertices adjacent to v_1 and l pendant vertices adjacent to v_d . Note that $T(1, 1, d)$ is a path on $d + 2$ vertices.

We define a specific subclass of graphs in $\mathfrak{H}_{n,0}$ as follows. Let m_1, m_2 and n be positive integers with $m_1, m_2 \geq 3$ and $n \geq m_1 + m_2 - 1$. If $n > m_1 + m_2 - 1$, take a path on $n - (m_1 + m_2) + 2$ vertices and identify one pendant vertex of the path with a vertex of C_{m_1} and another pendant vertex with a vertex of C_{m_2} . If $n = m_1 + m_2 - 1$, then identify one vertex of C_{m_1} with a vertex of C_{m_2} . We denote this graph by C_{m_1, m_2}^n .

In this paper, we prove the following results:

Theorem 1.1. *Let $0 \leq k \leq n - 2$ and let $G \in \mathfrak{H}_{n,k}$. Then*

(i) *for $2 \leq k \leq n - 2$, $W(G) \leq W(T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n - k))$ and equality happens if and only if $G = T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n - k)$. Furthermore, $W(T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n - k)) =$*

$$\begin{cases} \binom{n-k+1}{3} + \frac{k^2}{4}(n-k+3) + \frac{k}{2}[(n-k)^2 + n - k - 2] & \text{if } k \text{ is even} \\ \binom{n-k+1}{3} + \frac{k^2-1}{4}(n-k+3) + \frac{k}{2}[(n-k)^2 + n - k - 2] + 1 & \text{if } k \text{ is odd.} \end{cases}$$

(ii) *for $k = 1$, $W(G) \leq W(U_{n,3}^l)$ and equality holds if and only if $G = U_{n,3}^l$. Furthermore,*

$$W(U_{n,3}^l) = \frac{n^3 - 7n + 12}{6}.$$

(iii) *for $k = 0$ and $n \geq 7$, $W(G) \leq W(C_{3,3}^n)$ and equality holds if and only if $G = C_{3,3}^n$. Furthermore,*

$$W(C_{3,3}^n) = \frac{n^3 - 13n + 24}{6}.$$

For $0 \leq k \leq n - 3$ and $n \geq 4$, let P_n^k be the graph obtained by adding k pendant vertices at one vertex of the complete graph K_{n-k} .

Theorem 1.2. *Let $0 \leq k \leq n - 2$ and let $G \in \mathfrak{H}_{n,k}$. Then*

(i) for $0 \leq k \leq n-3$, $W(P_n^k) \leq W(G)$ and equality holds if and only if $G = P_n^k$. Furthermore,

$$W(P_n^k) = \binom{n-k}{2} + k^2 + 2k(n-k-1).$$

(ii) for $k = n-2$, $W(T(1, n-3, 2)) \leq W(G)$ and equality holds if and only if $G = T(1, n-3, 2)$. Furthermore,

$$W(T(1, n-3, 2)) = n^2 - n - 2.$$

Let $T_{n,k} \in \mathfrak{T}_{n,k}$ be the tree that has a vertex v of degree k and $T_{n,k} \setminus v = rP_{q+1} \cup (k-r)P_q$, where $q = \lfloor \frac{n-1}{k} \rfloor$ and $r = n-1-kq$. Here, we have $0 \leq r < k$.

Theorem 1.3. *Let $2 \leq k \leq n-2$ and $T \in \mathfrak{T}_{n,k}$. Then $W(T_{n,k}) \leq W(T)$ and equality holds if and only if $T = T_{n,k}$.*

Let $\mathfrak{C}_{n,s}$ be the set of all connected graphs on n vertices and s cut vertices. For $2 \leq m \leq n$, let v_1, v_2, \dots, v_m be the vertices of a complete graph K_m . For $i = 1, 2, \dots, m$ consider the paths P_{l_i} such that $l_1 + l_2 + \dots + l_m = n$. Identify a pendant vertex of the path P_{l_i} with the vertex v_i , for $i = 1, 2, \dots, m$ to obtain a graph on n vertices and we denote it by $K_m^n(l_1, l_2, \dots, l_m)$.

Theorem 1.4. *Let $0 \leq s \leq n-3$ and $i, j \in \{1, 2, \dots, n-s\}$. Then the graph $K_{n-s}^n(l_1, l_2, \dots, l_{n-s})$ with $|l_i - l_j| \leq 1$ has the minimum Wiener index over $\mathfrak{C}_{n,s}$.*

In the next section we will discuss some results related to Wiener index of graphs which are useful to prove our main theorems.

2 Preliminaries

We start this section with the following lemma.

Lemma 2.1. *Let G be a graph and $u, v \in V(G)$ are non adjacent. Let G' be the graph obtained from G by joining the vertices u and v by an edge. Then $W(G') < W(G)$.*

It follows from Lemma 2.1 that among all connected graphs on n vertices, the Wiener index is minimized by the complete graph K_n and maximized by a tree. Among all trees on n vertices, the Wiener index is minimized by the star $K_{1,n-1}$ and maximized by the path P_n (see [18], Theorem 2.1.14). It is easy to determine the Wiener index of the following graphs (see [18]): (i) $W(K_n) = \binom{n}{2}$ (ii) $W(P_n) = \binom{n+1}{3}$ (iii) $W(K_{1,n-1}) = (n-1)^2$. The Wiener index of the cycle C_n is (see [10], Theorem 5)

$$W(C_n) = \begin{cases} \frac{1}{8}n^3 & \text{if } n \text{ is even} \\ \frac{1}{8}n(n^2 - 1) & \text{if } n \text{ is odd.} \end{cases} \quad (1)$$

Also for $u \in V(C_n)$

$$D_{C_n}(u) = \begin{cases} \frac{n^2}{4} & \text{if } n \text{ is even} \\ \frac{n^2-1}{4} & \text{if } n \text{ is odd.} \end{cases} \quad (2)$$

The following lemma is very useful.

Lemma 2.2. ([2], Lemma 1.1) *Let G be a graph and u be a cut vertex in G . Let G_1 and G_2 be two subgraphs of G with $G = G_1 \cup G_2$ and $V(G_1) \cap V(G_2) = \{u\}$. Then*

$$W(G) = W(G_1) + W(G_2) + (|V(G_1)| - 1)D_{G_2}(u) + (|V(G_2)| - 1)D_{G_1}(u).$$

Corollary 2.3. *Let G and H be two connected graphs having at least 2 vertices each. Let $u, v \in V(G)$ and $w \in V(H)$. Let G_1 and G_2 be the graphs obtained from G and H by identifying the vertex w of H with the vertices u and v of G , respectively. If $D_G(v) \geq D_G(u)$ then $W(G_2) \geq W(G_1)$ and equality happens if and only if $D_G(v) = D_G(u)$.*

Proof. By Lemma 2.2,

$$W(G_1) = W(G) + W(H) + (|V(G)| - 1)D_H(w) + (|V(H)| - 1)D_G(u)$$

and

$$W(G_2) = W(G) + W(H) + (|V(G)| - 1)D_H(w) + (|V(H)| - 1)D_G(v).$$

So

$$W(G_2) - W(G_1) = (|V(H)| - 1)(D_G(v) - D_G(u))$$

and the result follows. \square

Let G be a connected graph on $n \geq 2$ vertices. Let v be a vertex of G . For $l, k \geq 1$, let $G_{k,l}$ be the graph obtained from G by attaching two new paths $P : vv_1v_2 \cdots v_k$ and $Q : vu_1u_2 \cdots u_l$ of lengths k and l respectively, at v , where u_1, u_2, \dots, u_l and v_1, v_2, \dots, v_k are distinct new vertices. Let $\tilde{G}_{k,l}$ be the graph obtained from $G_{k,l}$ by removing the edge $\{v_{k-1}, v_k\}$ and adding the edge $\{u_l, v_k\}$. Observe that the graph $\tilde{G}_{k,l}$ is isomorphic to the graph $G_{k-1, l+1}$. We say that $\tilde{G}_{k,l}$ is obtained from $G_{k,l}$ by *grafting* an edge.

Consider the path $P_n : v_1v_2 \cdots v_n$ on n vertices with v_i adjacent to v_{i-1} and v_{i+1} for $2 \leq i \leq n-1$. Then for $i = 1, 2, \dots, n$,

$$D_{P_n}(v_i) = D_{P_n}(v_{n-i+1}) = \frac{(n-i)(n-i+1) + i(i-1)}{2}.$$

So, if n is odd, then

$$D_{P_n}(v_1) > D_{P_n}(v_2) > \cdots > D_{P_n}(v_{\frac{n+1}{2}}) < D_{P_n}(v_{\frac{n+3}{2}}) < \cdots < D_{P_n}(v_{n-1}) < D_{P_n}(v_n)$$

and if n is even, then

$$D_{P_n}(v_1) > D_{P_n}(v_2) > \cdots > D_{P_n}(v_{\frac{n}{2}}) = D_{P_n}(v_{\frac{n+2}{2}}) < \cdots < D_{P_n}(v_{n-1}) < D_{P_n}(v_n).$$

The next result follows from the above and Corollary 2.3.

Corollary 2.4. ([13], Lemma 2.4) *If $1 \leq k \leq l$, then $W(G_{k-1, l+1}) > W(G_{k,l})$.*

The following result compares the Wiener index of two graphs, where one is obtained from the other by moving one component from a vertex to another vertex.

Lemma 2.5. ([12], Lemma 2.4) *Let H, X, Y be three connected pairwise vertex disjoint graphs having at least 2 vertices each. Suppose that u and v are two distinct vertices of H , x is a vertex of X and y is a vertex of Y . Let G be the graph obtained from H, X, Y by identifying u with x and v with y , respectively. Let G_1^* be the graph obtained from H, X, Y by identifying vertices u, x, y and let G_2^* be the graph obtained from H, X, Y by identifying vertices v, x, y (see figure 1). Then $W(G_1^*) < W(G)$ or $W(G_2^*) < W(G)$.*

Corollary 2.6. *Let G be a connected graph on $n \geq 2$ vertices and let $u, v \in V(G)$. For $n_1, n_2 \geq 0$, let $G_{uv}(n_1, n_2)$ be the graph obtained from G by attaching n_1 pendant vertices at u and n_2 pendant vertices at v . If $n_1, n_2 \geq 1$ then*

$$W(G_{uv}(n_1 + n_2, 0)) < W(G_{uv}(n_1, n_2)) \text{ or } W(G_{uv}(0, n_1 + n_2)) < W(G_{uv}(n_1, n_2)).$$

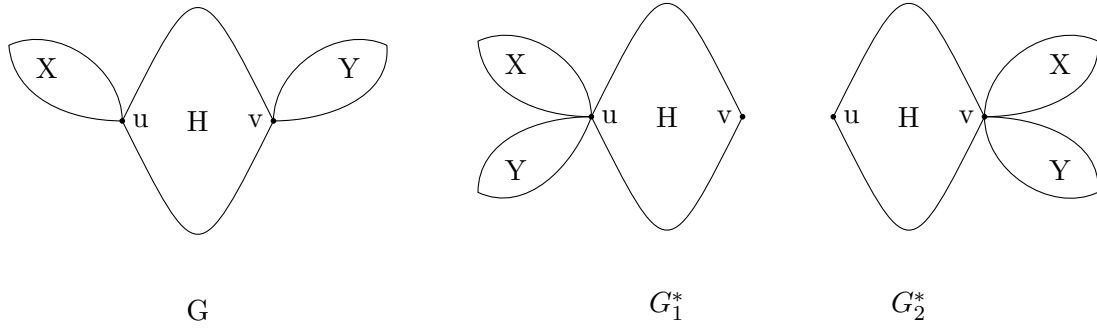


Figure 1: Movement of a component from one vertex to other

In [24], Lemma 2.6, if we take $G_0 = P_{n_0}$ and u_0 and v_0 as two distinct pendant vertices of G_0 , then $G_0 \cong G_1 \cong G_2$. So, $W(G_0) = W(G_1) = W(G_2)$, hence the statement of the mentioned lemma is not true. In the following result, we have given a proof of the corrected version of it.

Lemma 2.7. *Let G be a connected graph on $n \geq 3$ vertices and $u, v \in V(G)$. For $l, k \geq 1$, let $G_{uv}^p(l, k)$ be the graph obtained from G by identifying a pendant vertex of the path P_l with u and identifying a pendant vertex of the path P_k with v . Suppose $l, k \geq 2$. If G is not the u - v path and $D_G(u) \geq D_G(v)$ then*

$$W(G_{uv}^p(l+k-1, 1)) > W(G_{uv}^p(l, k)).$$

Proof. First consider the graph $G_{u,v}^p(l, 1)$ as H and let w be the pendant vertex of H corresponding to P_l . Then by Lemma 2.2,

$$W(G_{u,v}^p(l, k)) = W(H) + W(P_k) + (|V(H)| - 1)D_{P_k}(v) + (k-1)D_H(v)$$

and

$$W(G_{u,v}^p(l+k-1, 1)) = W(H) + W(P_k) + (|V(H)| - 1)D_{P_k}(w) + (k-1)D_H(w).$$

As $D_{P_k}(v) = D_{P_k}(w)$ we get,

$$W(G_{u,v}^p(l+k-1, 1)) - W(G_{u,v}^p(l, k)) = (k-1)(D_H(w) - D_H(v)).$$

Now

$$D_H(w) = D_{P_{l-1}}(w) + (l-1)|V(G)| + D_G(u)$$

and

$$D_H(v) = D_G(u) + (l-1)(d_G(u, v) + 1) + D_{P_{l-1}}(u')$$

where u' is the vertex on the path P_l adjacent to u . Since $D_{P_{l-1}}(w) = D_{P_{l-1}}(u')$, so

$$D_H(w) - D_H(v) = (l-1)(|V(G)| - d_G(u, v) - 1) + D_G(u) - D_G(v).$$

As $l \geq 2$ and G is not the u - v path, so $(l-1)(|V(G)| - d_G(u, v) - 1) > 0$. Hence the result follows from the given condition $D_G(u) \geq D_G(v)$. \square

The Wiener index of $U_{n,g}^p$ and $U_{n,g}^l$ are useful for our results and can be found in [24](see Theorem 1.1).

$$W(U_{n,g}^p) = \begin{cases} \frac{g^3}{8} + (n-g)(\frac{g^2}{4} + n-1) & \text{if } g \text{ is even} \\ \frac{g(g^2-1)}{8} + (n-g)(\frac{g^2-1}{4} + n-1) & \text{if } g \text{ is odd} \end{cases} \quad (3)$$

$$W(U_{n,g}^l) = \begin{cases} \frac{g^3}{8} + (n-g)(\frac{n^2+ng+3g-1}{6} - \frac{g^2}{12}) & \text{if } g \text{ is even} \\ \frac{g(g^2-1)}{8} + (n-g)(\frac{n^2+ng+3g-1}{6} - \frac{g^2}{12} - \frac{1}{4}) & \text{if } g \text{ is odd} \end{cases} \quad (4)$$

We next calculate the Wiener index of some more trees, which we need for the extremal bounds in some of our results. Let $S_{d,k}$ be the tree obtained by identifying a pendant vertex of the path P_d with the central vertex of the star $K_{1,k}$. By using Lemma 2.2, it is easy to see that

$$W(S_{d,k}) = \binom{d+1}{3} + k^2 + (d-1)k + \frac{d(d-1)k}{2}. \quad (5)$$

Then by Lemma 2.2 and using the value of $W(S_{d,k})$ and $W(K_{1,l})$, we get

$$W(T(l,k,d)) = \binom{d+1}{3} + l^2 + k^2 + \frac{(d^2+d-2)(k+l)}{2} + (d+1)kl. \quad (6)$$

For $l \geq 2$ and $q \geq 1$, let T_l^q be the tree on $lq+1$ vertices with l pendant vertices having one vertex v of degree l and $T_l^q - v = lP_q$ (l copies of P_q). Note that T_1^q is the path P_{q+1} . Then

$$D_{T_l^q}(v) = l + 2l + \dots + ql = \frac{lq(q+1)}{2}. \quad (7)$$

Now by lemma 2.2,

$$\begin{aligned} W(T_l^q) &= W(T_{l-1}^q) + W(T_1^q) + (l-1)qD_{T_1^q}(v) + qD_{T_{l-1}^q}(v) \\ &= W(T_{l-1}^q) + \binom{q+2}{3} + (l-1)q^2(q+1). \end{aligned}$$

Solving this recurrence relation we get,

$$W(T_l^q) = l \binom{q+2}{3} + \frac{q^2l(q+1)(l-1)}{2}. \quad (8)$$

3 Proofs of Theorem 1.1, Theorem 1.2 and Theorem 1.3

We first recall three known results related to Wiener index of graphs.

Theorem 3.1. ([15], Theorem 4) For $2 \leq k \leq n-2$, the tree $T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n-k)$ maximizes the Wiener index over $\mathfrak{T}_{n,k}$.

Theorem 3.2. ([24], Corollary 1.2) Among all unicyclic graphs on $n > 4$ vertices, the graph $U_{n,3}^l$ has the maximum Wiener index.

Theorem 3.3. ([10], Theorem 5) Let G be a two connected graph with n vertices then $W(G) \leq W(C_n)$ and equality holds if and only if $G = C_n$.

We now compare the Wiener index of the graphs $C_{3,3}^n$ and C_n .

Lemma 3.4. For $n \geq 6$, $W(C_n) \leq W(C_{3,3}^n)$ and equality happens if and only if $n = 6$.

Proof. By (4), we have $W(U_{n,3}^l) = \frac{n^3-7n+12}{6}$. If u is the pendant vertex of $U_{n,3}^l$ then $D_{U_{n,3}^l}(u) = D_{P_{n-2}}(u) + 2(n-2) = \frac{(n-3)(n-2)}{2} + 2n - 4 = \frac{n^2-n-2}{2}$. For $n \geq 6$, let u be the cut-vertex common to C_3 and $U_{n-2,3}^l$ of $C_{3,3}^n$. Then by Lemma 2.2,

$$\begin{aligned} W(C_{3,3}^n) &= W(C_3) + W(U_{n-2,3}^l) + 2D_{U_{n-2,3}^l}(u) + 2(n-3) \\ &= 3 + \frac{(n-2)^3 - 7(n-2) + 12}{6} + (n-2)^2 - (n-2) - 2 + 2n - 6 \\ &= \frac{n^3 - 13n + 24}{6} \end{aligned} \quad (9)$$

By (1) and (9), we have

$$W(C_{3,3}^n) - W(C_n) = \begin{cases} \frac{n(n^2-52)}{24} + 4, & \text{if } n \text{ is even} \\ \frac{n(n^2-49)}{24} + 4, & \text{if } n \text{ is odd.} \end{cases}$$

Hence the result follows. \square

Lemma 3.5. *Let $m_1, m_2 \geq 3$ be two integers and let $n = m_1 + m_2 - 1$. Then $W(C_n) > W(C_{m_1, m_2}^n)$.*

Proof. Let v be the vertex of degree 4 in C_{m_1, m_2}^n . First suppose n is even. Then one of m_1 or m_2 is odd and other is even. Without loss of generality, suppose m_1 is odd and m_2 is even. Then by Lemma 2.2, (1) and (2) we have

$$\begin{aligned} W(C_{m_1, m_2}^n) &= W(C_{m_1}) + W(C_{m_2}) + (m_2 - 1)D_{C_{m_1}}(v) + (m_1 - 1)D_{C_{m_2}}(v) \\ &= \frac{m_1^3 - m_1}{8} + \frac{m_2^3}{8} + (m_2 - 1)\frac{m_1^2 - 1}{4} + (m_1 - 1)\frac{m_2^2}{4} \\ &= \frac{1}{8}(m_1^3 + m_2^3 + 2m_1^2m_2 + 2m_1m_2^2 - 2m_1^2 - 2m_2^2 - m_1 - 2m_2 + 2) \end{aligned}$$

and

$$\begin{aligned} W(C_n) &= \frac{1}{8}(m_1 + m_2 - 1)^3 \\ &= \frac{1}{8}(m_1^3 + m_2^3 + 3m_1^2m_2 + 3m_1m_2^2 - 3m_1^2 - 3m_2^2 - 6m_1m_2 + 3m_1 + 3m_2 - 1) \end{aligned}$$

The difference is

$$\begin{aligned} W(C_n) - W(C_{m_1, m_2}^n) &= \frac{1}{8}(m_1^2m_2 + m_1m_2^2 - m_1^2 - m_2^2 - 6m_1m_2 + 4m_1 + 5m_2 - 3) \\ &= \frac{1}{8}((m_2 - 1)m_1^2 + (m_1 - 1)m_2^2 + 4m_1 + 5m_2 - 6m_1m_2 - 3) \end{aligned}$$

An easy calculation gives

$$W(C_n) - W(C_{m_1, m_2}^n) \begin{cases} = \frac{1}{4}m_2(m_2 - 2), & \text{if } m_1 = 3 \\ \geq \frac{1}{8}(3(m_1 - m_2)^2 + 4m_1 + 5m_2 - 3), & \text{if } m_1 \geq 5 \end{cases}$$

which is greater than 0.

Now suppose n is odd. Then there are two possibilities.

Case 1: Both m_1 and m_2 are even.

$$\begin{aligned} W(C_{m_1, m_2}^n) &= W(C_{m_1}) + W(C_{m_2}) + (m_2 - 1)D_{C_{m_1}}(v) + (m_1 - 1)D_{C_{m_2}}(v) \\ &= \frac{m_1^3}{8} + \frac{m_2^3}{8} + (m_2 - 1)\frac{m_1^2}{4} + (m_1 - 1)\frac{m_2^2}{4} \\ &= \frac{1}{8}(m_1^3 + m_2^3 + 2m_2m_1^2 + 2m_1m_2^2 - 2m_1^2 - 2m_2^2) \end{aligned}$$

$$\begin{aligned} W(C_n) &= W(C_{m_1+m_2-1}) \\ &= \frac{1}{8}((m_1 + m_2 - 1)^3 - (m_1 + m_2 - 1)) \\ &= \frac{1}{8}(m_1^3 + m_2^3 + 3m_1^2m_2 + 3m_1m_2^2 - 3m_1^2 - 3m_2^2 - 6m_1m_2 + 2m_1 + 2m_2) \end{aligned}$$

The difference is

$$\begin{aligned} W(C_n) - W(C_{m_1, m_2}^n) &= \frac{1}{8}((m_1 - 1)m_2^2 + (m_2 - 1)m_1^2 - 6m_1m_2 + 2m_1 + 2m_2) \\ &\geq \frac{1}{8}(3(m_1 - m_2)^2 + 2m_1 + 2m_2) \\ &> 0 \end{aligned}$$

Case 2: Both m_1 and m_2 are odd.

$$\begin{aligned} W(C_{m_1, m_2}^n) &= \frac{m_1^3 - m_1}{8} + \frac{m_2^3 - m_2}{8} + (m_2 - 1)\frac{m_1^2 - 1}{4} + (m_1 - 1)\frac{m_2^2 - 1}{4} \\ &= \frac{1}{8}(m_1^3 + m_2^3 + 2m_2m_1^2 + 2m_1m_2^2 - 2m_1^2 - 2m_2^2 - 3m_1 - 3m_2 + 4) \end{aligned}$$

and the difference is

$$W(C_n) - W(C_{m_1, m_2}^n) = \frac{1}{8}((m_1 - 1)m_2^2 + (m_2 - 1)m_1^2 - 6m_1m_2 + 5m_1 + 5m_2 - 4).$$

An easy calculation gives

$$W(C_n) - W(C_{m_1, m_2}^n) \begin{cases} > \frac{1}{8}(3(m_1 - m_2)^2 + 5m_1 + 5m_2 - 4), & \text{if } m_1, m_2 \geq 5 \\ = \frac{1}{8}(2m_2^2 - 4m_2 + 2), & \text{if } m_1 = 3 \\ = \frac{1}{8}(2m_1^2 - 4m_1 + 2), & \text{if } m_2 = 3 \end{cases}$$

which is greater than 0 and this completes the proof. \square

Lemma 3.6. *Let u be the pendant vertex and v be a non-pendant vertex of the unicyclic graph $U_{n,g}^l$. Then $D_{U_{n,g}^l}(u) > D_{U_{n,g}^l}(v)$.*

Proof. Let g be the vertex of degree 3 in $U_{n,g}^l$ and let $g+1$ be the vertex adjacent to g not on the g -cycle of $U_{n,g}^l$. Then

$$D_{U_{n,g}^l}(u) = D_{P_{n-g+1}}(u) + (g-1)(n-g) + D_{C_g}(g). \quad (10)$$

If v is a vertex on the cycle C_g of $U_{n,g}^l$ then

$$D_{U_{n,g}^l}(v) = D_{C_g}(v) + d(v, g)(n - g) + D_{P_{n-g+1}}(g)$$

and if w is a non pendant vertex of $U_{n,g}^l$ which is not on the cycle then

$$D_{U_{n,g}^l}(w) = D_{P_{n-g+1}}(w) + d(w, g)(g - 1) + D_{C_g}(g)$$

Since $D_{P_{n-g+1}}(u) = D_{P_{n-g+1}}(g), D_{P_{n-g+1}}(u) > D_{P_{n-g+1}}(w)$ and $D_{C_g}(g) = D_{C_g}(v)$, so

$$D_{U_{n,g}^l}(u) - D_{U_{n,g}^l}(v) = (n - g)(g - 1 - d(v, g)) > 0$$

$$D_{U_{n,g}^l}(u) - D_{U_{n,g}^l}(w) > (g - 1)(n - g - d(w, g)) > 0.$$

□

The next corollary follows from Lemma 3.6 and Corollary 2.3.

Corollary 3.7. *Let G be a connected graph with at least two vertices and let $u \in V(G)$. Suppose v is the pendant vertex of $U_{n,g}^l$ and w is a non-pendant vertex of $U_{n,g}^l$. Let G_1 and G_2 be the graph obtained from G and H by identifying u of G with the vertices with v and w of $U_{n,g}^l$, respectively. Then $W(G_1) > W(G_2)$.*

Lemma 3.8. *Let u be a vertex of a connected graph G . For $m \geq 4$, let G_1 be the graph obtained by identifying the vertex u of G with the pendant vertex of $U_{m+1,m}^l$ and G_2 be the graph obtained by identifying the vertex u with the pendant vertex of $U_{m+1,3}^l$. Then $W(G_2) > W(G_1)$.*

Proof. By Lemma 2.2, we have

$$W(G_1) = W(G) + W(U_{m+1,m}^l) + (|V(G)| - 1)D_{U_{m+1,m}^l}(u) + mD_G(u)$$

and

$$W(G_2) = W(G) + W(U_{m+1,3}^l) + (|V(G)| - 1)D_{U_{m+1,3}^l}(u) + mD_G(u).$$

By Theorem 3.2, $W(U_{m+1,3}^l) > W(U_{m+1,m}^l)$. So, the difference is

$$W(G_2) - W(G_1) > (|V(G)| - 1)(D_{U_{m+1,3}^l}(u) - D_{U_{m+1,m}^l}(u)).$$

By (10), we have $D_{U_{m+1,3}^l}(u) = \frac{(m-1)(m+2)}{2}$ and

$$D_{U_{m+1,m}^l}(u) = \begin{cases} m + \frac{m^2}{4} & \text{if } m \text{ is even} \\ m + \frac{m^2-1}{4} & \text{if } m \text{ is odd.} \end{cases}$$

So,

$$D_{U_{m+1,3}^l}(u) - D_{U_{m+1,m}^l}(u) = \begin{cases} \frac{m^2-2m-4}{4} & \text{if } m \text{ is even} \\ \frac{m^2-2m-3}{4} & \text{if } m \text{ is odd} \end{cases}$$

which is greater than 0 and this completes the proof. □

Corollary 3.9. *Let $m_1, m_2 \geq 3$ be two integers and let $m_1 + m_2 \leq n$. Then $W(C_{3,3}^n) \geq W(C_{m_1, m_2}^n)$ and equality happens if and only if $m_1 = m_2 = 3$.*

Proof of Theorem 1.1: (i) Let $G \in \mathfrak{H}_{n,k}$. Construct a spanning tree G' from G by deleting some edges if required. Then by Lemma 2.1, $W(G') \geq W(G)$. The number of pendent vertices of G' is greater than or equal to k . Suppose G' has more than k pendant vertices. Since $k \geq 2$, G' has at least one vertex of degree greater than 2 and two paths attached to it. Consider a vertex v of G' with $d(v) \geq 3$ and two paths P_{l_1}, P_{l_2} , $l_1 \geq l_2$ attached at v . Using grafting of edge operation on G' , we get a new tree \tilde{G} with number of pendant vertices one less than the number of pendant vertices of G' and by Corollary 2.4, $W(\tilde{G}) > W(G')$. Continue this process till we get a tree with k pendant vertices from \tilde{G} . By Lemma 2.4, every step in this process the Wiener index will increase. So, we will reach at a tree of order n with k pendant vertices. Hence the result follows from Theorem 3.1. Then replacing d, l and k by $n - k, \lfloor \frac{k}{2} \rfloor$ and $\lceil \frac{k}{2} \rceil$, respectively in (6), we get $W(T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n - k))$.

- (ii) Let $G \in \mathfrak{H}_{n,1}$. Since G is connected and has exactly one pendent vertex, it must contain a cycle. Let C_g be a cycle in G . If G has more than one cycle, then construct a new graph G' from G by deleting edges from all cycles other than C_g so that the graph remains connected. Then by Lemma 2.1, $W(G') > W(G)$ and G' is a unicyclic graph on n vertices with girth g . By Theorem 3.2, $W(U_{n,3}^l) \geq W(G')$ and equality happens if and only if $G' = U_{n,3}^l$. As $U_{n,3}^l \in \mathfrak{H}_{n,1}$, so the result follows and we get the value of $W(U_{n,3}^l)$ from (4).
- (iii) Let $n \geq 7$ and let $G \in \mathfrak{H}_{n,0}$. Then we have two cases:

Case 1: For some integers $m_1, m_2 \geq 3$ with $n = m_1 + m_2 - 1$ and C_{m_1, m_2}^n is a subgraph of G .

Since C_{m_1, m_2}^n is a subgraph of G , by deleting some edges from G we get $C_{m_1, m_2}^n \in \mathfrak{H}_{n,0}$ and by Lemma 2.1 $W(G) < W(C_{m_1, m_2}^n)$. Again by Lemma 3.5, $W(C_{m_1, m_2}^n) < W(C_n)$. Now the result follows from Lemma 3.4.

Case 2: There is no integers $m_1, m_2 \geq 3$ with $n = m_1 + m_2 - 1$ such that C_{m_1, m_2}^n is a subgraph of G .

If G is a two connected graph then by Theorem 3.3, $W(G) \leq W(C_n)$ and the result follows from Lemma 3.4. So let G has at least one cut vertex.

Claim: $W(G) \leq W(C_{g_1, g_2}^n)$ for some $g_1, g_2 \geq 3$ and the equality holds if and only if $G = C_{g_1, g_2}^n$.

Since G has a cut-vertex and no pendant vertices, so G contains two cycles with at most one common vertex. Let C_{g_1} and C_{g_2} be two cycles of G with at most one common vertex. Since C_{m_1, m_2}^n with $m_1 + m_2 - 1 = n$ is not a subgraph of G , so $g_1 + g_2 \leq n$. Clearly G has at least $n + 1$ edges.

If G has exactly $n + 1$ edges, then there is no common vertex between C_{g_1} and C_{g_2} and $G = C_{g_1, g_2}^n$. So, let G has at least $n + 2$ edges. Suppose $|E(G)| = n + k$, where $k \geq 2$. Choose $k - 1$ edges $\{e_1, \dots, e_{k-1}\} \subset E(G)$ such that $e_i \notin E(C_{g_1}) \cup E(C_{g_2})$, $i = 1, \dots, k - 1$ and $G \setminus \{e_1, \dots, e_{k-1}\}$ is connected. Let $G_1 = G \setminus \{e_1, \dots, e_{k-1}\}$ (G_1 may have some pendant vertices). Then by Lemma 2.1, $W(G_1) > W(G)$. If G_1 has no pendant vertices then $G_1 = C_{g_1, g_2}^n$.

Let G_1 has some pendant vertices. Then for some $l < n$, C_{g_1, g_2}^l is a subgraph of G_1 . By grafting of edges operation(if required), we can form a new graph G_2 from G_1 where G_2 is a connected graph on n vertices obtained by attaching some paths to some vertices of C_{g_1, g_2}^l . Then by Corollary 2.4, $W(G_2) > W(G_1)$. If more than one paths are attached to

different vertices of C_{g_1, g_2}^l in G_2 , then using the graph operation as mentioned in Lemma 2.7, form a new graph G_3 from G_2 , where G_3 has exactly one path attached to C_{g_1, g_2}^l . Then by Lemma 2.7, $W(G_3) > W(G_2)$. Let the path attached to the vertex u in C_{g_1, g_2}^l of G_3 . Then again we have two cases:

Case-i: $u \in V(C_{g_1}) \cup V(C_{g_2})$

Without loss of generality, assume that $u \in V(C_{g_1})$. Then the induced subgraph of G_3 containing the vertices of C_{g_1} and the vertices of the path attached to it, is the graph U_{k, g_1}^l for some $k > g_1$. Let v be the pendant vertex of U_{k, g_1}^l . Since the two cycles C_{g_1} and C_{g_2} have at most one vertex in common, so we have two subcases:

Subcase-1: $V(C_{g_1}) \cap V(C_{g_2}) = \{w\}$

Let H_1 be the induced subgraph of G_3 containing the vertices $\{V(G_3) \setminus V(U_{k, g_1}^l)\} \cup \{w\}$. Clearly H_1 is the cycle C_{g_2} . Then identify the vertex v of U_{k, g_1}^l with the vertex w of H_1 to form a new graph G_4 . By Corollary 3.7, $W(G_4) > W(G_3)$ and G_4 is the graph C_{g_1, g_2}^n .

Subcase-2: $V(C_{g_1}) \cap V(C_{g_2}) = \phi$

Let H_2 be the induced subgraph of G_3 containing the vertices $V(G_3) \setminus V(U_{k, g_1}^l)$. In G_3 exactly one vertex $w_1 \in U_{k, g_1}^l$ adjacent to exactly one vertex w_2 of H_2 . Form a new graph G_5 from G_3 by deleting the edge $\{w_1, w_2\}$ and adding the edge $\{v, w_2\}$. By Corollary 3.7, $W(G_5) > W(G_3)$ and G_5 is the graph C_{g_1, g_2}^n .

Case-ii: $u \notin V(C_{g_1}) \cup V(C_{g_2})$

Let w be the pendant vertex of G_3 and let w_3 be a vertex in C_{g_1, g_2}^l of G_3 adjacent to u . Form a new graph G_6 from G_3 by deleting the edge $\{u, w_3\}$ and adding the edge $\{w, w_3\}$. By Corollary 3.7, $W(G_6) > W(G_3)$ and G_6 is the graph C_{g_1, g_2}^n . This proves our claim.

Now from Corollary 3.9, it follows that $W(G) \leq W(C_{3,3}^n)$ and by (9) $W(C_{3,3}^n) = \frac{n^3 - 13n + 24}{6}$. This completes the proof. □

It can be checked easily that for $n \leq 5$, the cycle C_n has the maximum Wiener index over $\mathfrak{H}_{n,0}$ and for $n = 6$, the Wiener index is maximized by both the graphs C_6 and $C_{3,3}^n$.

Proof of Theorem 1.2: (i) Let $G \in \mathfrak{H}_{n,k}$ and let v_1, v_2, \dots, v_{n-k} be the non-pendant vertices of G . If the induced subgraph $G[v_1, v_2, \dots, v_{n-k}]$ is not complete, then form a new graph G' from G by joining all the non-adjacent non-pendant vertices of G with new edges. Then $G' \in \mathfrak{H}_{n,k}$ and by Lemma 2.1 $W(G') < W(G)$. If $G' = P_n^k$ then we are done, otherwise G' has at least two vertices of degree greater than or equal to $n - k$. Form a new graph G'' from G' by moving all the pendant vertices to one of the vertex v_1, v_2, \dots, v_{n-k} . Then $G'' = P_n^k$ and by Corollary 2.6, the result follows. Let $u \in V(P_n^k)$ be a vertex of degree $n - 1$. Then by Lemma 2.2, we have

$$\begin{aligned} W(P_n^k) &= W(K_{n-k}) + W(K_{1,k}) + (|V(K_{n-k})| - 1)k + kD_{K_{n-k}}(u) \\ &= \binom{n-k}{2} + k^2 + 2k(n-k-1). \end{aligned}$$

(ii) Let $G \in \mathfrak{H}_{n,n-2}$. Then G is isomorphic to a tree $T(k, l, 2)$ for some $k, l \geq 1$. If k and l both greater than or equal to 2 then form the tree $T(1, n-3, 2)$ from G by moving pendant vertices from one end to other. Then by Corollary 2.6, $W(T(1, n-3, 2)) < W(G)$ and by taking $d = 2, l = 1$ and $k = n - 3$ in (6), we have $W(T(1, n-3, 2)) = n^2 - n - 2$. □

Proof of Theorem 1.3. We first prove that for $k \geq 3$, if $T \in \mathfrak{T}_{n,k}$ has minimum Wiener index then there is a unique vertex $v \in V(T)$ with $d(v) \geq 3$. Let there be two vertices $u, v \in V(T)$ with $d(u) = n_1 \geq 3$, $d(v) = n_2 \geq 3$. Let $N_T(u) = \{u_1, u_2, \dots, u_{n_1}\}$ and $N_T(v) = \{v_1, v_2, \dots, v_{n_2}\}$ where u_1 and v_1 lie on the path joining u and v (u_1 may be v and v_1 may be u). Let T_1 be the largest subtree of T consisting of $u, u_2, u_3, \dots, u_{n_1-1}$ but not u_1, u_{n_1} and T_2 be the largest subtree of T containing $v, v_2, v_3, \dots, v_{n_2-1}$ but not v_1, v_{n_2} . We rename the vertices $u \in V(T_1)$ and $v \in V(T_2)$ by u' and v' , respectively. Let $H = T \setminus \{u_2, u_3, \dots, u_{n_1-1}, v_2, v_3, \dots, v_{n_2-1}\}$. Construct two trees T' and T'' from H , T_1 and T_2 by identifying the vertices u, u', v' and v, u', v' , respectively. Clearly both $T', T'' \in \mathfrak{T}_{n,k}$ and by Lemma 2.5, either $W(T') < W(T)$ or $W(T'') < W(T)$ which is a contradiction.

Let T be the tree which minimizes the Wiener index in $\mathfrak{T}_{n,k}$. For $k = 2$, the only possible tree is the path P_n which is isomorphic to $T_{n,2}$. So assume $3 \leq k \leq n - 2$. Then there exists a unique vertex $v \in V(T)$ with $d(v) \geq 3$. Hence the result follows from Corollary 2.4. \square

For $r = 0$, the tree $T_{n,k}$ is isomorphic to the tree T_k^q and hence by (8),

$$W(T_{n,k}) = k \binom{q+2}{3} + \frac{q^2(q+1)k(k-1)}{2}.$$

For $1 \leq r < k$, by Lemma 2.2, we have

$$W(T_{n,k}) = W(T_r^{q+1}) + W(T_{k-r}^q) + r(q+1)D_{T_{k-r}^q}(v) + (k-r)qD_{T_r^{q+1}}(v),$$

where v is the vertex of $T_{n,k}$ with $T_{n,k} \setminus v = rP_{q+1} \cup (k-r)P_q$. Thus by using (7) and (8) the value of $W(T_{n,k})$ can be obtained.

4 Proof of Theorem 1.4

Any graph on n vertices has at most $n - 2$ cut vertices. The path P_n is the only graph on n vertices with $n - 2$ cut vertices. Hence for $\mathfrak{C}_{n,s}$, we consider $0 \leq s \leq n - 3$. Let $\mathfrak{C}_{n,s}^t$ be the set of all trees on n vertices with s cut vertices. In a tree every vertex is either a pendant vertex or a cut vertex. So, $\mathfrak{C}_{n,s}^t = \mathfrak{T}_{n,n-s}$. Hence the next result follows from Theorem 3.1 and Theorem 1.3.

Theorem 4.1. *For $0 \leq s \leq n - 3$, the tree $T(\lfloor \frac{n-s}{2} \rfloor, \lceil \frac{n-s}{2} \rceil, s)$ maximizes the Wiener index and the tree $T_{n,n-s}$ minimizes the Wiener index over $\mathfrak{C}_{n,s}^t$.*

A block in a graph G is a maximal connected component without any cut vertices in it. Let B_G be the graph corresponding to G with $V(B_G)$ as the set of blocks of G and two vertices u and v of B_G are adjacent whenever the corresponding blocks contains a common cut vertex of G . A vertex of G with minimum eccentricity is called a central vertex. We call a block B in G , a pendant block if there is exactly one cut vertex of G in B . The block corresponding to a central vertex in B_G is called a central block of G .

Lemma 4.2. *Let G be a graph which minimizes the Wiener index over $\mathfrak{C}_{n,s}$. Then every block of G is a complete graph.*

Proof. Let B be a block of G which is not complete. Then there are at least two non adjacent vertices in B . Let u and v be two non adjacent vertices in B . Form a new graph G' from G by joining the edge $\{u, v\}$. Clearly $G' \in \mathfrak{C}_{n,s}$ and by Lemma 2.1 $W(G') < W(G)$, which is a contradiction. \square

Lemma 4.3. *Let G be a graph which minimizes the Wiener index over $\mathfrak{C}_{n,s}$. Then every cut vertex of G is shared by exactly two blocks.*

Proof. Let c be a cut vertex in G shared by more than two blocks say $B_1, B_2, \dots, B_k, k \geq 3$. Construct a new graph G' from G by joining all the non adjacent vertices of $\cup B_i, i = 2, 3, \dots, k$. Then $G' \in \mathfrak{C}_{n,s}$ and by Lemma 2.1, $W(G') < W(G)$ which is a contradiction. \square

Lemma 4.4. *Let $m \geq 3$. For $i, j \in \{1, 2, \dots, m\}$, if $l_i \leq l_j - 2$, then*

$$W(K_m^n(l_1, \dots, l_i + 1, \dots, l_j - 1, \dots, l_m)) < W(K_m^n(l_1, \dots, l_i, \dots, l_j, \dots, l_m)).$$

Proof. Let u be the pendant vertex of $K_m^n(l_1, \dots, l_i + 1, \dots, l_j - 1, \dots, l_m)$ on the path P_{l_i+1} and v be the pendant vertex of $K_m^n(l_1, \dots, l_i, \dots, l_j, \dots, l_m)$ on the path P_{l_j} . Let w_1 and w_2 be the vertices adjacent to u and v , respectively. Then using Lemma 2.2 we have

$$\begin{aligned} & W(K_m^n(l_1, \dots, l_i + 1, \dots, l_j - 1, \dots, l_m)) - W(K_m^n(l_1, \dots, l_i, \dots, l_j, \dots, l_m)) \\ &= D_{K_m^{n-1}(l_1, \dots, l_i, \dots, l_j-1, \dots, l_m)}(w_1) - D_{K_m^{n-1}(l_1, \dots, l_i, \dots, l_j-1, \dots, l_m)}(w_2). \end{aligned}$$

Since $l_i < l_j - 1$ and $m \geq 3$, so the result follows. \square

Let G be a graph in which every cut vertex is shared by exactly two blocks. Then B_G is a tree. So, B_G has either one central vertex or two adjacent central vertices and hence G has either one central block or two central blocks with a common cut vertex.

Lemma 4.5. *Let G be a graph which minimizes the Wiener index over $\mathfrak{C}_{n,s}$. If $s \geq 2$, then every pendant block of G is K_2 .*

Proof. All the blocks in G are complete by Lemma 4.2. Suppose B is a pendant block of G which is not K_2 . Let $V(B) = \{v_1, v_2, \dots, v_m\}$ with $m > 2$. Assume v_1 is the cut vertex of G in B which is shared by another block B' with $V(B') = \{v_1 = u_1, u_2, \dots, u_r\}$ and $r \geq 2$. Construct a new graph G' from G as follows: Delete the edges $\{v_2, v_j\}, j = 3, 4, \dots, m$ and add the edges $\{v_j, u_i\}, j = 3, 4, \dots, m$ and $i = 2, 3, \dots, r$. When G changes to G' the only type of distances which increase are $d(v_2, v_j), j = 3, 4, \dots, m$. Each such distance increases by one and hence the total increment in distances for $v_j, j = \{3, \dots, m\}$ is exactly $m - 2$. The distance $d(v_j, u_i), j = 3, 4, \dots, m, i = 2, 3, \dots, r$ decreases by one. Since $r \geq 2$, the total distance decreases by such pair of vertices is at least $m - 2$. Since $s \geq 2$ there exists a vertex w belonging to some other block B'' such that $d(v_j, w), j = 3, 4, \dots, m$ decreases by one. So $W(G') < W(G)$, which is a contradiction. \square

Let G be a graph in which every block is complete and every cut vertex is shared by exactly two blocks. Let B be a central block in G . Let B_1 be a non central non pendant block of G and $c_1, c_2 \in V(B_1)$ be two cut vertices of G . Suppose that the vertex c_1 is identified by a pendant vertex of a path P_l and c_2 is shared by another block B_2 such that the vertices corresponding to B_1, B_2 and B in the tree B_G lie on a path. Let $V(B_1) = \{c_1 = u_1, u_2, \dots, u_{m_1} = c_2\}$ and $V(B_2) = \{v_1, v_2, \dots, v_{m_2} = c_2\}$. Construct a new graph G' from G as follow: Delete the edges $\{c_1, u_i\}$ for all $u_i \in V(B_1) \setminus \{c_1, c_2\}$ and add the edges $\{u_i, v_j\}$ for all $u_i \in V(B_1) \setminus \{c_1, c_2\}$ and $v_j \in V(B_2) \setminus \{c_2\}$.

Lemma 4.6. *Let G and G' be the graphs defined as above. Then $W(G') < W(G)$.*

Proof. For $i = 2, \dots, m_1 - 1$, let H_i be the maximal connected component of G containing exactly one vertex u_i of B_1 . Let $P_l : t_1 t_2 \dots t_l$ be the path with t_1 identified with c_1 . When G changes to G' , the only type of distances which increase in G' are $d_{G'}(u, t_j)$ where $u \in \cup_{i=2}^{m_1-1} V(H_i)$ and $j =$

$1, 2, \dots, l$. Each such distance increases by one in G' . For any other pair of vertices, the distance between them either decreases or remains the same. Since B_1 is not a central block, for each $t_j, j = 1, 2, \dots, l$ there exists a vertex $t'_j \in V(G) \setminus \left(\cup_{i=2}^{m_1-1} V(H_i) \cup \{t_1, t_2, \dots, t_l, v_1, v_2, \dots, v_{m_2}\} \right)$ such that $d_{G'}(u, t'_j)$ decreases by one where $u \in \cup_{i=2}^{m_1-1} V(H_i)$. So, the increment in distance by the pairs u, t_j are neutralized by the pairs u, t'_j . Apart from this at least the distances $d_{G'}(u_i, v_j)$ for $i = 2, 3, \dots, m_1 - 1$ and $j = 1, 2, \dots, m_2 - 1$ decreases by one. So $W(G') < W(G)$. \square

Proof of Theorem 1.4: Let G be a graph which minimizes the Wiener index over $\mathfrak{C}_{n,s}$. We first claim that G is isomorphic to $K_{n-s}^n(l_1, \dots, l_{n-s})$ for some l_1, l_2, \dots, l_{n-s} .

By Lemma 4.2 and Lemma 4.3, every block of G is complete and every cut vertex of G is shared by exactly two blocks. If $s = 0$, then G has exactly one block and $G = K_n$ also K_n is isomorphic to $K_n^n(1, 1, \dots, 1)$.

For $s = 1$, G has exactly two complete blocks with a common vertex w (say). Let B_1 and B_2 be the two blocks of G . If any of B_1 or B_2 is K_2 then G is isomorphic to $K_{n-1}^n(2, 1, \dots, 1)$. Otherwise, let $V(B_1) = \{u_1, u_2, \dots, u_{m_1} = w\}$ and $V(B_2) = \{v_1, v_2, \dots, v_{m_2} = w\}$ with $m_1, m_2 > 2$. Construct a new graph G' from G as follow: Delete the edges $\{u_1, u_i\}, i = 2, 3, \dots, m_1 - 1$ and add the edges $\{u_i, v_j\}, i = 2, 3, \dots, m_1 - 1; j = 1, 2, \dots, m_2 - 1$. Clearly $G' \in \mathfrak{C}_{n,s}$. Then the only type of distances which increase are $d(u_1, u_j), j = 2, 3, \dots, m_1 - 1$ and each such distance increases by one. So total increment in distance is exactly $m_1 - 2$. Also each distance $d(u_i, v_j), i = 2, 3, \dots, m_1 - 1; j = 2, 3, \dots, m_2 - 1$ decreases by one. The total decrement is $(m_1 - 2)(m_2 - 1)$. Since $m_1, m_2 > 2$, so $W(G') < W(G)$, which is a contradiction. Hence G is isomorphic to $K_{n-1}^n(2, 1, \dots, 1)$.

Now suppose $s \geq 2$. Then G has $s + 1$ blocks and also G has either one central block or two adjacent central blocks.

Claim: All non central blocks of G are K_2 .

Suppose B is a non central block of G which is not K_2 . Then by Lemma 4.5, B must be a non pendant block. Construct G' from G as in Lemma 4.6. Clearly $G' \in \mathfrak{C}_{n,s}$ and by Lemma 4.6, $W(G') < W(G)$ which is a contradiction.

If G has exactly one central block, then G is isomorphic to $K_{n-s}^n(l_1, \dots, l_{n-s})$ for some l_1, l_2, \dots, l_s . Suppose G has two central blocks and G is not isomorphic to $K_{n-s}^n(l_1, \dots, l_{n-s})$ for any l_1, l_2, \dots, l_{n-s} . Then each of the central blocks of G has at least 3 vertices. Let B_1 and B_2 be the two central blocks with a common vertex w . Let $V(B_1) = \{u_1, u_2, \dots, u_{m_1} = w\}$ and $V(B_2) = \{v_1, v_2, \dots, v_{m_2} = w\}$ with $m_1, m_2 > 2$. Let $H_1(H_2)$ be the maximal connected component of G containing exactly one vertex w of $B_2(B_1)$. Let $P_l : wu_1t_3 \dots t_l$ be the longest path in H_1 starting at w containing u_1 such that non of the vertex t_3, \dots, t_l belongs to B_1 . Take w as t_1 and u_1 as t_2 in P_l . Since B_1 and B_2 are central blocks, so there exists a path $P'_l : t'_1t'_2 \dots t'_l$ on l vertices in H_2 starting at $w = t'_1$ and containing exactly two vertices of B_2 . Construct a new graph G' from G as follow: Delete the edges $\{u_1, u_i\}, i = 2, 3, \dots, m_1 - 1$ and add the edges $\{u_i, v_j\}, i = 2, 3, \dots, m_1 - 1; j = 1, 2, \dots, m_2 - 1$. Clearly $G' \in \mathfrak{C}_{n,s}$. The only type of distances which increase in G' are $d_{G'}(u, t_j)$ where $u \in V(H_1) \setminus V(P_l)$ and $j = 2, \dots, l$ also each such distance increases by one. The distance $d_{G'}(u, t'_j)$ decreases by one where $u \in V(H_1) \setminus V(P_l)$ and $j = 2, \dots, l$. So, the increment in distance by the pairs u, t_j are neutralized by the pairs u, t'_j . Since $m_2 \geq 3$, there exist at least one vertex w' in B_2 which is not in P'_l . For each $u \in V(H_1) \setminus V(P_l)$, the distance $d_{G'}(u, w')$ decreases by one. So, $W(G') < W(G)$, which is a contradiction. Hence G is $K_{n-s}^n(l_1, \dots, l_{n-s})$ for some l_1, l_2, \dots, l_{n-s} . Now the result follows from Lemma 4.4. \square

References

- [1] I. Althfer, Average distances in undirected graphs and the removal of vertices, *J. Combin. Theory Ser. B* 48 (1990), no. 1, 140-142.
- [2] R. Balakrishnan, N. Sridharan and K. Viswanathan Iyer, Wiener index of graphs with more than one cut-vertex, *Applied Mathematics Letters* 21 (2008), no. 9, 922-927.
- [3] F. Buckley and F. Harary, *Distance in Graphs*, Addison-Wesley, Redwood, 1990, p. 42.
- [4] P. Dankelmann, Average distance and independence number, *Discrete Appl. Math.* 51 (1994), no. 1-2, 75-83.
- [5] J. K. Doyle and J. E. Graver, Mean distance in a graph, *Discrete Math.* 17 (1977), no. 2, 147-154.
- [6] R. C. Entringer, D. E. Jackson, D. A. Synder, Distance in graphs, *Czech. Math. J.* 26 (1976), no. 2, 283-296.
- [7] I. Gutman, On distances in some bipartite graphs. *Publ. Inst. Math. (Beograd)* 43 (1988) 3-8.
- [8] I. Gutman, R. Cruz, J. Rada, Wiener index of Eulerian graphs, *Discrete Appl. Math.* 162 (2014) 247-250.
- [9] Y. Hong, H. Liu, X. Wu, On the Wiener index of unicyclic graphs, *Hacettepe Journal of Mathematics and Statistics* Volume 40 (1) (2011), 63-68
- [10] J. Plesnik, On the sum of all distances in a graph or digraph, *J. Graph Theory* 8 (1984), no. 1, 1-21.
- [11] F. Jelen and E. Triesch, Superdominance order and distance of trees with bounded maximum degree, *Discrete Appl. Math.*, 125 (2003), no. 2-3, 225-233.
- [12] H. Liu, M. Lu, A unified approach to extremal cacti for different indices, *MATCH Commun. Math. Comput. Chem.* 58 (2007), no. 1, 183-194.
- [13] H. Liu, X. Pan, On the Wiener index of trees with fixed diameter, *MATCH Commun. Math. Comput. Chem.* 60 (2008), no. 1, 85-94
- [14] D. Stevanovi, Maximizing Wiener index of graphs with fixed maximum degree, *MATCH Commun. Math. Comput. Chem.* 60 (2008), no. 1, 71-83.
- [15] R. Shi, The average distance of trees, *Systems Sci. Math. Sci.* 6 (1993),no. 1, 18-24.
- [16] S. W. Tan, The minimum Wiener index of unicyclic graphs with a fixed diameter, *J. Appl. Math. Comput.* 56 (2018), no. 1-2, 93-114.
- [17] S.W. Tan, Q. L. Wang, Y. Lin, The Wiener index of unicyclic graphs given number of pendant vertices or cut vertices, *J. Appl. Math. Comput.* 55 (2017), no. 1-2, 1-24.
- [18] D. B. West, *Introduction to Graph Theory*, Prentice Hall of India Private Limited, New Delhi, Second Edition, 2003.
- [19] P. Winkler, Mean distance in a tree, *Discrete Appl. Math.* 27 (1990), no. 1-2, 179-185.

- [20] H. Wang, The extremal values of the Wiener index of a tree with given degree sequence, *Discrete Appl. Math.* 156 (2008), no. 14, 2647-2654.
- [21] S. Wang, X. Guo, Trees with extremal Wiener indices, *MATCH Commun. Math. Comput. Chem.* 60 (2008), no. 2, 609-622.
- [22] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* 69 (1947), 17-20.
- [23] Y. N. Yeh and I. Gutman, On the sum of all distances in composite graphs, *Discrete Math.* 135 (1994), no. 1-3, 359-365.
- [24] G. Yu and L. Feng, On the Wiener index of unicyclic graphs with given girth, *Ars Comb.* 94 (2010), 361-369.
- [25] X. D. Zhang, Q.Y. Xiang, L. Q. Xu and R. Y. Pan, The Wiener index of Trees with given degree sequences, *MATCH Commun. Math. Comput. Chem.* 60 (2008), no. 2, 623-644.

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