

Extremal caterpillar-like trees relative to the Wiener index

Ndimphiwe Bradley Morné Dingile

The crest of Rhodes University is centered on the page. It features a shield with a red lion on a yellow background, a blue chief with a white cross, and a banner at the bottom with the motto 'VIR VIRTUS VERITAS'. The shield is supported by two black birds with yellow wings. Above the shield is a crown with a white cross.

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Declaration

I declare that the work in the dissertation entitled "Extremal caterpillar-like trees relative to the Wiener index" which I hereby submit for the degree, Master of Science at Rhodes University, is my own work. I also declare that this research has not been submitted by me for a degree at this or any other tertiary institution and that all the sources that I have used or quoted have been indicated and acknowledged by means of complete references.



Ndimphiwe Bradley Morné Dingile

Date signed

February 2, 2026

Abstract

The Wiener index of a graph G is the sum of the distances between all vertex pairs in G . A *caterpillar-like* tree is a tree where all its branching vertices (vertices of degree at least 3) lie on the same path. This project focuses on the class of caterpillar-like trees with given order and other restrictions such as number of leaves and maximum degree. The aim is to determine the structures of those caterpillar-like trees that reach the minimum (and maximum) Wiener index under the prescribed restrictions.

Acknowledgement

... by God's grace I am what I am,... 1 Corinthians 15:10

With a heart full of gratitude, I first bow in reverence to the One who carried me through every storm, every sleepless night, and every moment I thought I could not go on. Truly, it is by God's grace that I stand where I do today, not by strength, nor by might, but by mercy and divine favour.

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This dissertation is, above all, a tribute to my late mother *Thandiwe* whom I lost in 2016, my guiding light, my anchor, and my greatest source of strength. Mom, not a day passes without the weight of your absence. If I were to dedicate this entire research to measuring how deeply and endlessly you are missed, no equation could ever find a closed-form solution. You live in every decision I made to keep going, every late night I endured, every page written through exhaustion and perseverance. Though this work bears my name, its heartbeat is yours. I hope this makes you proud. I'm still trying, trying to be the man you always saw in me, long before I ever caught a glimpse of him myself. If I've done anything right here, it's because I never stopped the version of me you always knew I could be. Thank

you, Ma.

To my siblings, Thandeka and Baphelele, you are the reason I kept moving when it felt easier to stop. You have been my strength when mine failed, my hope when I was empty, my reminder of why I must never give up. You are the reason I pushed this far, the reason I fought to finish, the reason I dared to dream. I wanted you to see it was possible. I wanted to be proof that we can rise. This is ours, every page, every struggle, every victory.

"The first and greatest victory is to conquer yourself". To myself, I see you. Thank you for enduring, for holding on, and for rising through moments that felt impossible. This journey was never easy, but you stayed, you fought, and you finished. I honour that version of you who kept going, even when no one was watching.

1 | Introduction

In order to quantify the relationship between molecular structure and physical properties, particularly the boiling points of paraffin compounds (alkanes), Wiener [14] introduced the Wiener index in 1947 as a topological descriptor. Since then, the Wiener index has gained a lot of attention in pure mathematics and has established itself as a popular concept in the study of chemical graph theory. What started out as a chemically motivated invariant has developed into a topic of wide mathematical interest, leading to a large number of analytical frameworks and generalizations. These include concepts such as the transmission (also known as status) of a vertex and the distance of a graph, among others.

The development of extremal graph theory, as initiated by the pioneering work of Turán in 1941 [11], inspired a wide range of problems where the goal is to determine graphs that maximize or minimize specific parameters under given constraints. Within this context, the Wiener index is among the most studied parameters. A major part of this thesis involves extremal problems. The first mathematical paper on Wiener index was published in 1976 by Entringer et al. [7]. They proved that, out of all n -vertex trees, the path P_n achieves the maximum Wiener index, while the star $K_{1,n-1}$, or simply S_n , achieves the minimum Wiener index. Further extremal results were obtained for trees with given matching number [3], given degree sequence [1, 5, 12, 16], given number of leaves [5, 6], and given maximum degree [10, 13].

In particular, significant efforts have been directed towards understanding the behavior of the Wiener index under degree se-

quence and segment sequence constraints. Caterpillars and caterpillar-like trees often arise as extremal structures [2, 5, 15], while greedy tree constructions have been used to characterize trees minimizing and maximizing the Wiener index under various restrictions.

This thesis continues in this line of research by focusing on caterpillar-like trees (also known as quasi-caterpillars) of order n with given number of leaves ℓ and given maximum degree Δ . Our aim is to characterize the caterpillar-like trees with given number of leaves as well as the caterpillar-like trees with given maximum degree that achieve the minimum (and maximum) Wiener index.

1.1 Overview of the Thesis

This thesis is structured as follows. In Chapter 2, we present some preliminaries that we are going to need for the next chapters. In particular, in Section 2.1 we provide graph-theoretic notation and terminology that we shall adhere to throughout this thesis. Various families of graphs are also defined in Section 2.1. In Section 2.2, we define what we mean by the Wiener index of a graph, and we also present the explicit formulas for the Wiener index of some families of graphs. Furthermore, some known bounds for the Wiener Index of some graphs are presented in Section 2.2.

The gist of this thesis begins in Chapter 3, where we study caterpillar-like trees with a given number of leaves. In Section 3.1, we characterise the caterpillar-like tree of order n with given number of leaves ℓ and smallest Wiener index. Furthermore, the explicit formula for the Wiener index of such a tree is presented in Section 3.1. In Section 3.2, we characterise the caterpillar-like tree of order n with given number of leaves ℓ and largest Wiener index.

We continue in Chapter 4 by studying caterpillar-like trees with given maximum degree $\Delta \geq 3$. In Section 4.1, we obtained necessary conditions for the structure of the caterpillar-like tree of order n with given maximum degree $\Delta \geq 3$ and smallest Wiener index. In Section 4.2, we characterise the caterpillar-like tree of

order n with given maximum degree $\Delta \geq 3$ and largest Wiener index.

Chapter 5 provides some concluding remarks that summarize the results achieved in this thesis.

2 | Preliminaries

In this chapter, we discuss the necessary terminology and notation that we adhere to throughout this thesis. Moreover, we present some preliminary results on the Wiener index of a graph.

2.1 Basic Graph Theory

In layman's terms, a graph is any collection of objects, some of which are related. Formally, we define a (simple and undirected) graph as follows:

Definition 2.1 A *simple and undirected graph* G is an ordered pair of sets $(V(G), E(G))$, where the elements of $V(G)$ are called *vertices* and $E(G)$ is a set of 2-element subsets of $V(G)$ which are called *edges*.

Definition 2.2 The number of vertices in a graph G is the *order* of G , and is denoted by $n(G)$ or simply by n if the graph under consideration is clear. The number of edges in a graph G is the *size* of G , and is denoted by $m(G)$ or simply by m if the graph under consideration is clear.

Definition 2.3 If $e = \{u, v\}$ is an edge of a graph G that joins vertices u and v , then the vertices u and v are *adjacent* (or are *neighbours*) in G , while the edge e is *incident* to the vertices u and v in G . Two edges e_1 and e_2 of a graph G are *adjacent* in G if they share a common vertex; that is, $e_1 \cap e_2 \neq \emptyset$.

For simplicity, we often write uv to represent the edge that joins the vertices u and v instead of writing the set $\{u, v\}$. An example of

a graph $G = (V(G), E(G))$, where $V(G) = \{v_1, v_2, v_3, v_4\}$ and $E(G) = \{v_1v_2, v_2v_3, v_2v_4, v_3v_4\}$ is illustrated in Figure 2.1.

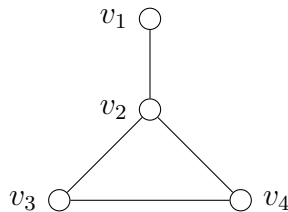


Figure 2.1: A graph G .

Note that in the graph G shown in Figure 2.1, the vertex v_1 is adjacent to the vertex v_2 , but the vertex v_1 is not adjacent to the vertex v_3 . In addition, the edge v_1v_2 is adjacent to the edge v_2v_3 , but the edge v_1v_2 is not adjacent to the edge v_3v_4 . Furthermore, the edge v_1v_2 is incident to both the vertices v_1 and v_2 .

Next, we define what is meant by the degree of a vertex.

Definition 2.4 The *degree* of a vertex v in a graph G , denoted $\deg_G(v)$, is the number of vertices adjacent to v in G . The *minimum degree* of G is

$$\delta(G) = \min\{\deg_G(v) \mid v \in V(G)\},$$

while the *maximum degree* of G is

$$\Delta(G) = \max\{\deg_G(v) \mid v \in V(G)\}.$$

Definition 2.5 Let G be a graph and $u, v \in V(G)$. A u - v *walk* W in G is an alternating sequence of vertices and edges $u = v_0, e_1, v_1, \dots, v_{k-1}, e_k, v_k = v$, where the edge e_i is incident to v_i and v_{i-1} for all $1 \leq i \leq k$. The *length* of W is the number of edges in it. We often denote a walk by its vertices only, i.e., $u = v_0, v_1, \dots, v_{k-1}, v_k = v$.

Definition 2.6 A graph G is *connected* if for every $u, v \in V(G)$, there exists a u - v walk in G , otherwise the graph G is *disconnected*.

2.1.1 Families of Graphs

In this subsection, we define some common families of graphs, some of which we use more often throughout this thesis.

Definition 2.7 A *complete graph* is a graph in which each vertex is adjacent to every other vertex. A complete graph of order n is denoted by K_n .

The complete graph of order 5 is shown in Figure 2.2.

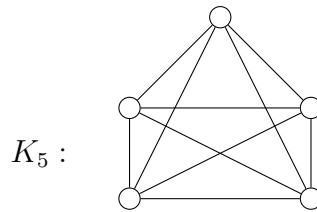


Figure 2.2: The complete graph K_5 .

Definition 2.8 Let G be a graph and $u, v \in V(G)$. If W is a u - v walk in G , and all the vertices of W are distinct, then W is called a u - v *path* in G . If all vertices of W are distinct except the first and the last, then W is a *cycle* of G . We denote the path and the cycle of order n by P_n and C_n , respectively.

The path of order 6 and the cycle of order 5 is shown in Figure 2.3.

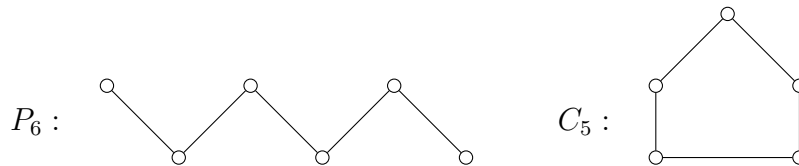


Figure 2.3: The path P_6 and the cycle C_5 .

Definition 2.9 A *tree* T is a connected graph that contains no cycles. A vertex of degree 1 in T is called a *leaf* of T . A vertex of

degree 2 in T is called an *internal vertex* of T . A vertex of degree at least 3 in T is called a *branching vertex* of T .

An example of a tree T is illustrated in Figure 2.4, where the vertex u of T is a leaf, the vertex v of T is an internal vertex, and the vertex w of T is a branching vertex.

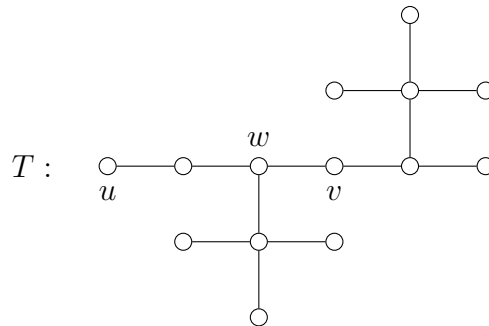


Figure 2.4: A tree T .

Definition 2.10 A *segment* S in a tree T is a path, where each terminal vertex of S is either a leaf or a branching vertex of T and all the other vertices of S are internal vertices of T . If S is a segment of a tree T and S contains a terminal vertex which is a leaf of T , then S is called a *pendant segment* of T .

In the tree T shown in Figure 2.4, the segment whose terminal vertices are u and w is a pendant segment of T since the vertex u is a leaf of T .

Definition 2.11 A *caterpillar* is a tree in which the removal of all the leaves yields a path.

An example of a caterpillar T is illustrated in Figure 2.5.

Definition 2.12 A *caterpillar-like tree* is a tree all whose branching vertices lie on a single path.

An example of a caterpillar-like tree T is illustrated in Figure 2.6.

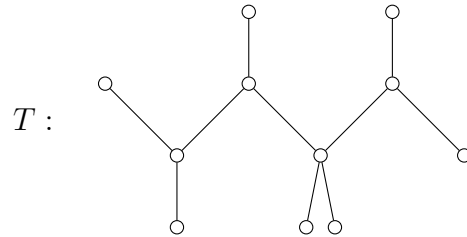


Figure 2.5: A caterpillar.

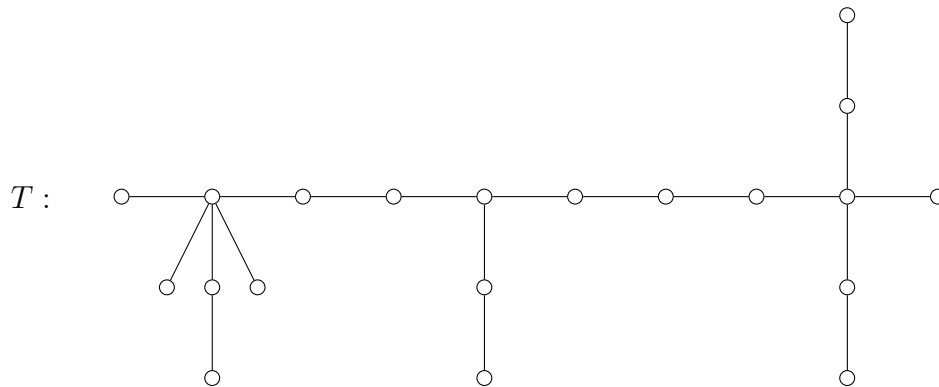


Figure 2.6: A caterpillar-like tree

Remark 2.13 Note that if T is a caterpillar, then T is a caterpillar-like tree all whose pendant segments have length exactly 1. Hence, we remark that a caterpillar is a special case of a caterpillar-like tree. In particular, a path and a star are caterpillar-like trees.

Definition 2.14 Let T be a caterpillar-like tree. The *backbone* of T is defined to be the longest path of T that contains all of its branching vertices.

Definition 2.15 A *broom*, denoted $B_{n,\ell}$, is a tree of order n obtained from a path $P_{n-\ell}$ by adding ℓ new vertices and joining them to exactly one end of $P_{n-\ell}$. A *double-broom*, denoted B_{n,ℓ_1,ℓ_2} , is a tree of order n obtained from a path $P_{n-\ell_1-\ell_2}$ by adding $\ell_1 + \ell_2$ new vertices and joining ℓ_1 vertices to one end of $P_{n-\ell_1-\ell_2}$, and ℓ_2 vertices to the other end of $P_{n-\ell_1-\ell_2}$.

2.2 The Wiener Index of a Graph

In this section we discuss the concept of the Wiener index. The Wiener index was first introduced by a chemist, Harry Wiener, in 1947, where he identified a correlation between this index and the boiling points of paraffins (saturated hydrocarbons or alkanes). This ignited the interest of many mathematicians to study the Wiener index and obtain results that exceed the class of chemical graphs; hence this index enjoys several applications in both chemistry and mathematics.

First, we define the distance between two vertices of a connected graph.

Definition 2.16 Let $G = (V(G), E(G))$ be a connected graph, and $u, v \in V(G)$. The *distance* between u and v in G , denoted $d_G(u, v)$, is the length of the shortest u - v path in G .

In the graph G shown in Figure 2.7, the v_1 - v_4 path $P_1 : v_1, v_2, v_3, v_4$ has length $\ell_1 = 3$, while the v_1 - v_4 path $P_2 : v_1, v_2, v_4$ has length $\ell_2 = 2$. Thus, the distance from v_1 to v_4 in G is $d_G(v_1, v_4) = \min\{\ell_1, \ell_2\} = \min\{2, 3\} = 2$.

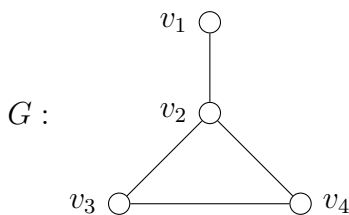


Figure 2.7: A graph G .

Next, we define the Wiener index of a connected graph. The Wiener index of a connected graph is the sum of the distances between pairs of vertices in it. More formally, the Wiener index is defined as follows:

Definition 2.17 Let G be a connected graph with vertex set $V(G)$. The Wiener index of G is defined as

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

2.2.1 Explicit Formulas for the Wiener Index of Some Graphs

In this subsection we present the explicit formula for the Wiener index of a complete graph K_n , star $K_{1,n-1}$ and a path P_n of order n . They are very well-know formulas, see for example [9].

Proposition 2.18 For any intergers $n \geq 1$.

$$W(K_n) = \binom{n}{2} \cdot (1) = \frac{n(n-1)}{2}.$$

Proof. Let G be a complete graph K_n . Then every vertex of G is adjacent to every other vertex of G , implying that all the $\binom{n}{2}$ pairs of vertices of G are at distance 1 from each other. Thus,

$$W(G) = W(K_n) = \binom{n}{2} \cdot (1) = \frac{n(n-1)}{2},$$

completing the proof. \square

Proposition 2.19 For any intergers $n \geq 1$.

$$W(K_{1,n-1}) = (n-1)^2.$$

Proof. Let G be a star $K_{1,n-1}$. Then there are $n-1$ vertices of G that are at distance 1 from a single (central) vertex, and there are $\binom{n-1}{2}$ vertices of G that are at distance 2 from each other. Thus,

$$W(G) = W(K_{1,n-1}) = (n-1) \cdot (1) + \binom{n-1}{2} \cdot (2) = (n-1)^2,$$

completing the proof. \square

Proposition 2.20 For any intergers $n \geq 1$.

$$W(P_n) = \frac{n^3 - n}{6}.$$

Proof. Let $P_n = v_1, v_2, \dots, v_n$ be a path of order n . Note that $d_{P_n}(v_i, v_j) = |j - i|$ for every $1 \leq i, j \leq n$. The Wiener index of P_n is, therefore, given by

$$\begin{aligned} W(P_n) &= \sum_{v_i, v_j \in V(P_n)} d_{P_n}(v_j, v_i) \\ &= \sum_{i=1}^{n-1} \sum_{j=i+1}^n (j - i) \\ &= \sum_{i=1}^{n-1} \left(\sum_{j=i+1}^n j - \sum_{j=i+1}^n i \right) \\ &= \sum_{i=1}^{n-1} \left(\frac{n(n+1)}{2} - \frac{i(i+1)}{2} - i(n-i) \right) \\ &= \sum_{i=1}^{n-1} \frac{n(n+1)}{2} - \sum_{i=1}^{n-1} \frac{i(i+1)}{2} - \sum_{i=1}^{n-1} in + \sum_{i=1}^{n-1} i^2 \\ &= \frac{n(n+1)}{2}(n-1) - \frac{1}{2} \sum_{i=1}^{n-1} i(i+1) - n \cdot \frac{n(n-1)}{2} \\ &\quad + \frac{n(n-1)(2n-1)}{6} \\ &= \frac{n(n+1)(n-1)}{2} - \frac{1}{2} \left(\sum_{i=1}^{n-1} i^2 + \sum_{i=1}^{n-1} i \right) - n \cdot \frac{(n-1)n}{2} \\ &\quad + \frac{(n-1)n(2n-1)}{6} \\ &= \frac{n(n+1)(n-1)}{2} - \frac{1}{2} \left(\sum_{i=1}^{n-1} i^2 \right) - \frac{1}{2} \left(\sum_{i=1}^{n-1} i \right) - n \cdot \frac{(n-1)n}{2} \\ &\quad + \frac{(n-1)n(2n-1)}{6} \\ &= \frac{n(n+1)(n-1)}{2} - \frac{1}{2} \left(\frac{n(n-1)(2n-1)}{6} \right) - \frac{1}{2} \left(\frac{n(n-1)}{2} \right) \end{aligned}$$

$$\begin{aligned}
& -n \cdot \frac{n(n-1)}{2} + \frac{n(n-1)(2n-1)}{6} \\
& = \frac{n^3 - n}{6},
\end{aligned}$$

which completes the proof. \square

2.2.2 Known Bounds for the Wiener Index of Some Graphs

In this subsection we present, some known lower (and upper) bounds for the Wiener index of some classes of graphs. More specifically, we present a lower (and upper) bound for the Wiener index of a graph G in terms of its number of vertices if G is any connected graph, and if G is any tree.

Bounds for Connected Graphs

One of the general bounds on the Wiener index comes from considering the extremal behavior in the class of all connected graphs of fixed order. The minimum Wiener index is attained by the complete graph, where the distance between each pair of distinct vertices is exactly 1.

Theorem 2.21 ([4]) *If G is a connected graph of order n , then*

$$W(G) \geq \frac{n(n-1)}{2},$$

with equality if and only if $G \cong K_n$.

Proof. In any connected graph, the shortest path between two distinct vertices is at least 1. The complete graph K_n achieves this lower bound for all $\binom{n}{2}$ pairs of vertices. Thus,

$$W(K_n) = \sum_{u,v \in V(G)} d(u,v) = \binom{n}{2} \cdot 1 = \frac{n(n-1)}{2}.$$

For any other connected graph G that is not complete, there exists at least one pair of vertices with distance greater than 1, which

increases the overall sum of distances. Therefore, $W(G) > W(K_n)$ unless $G \cong K_n$. \square

On the other hand, the largest Wiener index among all connected graphs with n vertices is achieved by the path graph P_n .

Theorem 2.22 ([4]) *If G is a connected graph of order n , then*

$$W(G) \leq \frac{n^3 - n}{6},$$

with equality if and only if $G \cong P_n$.

As in Proposition 2.20, this upper bound can be derived by summing all pairwise distances in a path graph, using known summation identities. This can be done using known summation formulas. Since this bound also holds for trees, we will revisit it later in a more specific way.

Bounds for Trees

The class of trees has received particular attention in the study of Wiener index due to its structural simplicity and relevance in both theoretical and applied contexts. In a landmark 1976 paper, Entringer et al. [7] established tight bounds on the Wiener index for trees of a given order. These results remain foundational and continue to be widely cited.

The following theorem provides a lower bound on the Wiener index for trees.

Theorem 2.23 ([7]) *If T is a tree of order n , then*

$$W(T) \geq (n - 1)^2,$$

with equality if and only if $T \cong K_{1,n-1}$.

Proof. Let T be a tree of order n with diameter d . For an integer i , where $1 \leq i \leq d$, define

$$D_i(T) = \{\{u, v\} \subseteq V(T) \mid d_T(u, v) = i\}.$$

Note that, $K_{1,n-1}$ has diameter 2, so

$$\begin{aligned} W(K_{1,n-1}) &= 1 \cdot |D_1(T)| + 2 \cdot |D_2(T)| \\ &= 1 \cdot (n-1) + 2 \cdot \binom{n-1}{2} \\ &= (n-1)^2. \end{aligned}$$

If $T \not\cong K_{1,n-1}$, then T has diameter d , where $d \geq 3$. Thus,

$$\begin{aligned} W(T) &= \sum_{i=1}^d i |D_i(T)| \\ &= 1 \cdot |D_1(T)| + 2 \cdot |D_2(T)| + \sum_{i=3}^d i |D_i(T)|. \end{aligned}$$

Let x be the number of pairs at distance 2, and y the number of pairs at distance at least 3. Then $x + y = \binom{n-1}{2}$. So

$$\begin{aligned} W(T) &= \sum_{i \geq 1} i |D_i(T)| \\ &= 1 \cdot |D_1(T)| + \sum_{i \geq 2} i |D_i(T)| \\ &\geq (n-1) + 2x + 3y \\ &> (n-1) + 2 \binom{n-1}{2} \\ &= W(K_{1,n-1}) \end{aligned}$$

as desired. This establishes the lower bound. \square

The maximum Wiener index for trees is again achieved by the path graph.

Theorem 2.24 ([7]) *If G is a tree of order n , then*

$$W(G) \leq \frac{n^3 - n}{6},$$

with equality if and only if $G \cong P_n$.

This result follows by computing the exact Wiener index of a path graph, where the distance between two vertices i and j is $|i - j|$, and summing over all such pairs:

$$W(P_n) = \sum_{i=1}^n \sum_{j=i+1}^n |i - j| = \sum_{k=1}^{n-1} k(n - k) = \frac{n^3 - n}{6}.$$

The derivation uses symmetry and classic summation formulas; details can be found in [7].

The proof uses symmetry and classic summation formulas; details can be found in [7].

Remark: The result of Theorem 2.23 and Theorem 2.24 completely characterises the extremal trees with respect to the Wiener index in the class of all trees with given order n .

The main results of this thesis are presented in Chapter 3 and Chapter 4, where the Wiener index is studied in the family of caterpillar-like trees which is a subfamily of the family of trees.

3 | Caterpillar-like trees with given number of leaves

In this chapter we study caterpillar-like trees with given order and given number of leaves relative to their Wiener index. More specifically, we determine the structure of those that have the largest or smallest Wiener index.

3.1 Minimal n -vertex caterpillar-like trees with given order and number of leaves

In this section we present a series of lemmas that intend to characterise the structure of a caterpillar-like tree with given order and given number of leaves that possesses the smallest Wiener index.

Definition 3.1 A tree is called *start-like* if it contains at most one vertex whose degree is greater than 2. Let n and ℓ be integers such that $n > \ell \geq 2$, and let $S_{n,\ell}$ be the star-like tree of order n , where each pendant segment of $S_{n,\ell}$ has length either $\lfloor \frac{n-1}{\ell} \rfloor$ or $\lceil \frac{n-1}{\ell} \rceil$.

Lemma 3.2 *Let T be a caterpillar-like tree of order n having ℓ leaves. If T has minimum Wiener index, then every segment of T is a pendant segment.*

Proof. Let T be a caterpillar-like tree of order n having ℓ leaves. Suppose, to the contrary, that T has minimum Wiener index and

there exists a segment $S : u_0, u_1, \dots, u_{r-1}, u_r$ in T such that S is not a pendant segment. Thus, both u_0 and u_r are branching vertices of T , and therefore have degrees at least 3 in T . Let $\deg_T(u_0) = q$ and $\deg_T(u_r) = t$. Furthermore, let $N_T(u_r) \setminus \{u_{r-1}\} = \{w_1, w_2, \dots, w_{t-1}\}$. Since T is a caterpillar-like tree, there must exist a vertex w_i , where $1 \leq i \leq t-1$, such that w_i lies on a pendant segment of T . Let u_r, u_{r+1}, \dots, u_s be a pendant segment of T . Without any loss of generality, we may assume that $w_{t-1} = u_{r+1}$.

Let $A = N_T(u_0) \setminus \{u_1\} = \{z_1, z_2, \dots, z_q\}$, $B = S$, C the path induced by the vertices of the set $\{u_i \mid r+1 \leq i \leq s\}$, and $D = T - A - B - C$ containing w_i for $1 \leq i \leq t-2$. Let $F = C \cup D$. Without any loss of generality, by flipping the tree T if necessary, we may assume that $A \geq F$. Hence $A \geq F > C$ (since $F = C \cup D$).

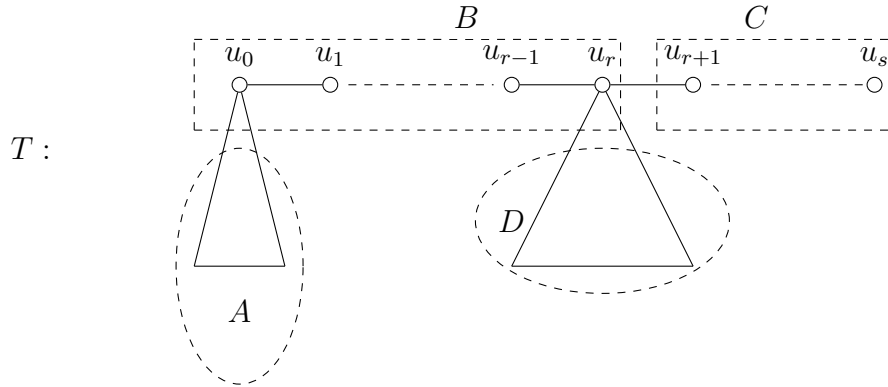


Figure 3.1: The tree T in the proof of Lemma 3.2

The Wiener index of T is

$$\begin{aligned}
 W(T) = & \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) + \sum_{u,v \in V(C)} d_T(u,v) \\
 & + \sum_{u,v \in V(D)} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(C)}} d_T(u,v) \\
 & + \sum_{\substack{u \in V(A) \\ v \in V(D)}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(C)}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(D)}} d_T(u,v)
 \end{aligned}$$

$$+ \sum_{\substack{u \in V(C) \\ v \in V(D)}} d_T(u, v).$$

Let T' be the graph obtained from T by deleting the edges in the set $\{u_r w_i \mid 1 \leq i \leq t-2\}$ and adding the edges in the set $\{u_0 w_i \mid 1 \leq i \leq t-2\}$.

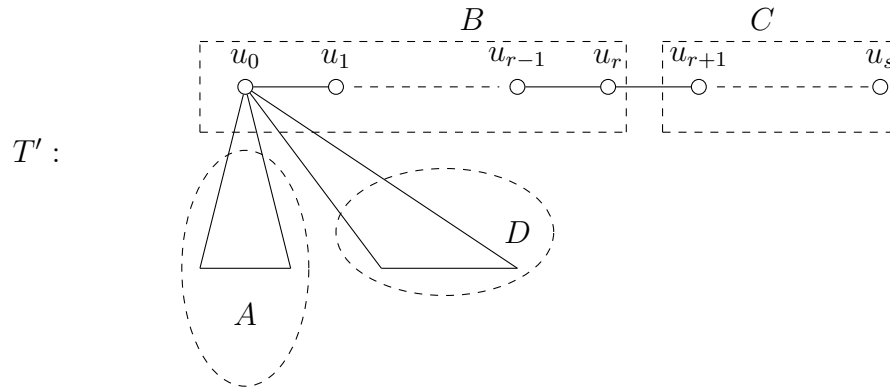


Figure 3.2: The tree T' in the proof of Lemma 3.2

Note that T' has the same number of leaves as T , so it is a caterpillar-like tree with ℓ leaves. The Wiener index of T' is

$$\begin{aligned} W(T') &= \sum_{u,v \in V(A)} d_{T'}(u, v) + \sum_{u,v \in V(B)} d_{T'}(u, v) + \sum_{u,v \in V(C)} d_{T'}(u, v) \\ &+ \sum_{u,v \in V(D)} d_{T'}(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_{T'}(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(C)}} d_{T'}(u, v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(D)}} d_{T'}(u, v) + \sum_{\substack{u \in V(B) \\ v \in V(C)}} d_{T'}(u, v) + \sum_{\substack{u \in V(B) \\ v \in V(D)}} d_{T'}(u, v) \\ &+ \sum_{\substack{u \in V(C) \\ v \in V(D)}} d_{T'}(u, v) \\ &= \sum_{u,v \in V(A)} d_T(u, v) + \sum_{u,v \in V(B)} d_T(u, v) + \sum_{u,v \in V(C)} d_T(u, v) \end{aligned}$$

$$\begin{aligned}
& + \sum_{u,v \in V(D)} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(C)}} d_T(u,v) \\
& + \sum_{\substack{u \in V(A) \\ v \in V(D)}} [d_T(u,v) - r] + \sum_{\substack{u \in V(B) \\ v \in V(C)}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(D)}} [d_T(u,v) \\
& + \sum_{\substack{u \in V(C) \\ v \in V(D)}} [d_T(u,v) + r] \\
& = W(T) - r|V(A)||V(D)| + r|V(C)||V(D)| \\
& = W(T) - r|V(D)|(|V(A)| - |V(C)|) \\
& < W(T).
\end{aligned}$$

The last inequality is strict because $r \geq 1$, $|V(D)| \neq \emptyset$, and $|V(A)| > |V(C)|$. \square

By iteration of Lemma 3.2, we deduce that the n -vertex tree T with smallest Wiener index is a star-like graph. Next, we show that all segments of T have lengths as close as possible.

Lemma 3.3 *Let T be a caterpillar-like tree of order n having ℓ leaves, and let S_1 and S_2 be any two segments of T such that S_1 and S_2 have lengths r and s , respectively. If T has minimum Wiener index, then $|s - r| \leq 1$.*

Proof. Let T be a caterpillar-like tree of order n having ℓ leaves, and let $S_1 : u_0, u_1, \dots, u_r$ and $S_2 : w_0, w_1, \dots, w_s$ be any two segments of T . Suppose, to the contrary, that T has minimum Wiener index and $|s - r| \geq 2$. Without any loss of generality, we may assume that $s > r$. By Lemma 3.2, T is a star-like tree and, therefore, all its segments are pendant segments. Thus, we may further assume that u_r and w_s are leaves of the segments S_1 and S_2 , respectively. Also, we deduce that $u_0 = w_0$.

Let $A = V(S_1) \cup V(S_2 \setminus w_s)$ and $B = V(T) \setminus A$.

The Wiener index of T is given by

$$W(T) = \sum_{u,v \in A} d_T(u,v) + \sum_{u,v \in B} d_T(u,v) + \sum_{\substack{u \in A \\ v \in B}} d_T(u,v)$$

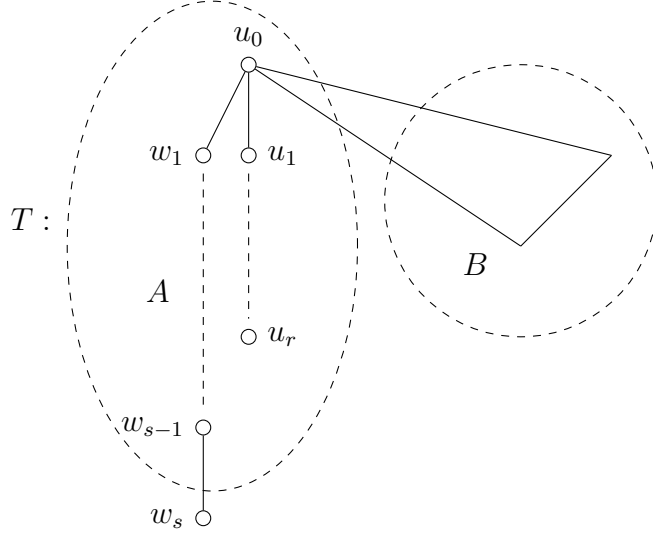


Figure 3.3: The tree T in the proof of Lemma 3.3

$$+ \sum_{v \in A} d_T(w_s, v) + \sum_{v \in B} d_T(w_s, v).$$

Let T' be the graph obtained from T by deleting the edge $w_{s-1}w_s$ and adding the edge $u_r w_s$.

Note that T' is a star-like tree with ℓ leaves. However, the Wiener index of T' is

$$\begin{aligned} W(T') &= \sum_{u, v \in A} d_{T'}(u, v) + \sum_{u, v \in B} d_{T'}(u, v) + \sum_{\substack{u \in A \\ v \in B}} d_{T'}(u, v) \\ &\quad + \sum_{v \in A} d_{T'}(w_s, v) + \sum_{v \in B} d_{T'}(w_s, v) \\ &= \sum_{u, v \in A} d_T(u, v) + \sum_{u, v \in B} d_T(u, v) + \sum_{\substack{u \in A \\ v \in B}} d_T(u, v) \\ &\quad + \sum_{v \in A} d_T(w_s, v) + \sum_{v \in B} [d_T(w_s, v) - (s - r)] \\ &= W(T) - (s - r)|B| \\ &< W(T) \end{aligned}$$

, since $s - r \geq 2$.

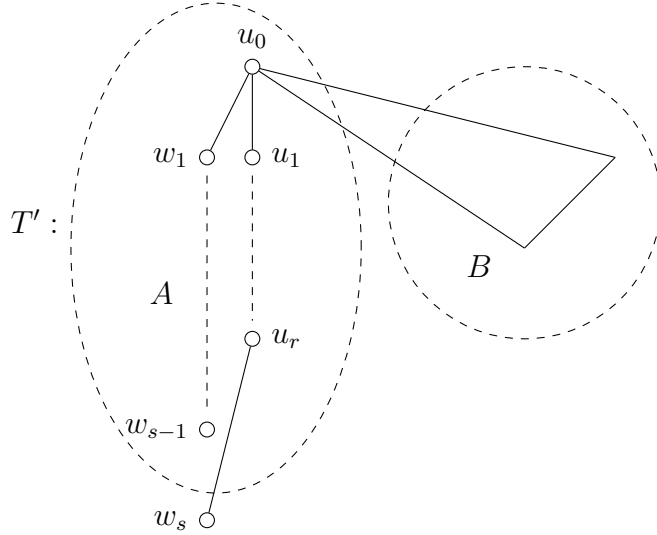


Figure 3.4: The tree T' in the proof of Lemma 3.3

This contradicts the fact that T has minimum Wiener index. □

We now find the formula for the Wiener index, $W(S_{n,\ell})$, of the star-like tree, $S_{n,\ell}$, described in Definition 3.1. We will express $W(S_{n,\ell})$ as a function, of the number n of vertices of $S_{n,\ell}$ and the number ℓ of leaves of $S_{n,\ell}$. Let $s = \lfloor \frac{n-1}{\ell} \rfloor$ and $t = \lceil \frac{n-1}{\ell} \rceil$ denote the length of the shortest and a longest (pendant) segment of $S_{n,\ell}$, respectively. Let k_1 be the number of segments of length s in $S_{n,\ell}$, and k_2 be the number of segments of length t in $S_{n,\ell}$.

Let S be the set of all segments of length s in $S_{n,\ell}$, and let T be the set of all segments of length t in $S_{n,\ell}$. If $P = v_0, v_1, \dots, v_s$ is a segment (or path), then $d(v_i, v_j) = |j - i|$. Let u and v be arbitrary vertices of $S_{n,\ell}$. The sum of the distance between all pairs u, v that lies on the same segment P of length s is

$$\sum_{P \in S} \sum_{u, v \in P} d(u, v) = k_1 \cdot \sum_{i=0}^{s-1} \sum_{j=i+1}^s (j - i)$$

$$\begin{aligned}
 &= k_1 \cdot \sum_{i=0}^{s-1} \left[\frac{(s - (i + 1) + 1)(s + i + 1)}{2} - i(s - (i + 1) + 1) \right] \\
 &= k_1 \cdot \sum_{i=0}^{s-1} \left[\frac{(s - i)(s + i + 1)}{2} - i(s - i) \right] \\
 &= k_1 \cdot \sum_{i=0}^{s-1} \left[\frac{(s - i)(s + i + 1) - 2i(s - i)}{2} \right] \\
 &= k_1 \cdot \sum_{i=0}^{s-1} \left[\frac{s^2 + s + i^2 - i - 2is}{2} \right] \\
 &= \frac{k_1}{2} \cdot \left[\sum_{i=0}^{s-1} (s - i)^2 + \sum_{i=0}^{s-1} (s - i) \right] \\
 &= \frac{k_1}{2} \cdot \left[\sum_{i=0}^s i^2 + \sum_{i=0}^s i \right] \\
 &= \frac{k_1}{2} \cdot \left[\frac{s(s + 1)(2s + 1)}{6} + \frac{s(s + 1)}{2} \right] \\
 &= k_1 \cdot \frac{s(s + 1)(s + 2)}{6}.
 \end{aligned}$$

Similarly, the sum of the distance between all pairs u, v that lies on the same segment P of length t is

$$\sum_{P \in T} \sum_{u, v \in P} d(u, v) = k_2 \cdot \frac{t(t + 1)(t + 2)}{6}.$$

The sum of the distance between all pairs u, v that lies on different segments of length s and t respectively, is

$$\begin{aligned}
 W_{st} &= k_1 k_2 \sum_{i=1}^s \sum_{j=1}^t (j + i) \\
 &= k_1 k_2 \sum_{i=1}^s \left[\frac{t(t + 1)}{2} + it \right] \\
 &= k_1 k_2 \left[\frac{t(t + 1)}{2} \cdot s + \frac{s(s + 1)}{2} \cdot t \right]
 \end{aligned}$$

$$= k_1 k_2 \left[\frac{t(t+1)}{2} \cdot s + \frac{s(s+1)}{2} \cdot t \right].$$

If u and v lie on different paths of length s in $S_{n,\ell}$, then the sum of the distances between u and v is

$$W_{ss} = \binom{k_1}{2} s^2 (s+1).$$

If u and v lie on different paths of length t in $S_{n,\ell}$, then the sum of the distances between u and v is

$$W_{tt} = \binom{k_2}{2} t^2 (t+1).$$

We now consider the following two cases.

Case I: $\frac{n-1}{\ell} \in \mathbb{Z}$.

Suppose that $\frac{n-1}{\ell} \in \mathbb{Z}$. Then, $t = s = \frac{n-1}{\ell}$, and $k_1 = k_2 = \ell$. Thus,

$$\begin{aligned} W(S_{n,\ell}) &= \sum_{P \in S} \sum_{u,v \in P} d(u,v) + W_{ss} \\ &= \ell \cdot \left[\frac{s(s+1)(s+2)}{6} \right] + \binom{\ell}{2} \cdot \left[\frac{s(s+1)}{2} \cdot s + \frac{s(s+1)}{2} \cdot s \right] \\ &= \ell \cdot \left[\frac{s(s+1)(s+2)}{6} \right] + \binom{\ell}{2} \cdot [s^2(s+1)] \\ &= \ell \cdot \left[\frac{s(s+1)(s+2)}{6} \right] + \frac{\ell(\ell-1)}{2} \cdot [s^2(s+1)] \\ &= \frac{\ell s(s+1)(s+2)}{6} + \frac{(\ell s)^2 (s+1)(\ell-1)}{2} \\ &= \frac{1}{6} \ell s(s+1)(s+2+3\ell s(\ell-1)) \\ &= \frac{1}{6} \ell \left(\frac{n-1}{\ell} \right) \left(\frac{n-1}{\ell} + 1 \right) \left(\frac{n-1}{\ell} + 2 + 3\ell \left(\frac{n-1}{\ell} \right) (\ell-1) \right) \\ &= \frac{1}{6} \ell \left(\frac{n-1}{\ell} \right) \left(\frac{n-1+\ell}{\ell} \right) \left(\frac{n-1+2\ell}{\ell} + 3\ell \left(\frac{n-1}{\ell} \right) (\ell-1) \right) \end{aligned}$$

$$= \left(\frac{n-1}{6\ell} \right)^2 (n-1+\ell)(1-\ell+3\ell^2).$$

Case II: $\frac{n-1}{\ell} \notin \mathbb{Z}$.

Suppose that $\frac{n-1}{\ell} \notin \mathbb{Z}$. Then, $t = s + 1$. Since $S_{n,\ell}$ has $n - 1$ edges and ℓ leaves, we have

$$k_1 + k_2 = \ell, \quad \text{and} \quad (3.1)$$

$$k_1 s + k_2 t = n - 1. \quad (3.2)$$

Thus,

$$\begin{aligned} k_1 s + k_2 (s + 1) = n - 1 &\implies (k_1 + k_2) s + k_2 = n - 1 \\ &\implies \ell s + k_2 = n - 1, \end{aligned}$$

or, equivalently,

$$k_2 = n - 1 - \ell s. \quad (3.3)$$

Substituting Equation (3.3) into Equation (3.1) gives

$$k_1 = \ell - (n - 1 - \ell s) = (s + 1)\ell - (n - 1). \quad (3.4)$$

The Wiener index of $S_{n,\ell}$ is,

$$\begin{aligned} W(S_{n,\ell}) &= \sum_{P \in S} \sum_{u,v \in V(P)} d(u,v) + \sum_{P \in T} \sum_{u,v \in V(P)} d(u,v) + W_{ss} + W_{tt} + W_{st} \\ &= k_1 \cdot \left[\frac{s(s+1)(s+2)}{6} \right] + k_2 \cdot \left[\frac{(s+1)(s+2)(s+3)}{6} \right] \\ &\quad + \binom{k_1}{2} \cdot [s^2(s+1)] + \binom{k_2}{2} \cdot [(s+1)^2(s+2)] \\ &\quad + k_1 k_2 \cdot \left[\frac{s(s+1)(s+2)}{2} + \frac{s(s+1)^2}{2} \right]. \end{aligned} \quad (3.5)$$

Note that if $\beta \in \mathbb{Z}$, then $\lfloor \frac{n-1}{\ell} \rfloor + \beta = \lfloor \frac{n-1}{\ell} + \beta \rfloor$. Substituting $s = \lfloor \frac{n-1}{\ell} \rfloor$ and Equations (3.3) and (3.4) into Equation (3.5) gives

$$\sum_{P \in S} \sum_{u,v \in V(P)} d(u,v) =$$

$$\frac{1}{6} \left(\left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \ell - (n-1) \right) \left\lfloor \frac{n-1}{\ell} \right\rfloor \left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \left\lfloor \frac{n-1+2\ell}{\ell} \right\rfloor,$$

$$\sum_{P \in T} \sum_{u,v \in V(P)} d(u,v) = \frac{1}{6} \left(n-1 - \ell \left\lfloor \frac{n-1}{\ell} \right\rfloor \right) \left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \left\lfloor \frac{n-1+2\ell}{\ell} \right\rfloor \left\lfloor \frac{n-1+3\ell}{\ell} \right\rfloor,$$

$$W_{ss} = \binom{\left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \ell - (n-1)}{2} \left\lfloor \frac{n-1}{\ell} \right\rfloor^2 \left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor,$$

$$W_{tt} = \binom{n-1 - \ell \left\lfloor \frac{n-1}{\ell} \right\rfloor}{2} \left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor^2 \left\lfloor \frac{n-1+2\ell}{\ell} \right\rfloor,$$

$$W_{st} = \frac{1}{2} \left(\left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \ell - (n-1) \right) \left(n-1 - \ell \left\lfloor \frac{n-1}{\ell} \right\rfloor \right) \\ \times \left[\left\lfloor \frac{n-1}{\ell} \right\rfloor \left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \left\lfloor \frac{n-1+2\ell}{\ell} \right\rfloor + \left\lfloor \frac{n-1}{\ell} \right\rfloor \left(\left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \right)^2 \right].$$

Thus,

$$W(S_{n,\ell}) = \sum_{P \in S} \sum_{u,v \in V(P)} d(u,v) + \sum_{P \in T} \sum_{u,v \in V(P)} d(u,v) + W_{ss} + W_{tt} + W_{st} \\ = k_1 \cdot \left[\frac{s(s+1)(s+2)}{6} \right] + k_2 \cdot \left[\frac{(s+1)(s+2)(s+3)}{6} \right] \\ + \binom{k_1}{2} \cdot [s^2(s+1)] + \binom{k_2}{2} \cdot [(s+1)^2(s+2)] \\ + k_1 k_2 \cdot \left[\frac{s(s+1)(s+2)}{2} + \frac{s(s+1)^2}{2} \right]. \\ = \frac{1}{6} \left(\left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \ell - (n-1) \right) \left\lfloor \frac{n-1}{\ell} \right\rfloor \left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \left\lfloor \frac{n-1+2\ell}{\ell} \right\rfloor \\ + \frac{1}{6} \left(n-1 - \ell \left\lfloor \frac{n-1}{\ell} \right\rfloor \right) \left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \left\lfloor \frac{n-1+2\ell}{\ell} \right\rfloor \left\lfloor \frac{n-1+3\ell}{\ell} \right\rfloor$$

$$\begin{aligned}
 &+ \binom{\lfloor \frac{n-1+\ell}{\ell} \rfloor \ell - (n-1)}{2} \left\lfloor \frac{n-1}{\ell} \right\rfloor^2 \left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \\
 &+ \binom{n-1 - \ell \lfloor \frac{n-1}{\ell} \rfloor}{2} \left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor^2 \left\lfloor \frac{n-1+2\ell}{\ell} \right\rfloor \\
 &+ \frac{1}{2} \left(\left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \ell - (n-1) \right) \left(n-1 - \ell \left\lfloor \frac{n-1}{\ell} \right\rfloor \right) \\
 &\times \left[\left\lfloor \frac{n-1}{\ell} \right\rfloor \left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \left\lfloor \frac{n-1+2\ell}{\ell} \right\rfloor + \left\lfloor \frac{n-1}{\ell} \right\rfloor \left(\left\lfloor \frac{n-1+\ell}{\ell} \right\rfloor \right)^2 \right].
 \end{aligned}$$

Lemmas 3.2 and 3.3 give the following characterisation of the n -vertex caterpillar-like tree with number of leaves and smallest Wiener index.

Theorem 3.4 *If T is a caterpillar-like tree of order n having ℓ leaves, then*

$$W(T) \geq W(S_{n,\ell}),$$

with equality if and only if $T \cong S_{n,\ell}$.

3.2 Maximal n -vertex caterpillar-like trees with given number of leaves

In this section we characterise the structure of a caterpillar-like tree with given order and given number of leaves that possesses the largest Wiener index. We begin with the following definition.

Definition 3.5 Let n and ℓ be integers such that $n > \ell \geq 2$, and let $\ell = \ell_1 + \ell_2$ for some $\ell_1, \ell_2 \in \mathbb{Z}$ with $\ell_1, \ell_2 \geq 1$. Denote by B_{n,ℓ_1,ℓ_2} the double-broom of order n obtained from the path $P_{n-(\ell_1+\ell_2)}$ by attaching ℓ_1 leaves to one end of $P_{n-(\ell_1+\ell_2)}$ and attaching ℓ_2 leaves to the other end of $P_{n-(\ell_1+\ell_2)}$.

In the remaining part of this section, we present, with proofs, a series of lemmas that lead to a characterisation the n -vertex

caterpillar-like tree with given number of leaves and largest Wiener index. We deduce from these lemmas that such an n -vertex caterpillar-like tree is none other than the double-broom $B_{n, \lfloor \frac{\ell}{2} \rfloor, \lfloor \frac{\ell}{2} \rfloor}$.

Lemma 3.6 *Let T be a caterpillar-like tree of order n having ℓ leaves and at least one non-pendant segment. If T has maximum Wiener index, then all the internal vertices of T (vertices of degree 2 in T) lie in one non-pendant segment.*

Proof. Let T be a caterpillar-like tree of order n having ℓ leaves and at least one non-pendant segment. Let $S : x_0, x_1, \dots, x_{k-1}, x_k$ be a non-pendant segment of T , where both x_0 and x_k are branching vertices of T . Let $\deg_T(x_0) = q$ and $\deg_T(x_k) = t$. Furthermore, let $N_T(x_k) \setminus \{x_{k-1}\} = \{w_1, w_2, \dots, w_{t-1}\}$. Suppose, to the contrary, that T maximizes the Wiener index and there exists a vertex v of degree 2 that lies on a pendant segment $P : x_k, x_{k+1}, \dots, x_s$ of T . Without any loss of generality, we may assume that $w_{t-1} = x_{k+1}$.

Let A be the component of $T - x_{k-1}x_k$ containing x_{k-1} and B be a component of $T - x_{k-1}x_k$ containing x_k . Assume that $|V(A)| \geq |V(B)|$. Furthermore, let B_1 be the component of $B - x_kx_{k+1}$ containing x_{k+1} and $B_2 = B - (V(B_1) \cup \{x_k\})$.

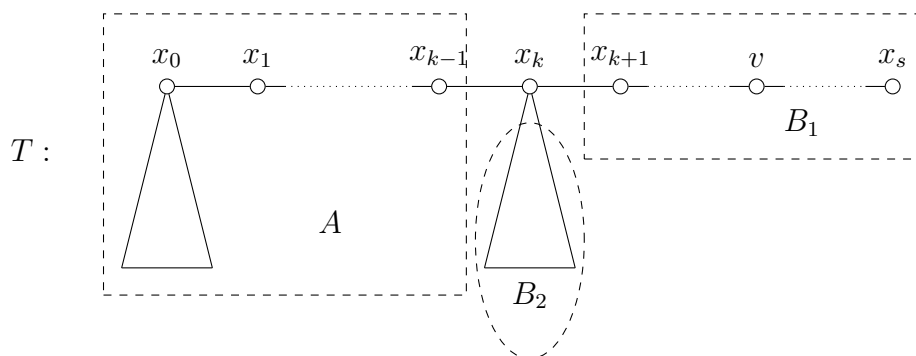


Figure 3.5: The tree T in the proof of Lemma 3.6

The Wiener index of T is

$$W(T) = \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(B_1)} d_T(u,v) + \sum_{u,v \in V(B_2)} d_T(u,v)$$

$$\begin{aligned}
 & + \sum_{\substack{u \in V(A) \\ v \in V(B_1)}} d_T(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(B_2)}} d_T(u, v) + \sum_{\substack{u \in V(B_1) \\ v \in V(B_2)}} d_T(u, v) \\
 & + \sum_{u \in V(A)} d_T(u, x_k) + \sum_{u \in V(B_1)} d_T(u, x_k) + \sum_{u \in V(B_2)} d_T(u, x_k).
 \end{aligned}$$

Let T' be the graph obtained from T by deleting the edges in the set $\{x_k w_i \mid 1 \leq i \leq t-2\}$ and adding the edges in the set $\{x_{k+1} w_i \mid 1 \leq i \leq t-2\}$.

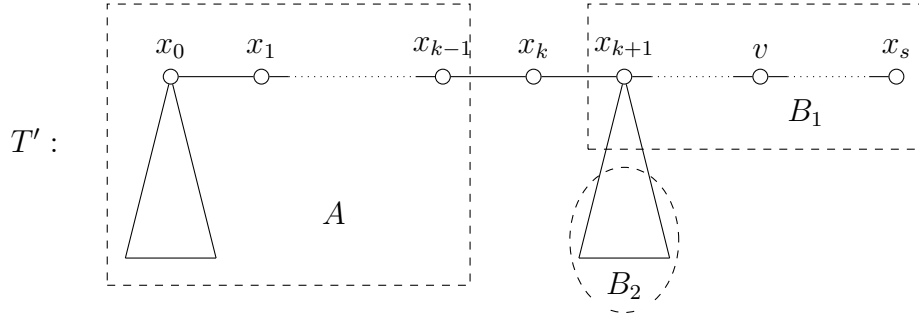


Figure 3.6: The tree T' in the proof of Lemma 3.6

Note that T' is a caterpillar-like tree with ℓ leaves. The Wiener index of T' is

$$\begin{aligned}
 W(T') &= \sum_{u, v \in V(A)} d_{T'}(u, v) + \sum_{u, v \in V(B_1)} d_{T'}(u, v) + \sum_{u, v \in V(B_2)} d_{T'}(u, v) \\
 &+ \sum_{\substack{u \in V(A) \\ v \in V(B_1)}} d_{T'}(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(B_2)}} d_{T'}(u, v) + \sum_{\substack{u \in V(B_1) \\ v \in V(B_2)}} d_{T'}(u, v) \\
 &+ \sum_{u \in V(A)} d_{T'}(u, x_k) + \sum_{u \in V(B_1)} d_{T'}(u, x_k) + \sum_{u \in V(B_2)} d_{T'}(u, x_k). \\
 &= \sum_{u, v \in V(A)} d_T(u, v) + \sum_{u, v \in V(B_1)} d_T(u, v) + \sum_{u, v \in V(B_2)} d_T(u, v) \\
 &+ \sum_{\substack{u \in V(A) \\ v \in V(B_1)}} d_T(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(B_2)}} [d_T(u, v) + 1] + \sum_{\substack{u \in V(B_1) \\ v \in V(B_2)}} [d_T(u, v) - 1]
 \end{aligned}$$

$$\begin{aligned}
 & + \sum_{u \in V(A)} d_T(u, x_k) + \sum_{u \in V(B_1)} d_T(u, x_k) + \sum_{u \in V(B_2)} [d_T(u, x_k) + 1] \\
 & = W(T) + |V(A)||V(B_2)| - |V(B_1)||V(B_2)| + |V(B_2)| \\
 & = W(T) + (|V(A)| - |V(B_1)| + 1)|V(B_2)|.
 \end{aligned}$$

Since $|V(A)| \geq |V(B)| = |V(B_1)| + |V(B_2)| + 1$, we deduce that $|V(A)| > |V(B_1)|$ and hence $(|V(A)| - |V(B_1)| + 1)|V(B_2)| > 0$. Thus, $W(T') > W(T)$, contradicting our supposition that T has maximum Wiener index.

Similarly, if $|A| < |B_1|$, let T'' be the graph obtained from T by deleting the edges in the set $\{x_k w_i \mid 1 \leq i \leq t - 2\}$ and adding the edges in the set $\{x_{k-1} w_i \mid 1 \leq i \leq t - 2\}$.

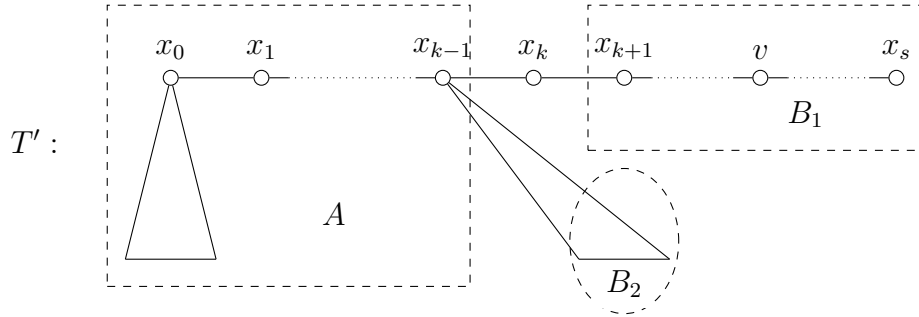


Figure 3.7: The tree T'' in the proof of Lemma 3.6

Note that T'' is a caterpillar-like tree with ℓ leaves. The Wiener index of T'' is

$$\begin{aligned}
 W(T'') & = \sum_{u,v \in V(A)} d_{T''}(u,v) + \sum_{u,v \in V(B_1)} d_{T''}(u,v) + \sum_{u,v \in V(B_2)} d_{T''}(u,v) \\
 & + \sum_{\substack{u \in V(A) \\ v \in V(B_1)}} d_{T''}(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(B_2)}} d_{T''}(u,v) + \sum_{\substack{u \in V(B_1) \\ v \in V(B_2)}} d_{T''}(u,v) \\
 & + \sum_{u \in V(A)} d_{T''}(u, x_k) + \sum_{u \in V(B_1)} d_{T''}(u, x_k) + \sum_{u \in V(B_2)} d_{T''}(u, x_k). \\
 & = \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(B_1)} d_T(u,v) + \sum_{u,v \in V(B_2)} d_T(u,v)
 \end{aligned}$$

$$\begin{aligned}
& + \sum_{\substack{u \in V(A) \\ v \in V(B_1)}} d_T(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(B_2)}} [d_T(u, v) - 1] + \sum_{\substack{u \in V(B_1) \\ v \in V(B_2)}} [d_T(u, v) + 1] \\
& + \sum_{u \in V(A)} d_T(u, x_k) + \sum_{u \in V(B_1)} d_T(u, x_k) + \sum_{u \in V(B_2)} [d_T(u, x_k) + 1] \\
& = W(T) - |V(A)||V(B_2)| + |V(B_1)||V(B_2)| + |V(B_2)| \\
& = W(T) + (|V(B_1)| - |V(A)| + 1)|V(B_2)| \\
& > W(T)
\end{aligned}$$

again contradicting the maximality of T . Thus, all the internal vertices of T (vertices of degree 2 in T) lie in one non-pendant segment. \square

Lemma 3.7 *Let T be an n -vertex caterpillar-like tree with ℓ leaves. If T has maximum Wiener index, then T has at most one non-pendant segment.*

Proof. Let T be a caterpillar-like tree of order n having ℓ leaves. Furthermore, let $Q = x_0, x_1, \dots, x_k$ be the backbone of T . It is sufficient to prove that if T has maximum Wiener index, then $\deg_T(x_i) = 2$ for all i , where $1 \leq i \leq k - 1$. Suppose, to the contrary, that T attains the maximum Wiener index and $\deg_T(x_i) \geq 3$ for some i , where $1 \leq i \leq k - 1$. Let $N_T(x_i) \setminus \{x_{i-1}, x_{i+1}\} = \{w_1, w_2, \dots, w_t\}$, where $t = \deg_T(x_i) - 2$. Since T is a caterpillar-like tree, there must exist j , where $1 \leq j \leq t$ such that w_j lie on a pendant segment of T . Without any loss of generality, let $S = x_i, w_1^*, w_2^*, \dots, w_r^*$, where $r \geq 1$ is an integer and $w_1^* = w_1$.

Let A be the component of $T - x_{i-1}x_i$ containing x_{i-1} and B be the component of $T - x_{i-1}x_i$ containing x_i . Without any loss of generality, we may assume that $|V(A)| \leq |V(B_1)|$. Furthermore, let B_1 be the component of $B - x_i x_{i+1}$ containing x_{i+1} , and $B_2 = B - V(B_1) - V(S)$.

The Wiener index of T is

$$W(T) = \sum_{u, v \in V(A)} d_T(u, v) + \sum_{u, v \in V(B_1)} d_T(u, v) + \sum_{u, v \in V(B_2)} d_T(u, v)$$

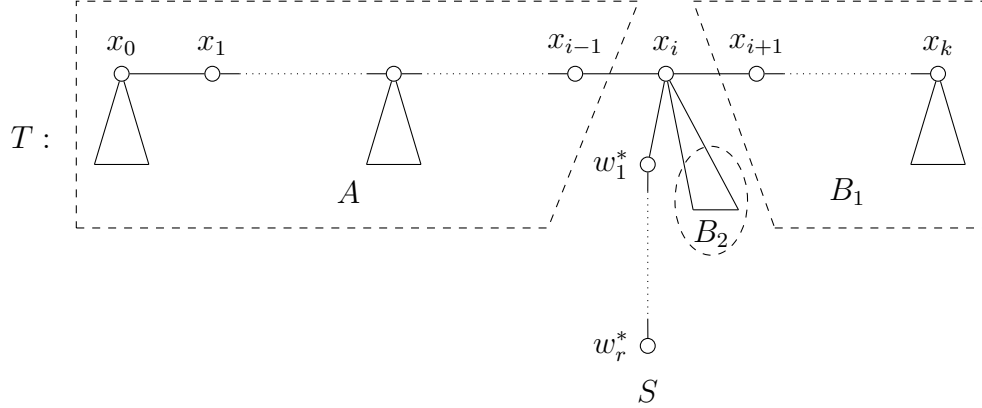


Figure 3.8: The tree T in the proof of Lemma 3.7

$$\begin{aligned}
 & + \sum_{u,v \in V(S)} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(B_1)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(B_2)}} d_T(u,v) \\
 & + \sum_{\substack{u \in V(A) \\ v \in V(S)}} d_T(u,v) + \sum_{\substack{u \in V(B_1) \\ v \in V(B_2)}} d_T(u,v) + \sum_{\substack{u \in V(B_1) \\ v \in V(S)}} d_T(u,v) \\
 & + \sum_{\substack{u \in V(B_2) \\ v \in V(S)}} d_T(u,v).
 \end{aligned}$$

Let T' be the graph obtained from T by removing B_2 and adding it x_{i-1} .

Note that T' is a caterpillar-like tree. The Wiener index of T' is

$$\begin{aligned}
 W(T') & = \sum_{u,v \in V(A)} d_{T'}(u,v) + \sum_{u,v \in V(B_1)} d_{T'}(u,v) + \sum_{u,v \in V(B_2)} d_{T'}(u,v) \\
 & + \sum_{u,v \in V(S)} d_{T'}(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(B_1)}} d_{T'}(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(B_2)}} d_{T'}(u,v) \\
 & + \sum_{\substack{u \in V(A) \\ v \in V(S)}} d_{T'}(u,v) + \sum_{\substack{u \in V(B_1) \\ v \in V(B_2)}} d_{T'}(u,v) + \sum_{\substack{u \in V(B_1) \\ v \in V(S)}} d_{T'}(u,v)
 \end{aligned}$$

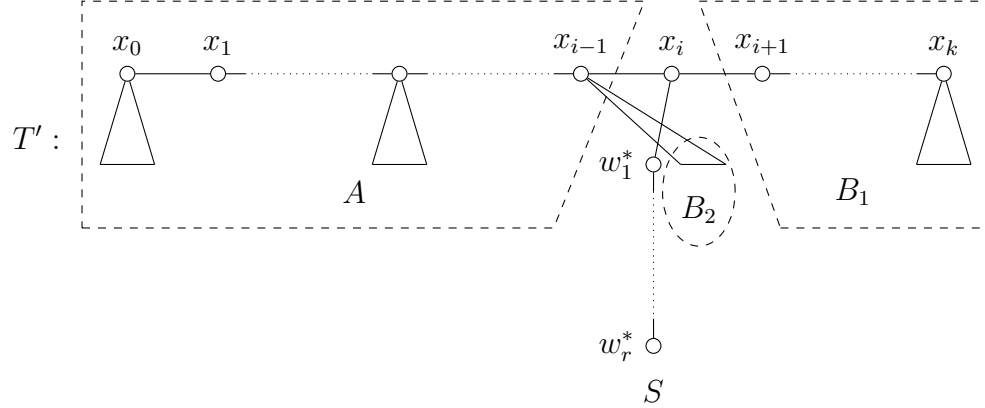


Figure 3.9: The tree T' in the proof of Lemma 3.7

$$\begin{aligned}
 & + \sum_{\substack{u \in V(B_2) \\ v \in V(S)}} d_{T'}(u, v) \\
 & = \sum_{u, v \in V(A)} d_T(u, v) + \sum_{u, v \in V(B_1)} d_T(u, v) + \sum_{u, v \in V(B_2)} d_T(u, v) \\
 & + \sum_{u, v \in V(S)} d_T(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(B_1)}} d_T(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(B_2)}} [d_T(u, v) - 1] \\
 & + \sum_{\substack{u \in V(A) \\ v \in V(S)}} d_T(u, v) + \sum_{\substack{u \in V(B_1) \\ v \in V(B_2)}} [d_T(u, v) + 1] + \sum_{\substack{u \in V(B_1) \\ v \in V(S)}} d_T(u, v) \\
 & + \sum_{\substack{u \in V(B_2) \\ v \in V(S)}} [d_T(u, v) + 1] \\
 & = W(T) - |V(A)||V(B_2)| + |V(B_1)||V(B_2)| + |V(B_2)||V(S)| \\
 & = W(T) + |V(B_2)|(|V(B_1)| + |V(S)| - |V(A)|) \\
 & > W(T).
 \end{aligned}$$

Since $|V(S)| \geq 1$, we have $|V(B_1)| + |V(S)| - |V(A)| \geq 1$, and since $B_2 \neq \emptyset$, $|V(B_2)| > 0$. \square

Lemma 3.8 *Let T be a caterpillar-like tree of order n having ℓ leaves and only one non-pendant segment S . If ℓ_1 and ℓ_2 are respectively*

the number of leaves in the two sides of S , then T reaches the maximum Wiener index if $|\ell_2 - \ell_1| \leq 1$.

Proof. Let T be a caterpillar-like tree of order n having ℓ leaves and only one non-pendant segment $S : w_0, w_1, \dots, w_{z-1}, w_z$. Furthermore, let $N_T(w_0) \setminus \{w_1\} = \{x_1, x_2, \dots, x_{\ell_1}\}$ and $N_T(w_z) \setminus \{w_{z-1}\} = \{v_1, v_2, \dots, v_{\ell_2}\}$. Suppose, to the contrary, that T has maximum Wiener index and $|\ell_2 - \ell_1| \geq 2$. Without any loss of generality, we may assume that $\ell_2 > \ell_1$. By Lemma 3.6, if T contains an internal vertex (a vertex of degree 2), then such a vertex lies on S , implying that each pendant segment of T has length exactly 1.

Let A^* be the component of $T - w_0w_1$ that contains w_0 and $A = A^* - w_0$. Furthermore, let B^* be a component of $T - w_{z-1}w_z$ that contains w_z and $B = B^* - \{w_z, v_{\ell_2}\}$.

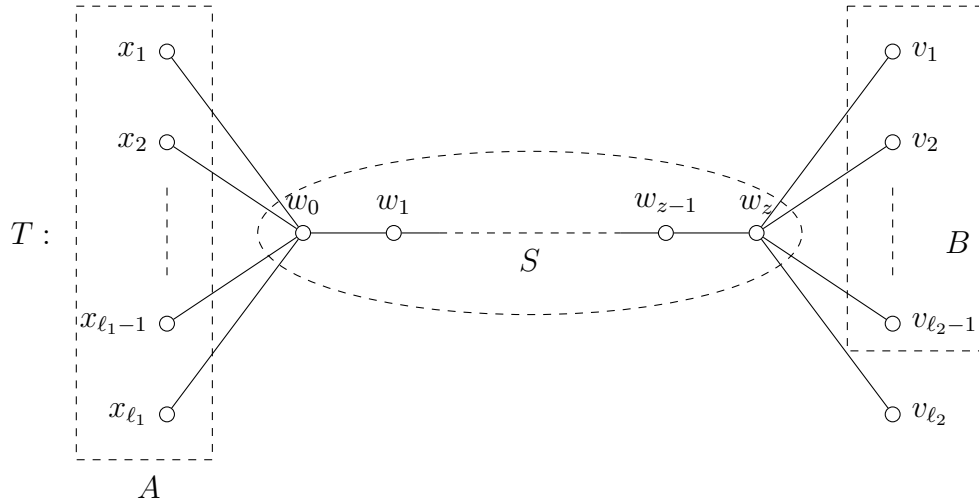


Figure 3.10: The tree T in the proof of Lemma 3.8

The Wiener index of T is

$$\begin{aligned}
 W(T) &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(S)} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) \\
 &+ \sum_{\substack{u \in V(A) \\ v \in V(S)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(S) \\ v \in V(B)}} d_T(u,v)
 \end{aligned}$$

$$+ \sum_{v \in V(A)} d_T(v_{\ell_2}, v) + \sum_{v \in V(S)} d_T(v_{\ell_2}, v) + \sum_{v \in V(B)} d_T(v_{\ell_2}, v).$$

Let $T' = T - w_z v_{\ell_2} + w_0 v_{\ell_2}$.

Note that T' is a caterpillar-like tree with ℓ leaves. The Wiener

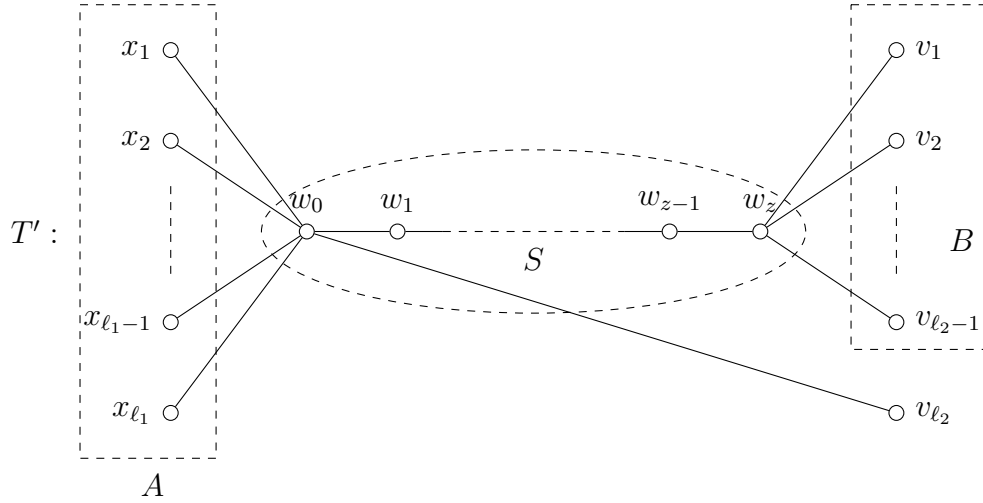


Figure 3.11: The tree T' in the proof of Lemma 3.8

index of T' is

$$\begin{aligned} W(T') &= \sum_{u,v \in V(A)} d_{T'}(u,v) + \sum_{u,v \in V(S)} d_{T'}(u,v) + \sum_{u,v \in V(B)} d_{T'}(u,v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(S)}} d_{T'}(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_{T'}(u,v) + \sum_{\substack{u \in V(S) \\ v \in V(B)}} d_{T'}(u,v) \\ &+ \sum_{v \in V(A)} d_{T'}(v_{\ell_2}, v) + \sum_{v \in V(S)} d_{T'}(v_{\ell_2}, v) + \sum_{v \in V(B)} d_{T'}(v_{\ell_2}, v) \\ &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(S)} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(S)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(S) \\ v \in V(B)}} d_T(u,v) \end{aligned}$$

$$\begin{aligned}
 & + \sum_{v \in V(A)} [d_T(v_{\ell_2}, v) - z] + \sum_{v \in V(S)} d_T(v_{\ell_2}, v) + \sum_{v \in V(B)} [d_T(v_{\ell_2}, v) + z] \\
 & = W(T) - z|V(A)| + z|V(B)| \\
 & = W(T) + z(|V(B)| - |V(A)|).
 \end{aligned}$$

By assumption, $\ell_2 \geq \ell_1 + 2$, so $|V(B)| = \ell_2 - 1 > \ell_1 = |V(A)|$. Thus, $|V(B)| - |V(A)| > 0$, implying that $W(T') > W(T)$. This contradicts the fact that T has maximum Wiener index. \square

Lemma 3.6, Lemma 3.7 and Lemma 3.8 give the following characterisation of the n -vertex caterpillar-like tree with given number of leaves and largest Wiener index.

Theorem 3.9 *If T is a caterpillar-like tree of order n having ℓ leaves, then*

$$W(T) \leq W(B_{n, \lceil \frac{\ell}{2} \rceil, \lfloor \frac{\ell}{2} \rfloor}),$$

with equality if and only if $T \cong B_{n, \lceil \frac{\ell}{2} \rceil, \lfloor \frac{\ell}{2} \rfloor}$.

4 | Caterpillar-like trees with given maximum degree.

In this chapter, we focus on finding extremal caterpillar-like trees with given order and fixed maximum degree. The first section is based on finding minimal graphs then we proceed to finding maximal graphs.

4.1 Minimal n -vertex caterpillar-like trees with given maximum degree.

In this section we present partial results on characterization of the n -vertex caterpillar-like tree with given maximum degree and has the smallest Wiener index. We also present corollaries for special cases in which a complete characterization is obtained.

Lemma 4.1 *Let T be a caterpillar-like tree of order n having a maximum degree $\Delta \geq 3$. If T has a minimum Wiener index then, all non-pendant segments in the backbone are of length 1.*

Proof. Let T be a caterpillar-like tree of order n having a maximum degree $\Delta \geq 3$. Furthermore, let $Q : x_{0,0}, x_{0,1}, \dots, x_{0,r}$ be any non-pendant segment of T . It follows, therefore, that $\deg_T(x_{0,0}) \geq 3$ and $\deg_T(x_{0,r}) \geq 3$. We want to show that if T has minimum Wiener index, then $r = 1$. Suppose, to the contrary, that T has minimum Wiener index and $r \geq 2$. Let $S_1 : x_{0,0}, x_{1,0}, \dots, x_{i,0}$ and $S_2 : x_{0,r}, x_{1,r}, \dots, x_{j,r}$ be any two pendant segments of T rooted at $x_{0,0}$ and $x_{0,r}$, respectively.

Let $H = T - (V(Q) \setminus \{x_{0,0}, x_{0,r}\})$. Then, H has two components, namely H_1 containing the vertex $x_{0,0}$ and H_2 containing the vertex $x_{0,r}$. Let $A = H_1 - V(S_1)$ and $B = H_2 - V(S_2)$. Without any loss of generality, we may assume that $j \geq i$.

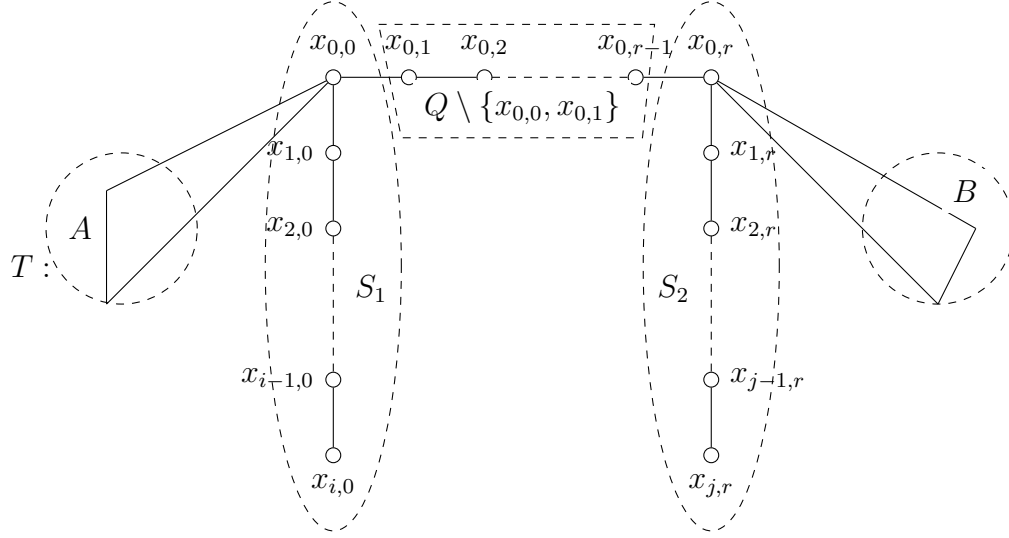


Figure 4.1: The tree T in the proof of Lemma 4.1

The Wiener index of T is, therefore, given by

$$\begin{aligned}
 W(T) = & \sum_{u,v \in A} d_T(u,v) + \sum_{u,v \in S_1} d_T(u,v) + \sum_{u,v \in S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}} d_T(u,v) \\
 & + \sum_{\substack{u \in A \\ v \in S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}}} d_T(u,v) + \sum_{\substack{u \in A \\ v \in S_1}} d_T(u,v) + \sum_{\substack{u \in S_1 \\ v \in S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}}} d_T(u,v) \\
 & + \sum_{u \in A} d_T(u, x_{0,1}) + \sum_{u \in S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}} d_T(u, x_{0,1}) + \sum_{u \in S_1} d_T(u, x_{0,1}).
 \end{aligned}$$

Let $T' = (T - \{x_{0,0}x_{0,1}\}) + \{x_{0,0}x_{0,2}\}$.

Note that T' is still a caterpillar-like tree with maximum degree Δ . However, the Wiener index of T' is given by

$$W(T') = \sum_{u,v \in A} d_{T'}(u,v) + \sum_{u,v \in S_1} d_{T'}(u,v) + \sum_{u,v \in S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}} d_{T'}(u,v)$$

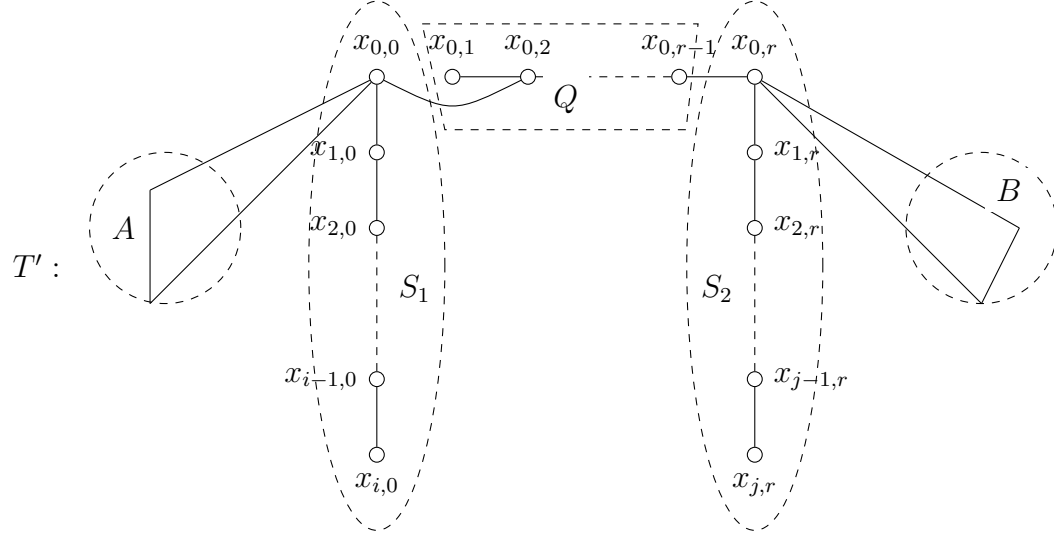


Figure 4.2: The tree T' in the proof of Lemma 4.1

$$\begin{aligned}
 & + \sum_{\substack{u \in A \\ v \in S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}}} d_{T'}(u, v) + \sum_{\substack{u \in A \\ v \in S_1}} d_{T'}(u, v) \\
 & + \sum_{\substack{u \in S_1 \\ v \in S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}}} d_{T'}(u, v) + \sum_{u \in A} d_{T'}(u, x_{0,1}) \\
 & + \sum_{u \in S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}} d_{T'}(u, x_{0,1}) + \sum_{u \in S_1} d_{T'}(u, x_{0,1}) \\
 & = \sum_{u, v \in A} d_T(u, v) + \sum_{u, v \in S_1} d_T(u, v) + \sum_{u, v \in S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}} d_T(u, v) \\
 & + \sum_{\substack{u \in A \\ v \in S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}}} [d_T(u, v) - 1] + \sum_{\substack{u \in A \\ v \in S_1}} d_T(u, v) \\
 & + \sum_{\substack{u \in S_1 \\ v \in S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}}} [d_T(u, v) - 1] \\
 & + \sum_{u \in S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}} [d_T(u, x_{0,1})]
 \end{aligned}$$

$$\begin{aligned}
& + \sum_{u \in A} [d_T(u, x_{0,1}) + 1] + \sum_{u \in S_1} [d_T(u, x_{0,1}) + 1] \\
& = W(T) - |A||S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}| \\
& \quad - |S_1||S_2 \cup B \cup Q \setminus \{x_{0,0}, x_{0,1}\}| + |A| + |S_1| \\
& = W(T) - |A|(j + (r - 1) + |B|) - (i + 1)(j + (r - 1) + |B|) \\
& \quad + |A| + |S_1| \\
& = W(T) - (j + r - 1 + |B|)(|A| + (i + 1)) + |A| + |S_1| \\
& = W(T) - (j + r - 1 + |B|)(|A| + (i + 1)) + |A| + (i + 1) \\
& = W(T) - (j + r + |B|)(|A| + (i + 1)) \\
& \leq W(T) - (3 + |B|)(|A| + 2) \\
& < W(T).
\end{aligned}$$

Since $r \geq 2$ and $j \geq i \geq 1$. □

Lemma 4.2 *Let T be a caterpillar-like tree of order n with maximum degree $\Delta \geq 3$, and let $P : x_0, \dots, x_i$ and $Q : y_0, \dots, y_j$ be pendant segments in T with $\deg_T x_0 \geq 3$ and $\deg_T y_0 \geq 3$ such that $d_T(x_0, y_0) \leq 1$. If T has minimum Wiener index, then $|j - i| \leq 1$.*

Proof. Let T be a caterpillar-like tree of order n with maximum degree $\Delta \geq 3$, and let $P : x_0, \dots, x_i$ and $Q : y_0, \dots, y_j$ be pendant segments in T with $\deg_T x_0 \geq 3$ and $\deg_T y_0 \geq 3$ such that $d_T(x_0, y_0) \leq 1$. Suppose, to the contrary, that T has minimum Wiener index and $|j - i| \geq 2$. Without any loss of generality, we may assume that $j = i + r$, where $r \geq 2$. We now consider two cases.

Case (i) Suppose $d_T(x_0, y_0) = 0$.

Then $x_0 = y_0$, so the pendant segments P and Q share a common vertex, say x_0 . Let $A = T - P \cup Q$.

The Wiener index of T is, therefore, given by

$$\begin{aligned}
W(T) & = \sum_{u, v \in V(A)} d_T(u, v) + \sum_{u, v \in V(P \cup Q) \setminus \{y_j\}} d_T(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(P \cup Q) \setminus \{y_j\}}} d_T(u, v) \\
& \quad + \sum_{u \in V(A)} d_T(u, y_j) + \sum_{u \in V(P \cup Q) \setminus \{y_j\}} d_T(u, y_j).
\end{aligned}$$

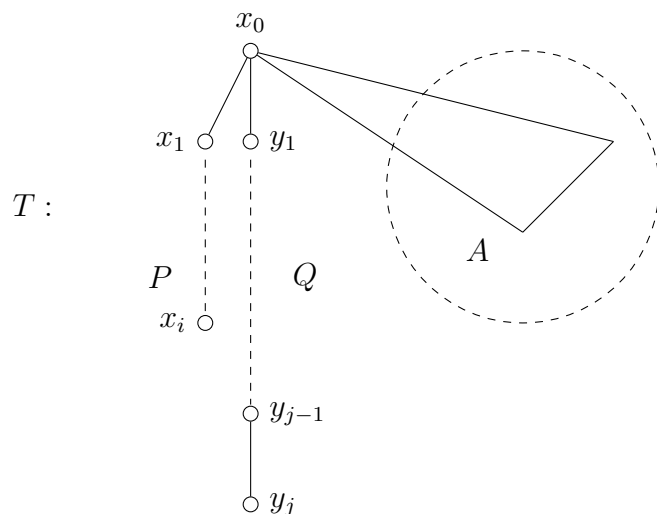


Figure 4.3: The tree T in the proof of Lemma 4.2 (case (i))

Let $T' = (T - y_{j-1}y_j) \cup \{x_i y_j\}$.

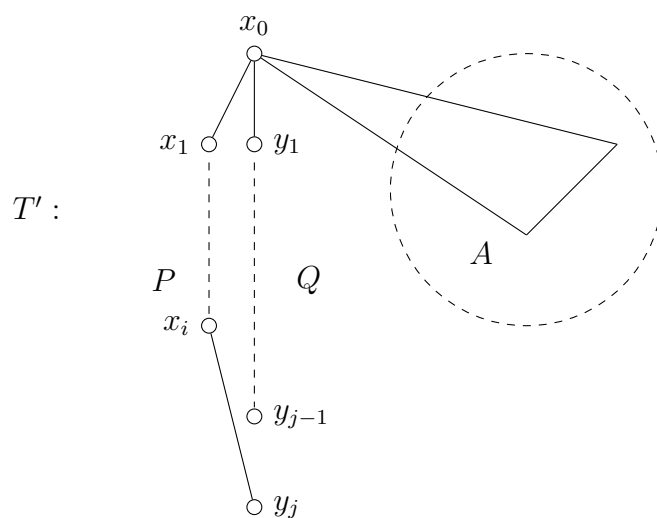


Figure 4.4: The tree T' in the proof of Lemma 4.2 (case (i))

Note that T' is a caterpillar-like tree with maximum degree $\Delta \geq$

3. However, the Wiener index of T' is

$$\begin{aligned}
 W(T') &= \sum_{u,v \in V(A)} d_{T'}(u,v) + \sum_{u,v \in V(P \cup Q) \setminus \{y_j\}} d_{T'}(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(P \cup Q) \setminus \{y_j\}}} d_{T'}(u,v) \\
 &\quad + \sum_{u \in V(A)} d_{T'}(u, y_j) + \sum_{u \in V(P \cup Q) \setminus \{y_j\}} d_{T'}(u, y_j) \\
 &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(P \cup Q) \setminus \{y_j\}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(P \cup Q) \setminus \{y_j\}}} d_T(u,v) \\
 &\quad + \sum_{u \in V(A)} [d_T(u, y_j) - (r-1)] + \sum_{u \in V(P \cup Q) \setminus \{y_j\}} d_T(u, y_j) \\
 &= W(T) - (r-1)|A|.
 \end{aligned}$$

Since $\deg_T(x_0) \geq 3$, we have $|A| \geq 1$. Furthermore, since $r \geq 2$, we have $r-1 \geq 1$. This implies that $(r-1)|A| \geq 1$, and so $W(T') < W(T)$. This, however, contradicts our assumption that T has the minimum Wiener index.

Case (ii) Suppose $d_T(x_0, y_0) = 1$.

Then, P and Q are pendant segments of T whose backbone vertices, x_0 and y_0 are neighbors in T . Let A' be the connected component of $T - x_0y_0$ that contain x_0 . Let $A = A' - P$ and let $B = T - A - P - Q$.

The Wiener index of T is, therefore, given by

$$\begin{aligned}
 W(T) &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(P \cup Q) \setminus \{y_j\}} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) \\
 &\quad + \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(P \cup Q) \setminus \{y_j\}}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(P \cup Q) \setminus \{y_j\}}} d_T(u,v) \\
 &\quad + \sum_{u \in V(A)} d_T(u, y_j) + \sum_{u \in V(P \cup Q) \setminus \{y_j\}} d_T(u, y_j) + \sum_{u \in V(B)} d_T(u, y_j).
 \end{aligned}$$

Let $T' = (T - y_{j-1}y_j) + \{x_iy_j\}$.

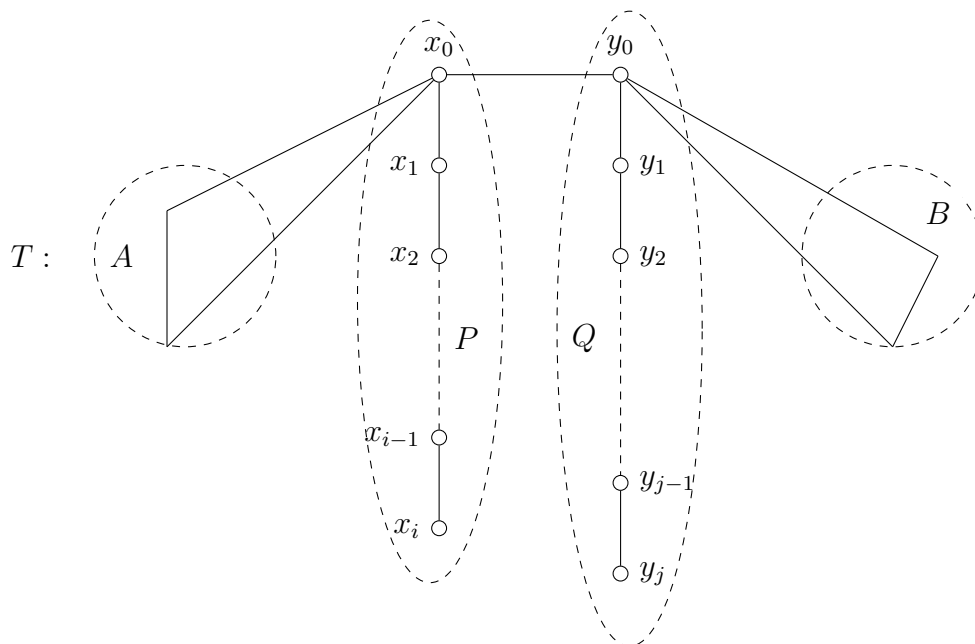


Figure 4.5: The tree T in the proof of Lemma 4.2 (case (ii))

Note that T' is still a caterpillar-like tree with maximum degree $\Delta \geq 3$. However, the Wiener index of T' is

$$\begin{aligned}
 W(T') &= \sum_{u,v \in V(A)} d_{T'}(u,v) + \sum_{u,v \in V(P \cup Q) \setminus \{y_j\}} d_{T'}(u,v) + \sum_{u,v \in V(B)} d_{T'}(u,v) \\
 &+ \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_{T'}(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(P \cup Q) \setminus \{y_j\}}} d_{T'}(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(P \cup Q) \setminus \{y_j\}}} d_{T'}(u,v) \\
 &+ \sum_{u \in V(A)} d_{T'}(u, y_j) + \sum_{u \in V(P \cup Q) \setminus \{y_j\}} d_{T'}(u, y_j) + \sum_{u \in V(B)} d_{T'}(u, y_j) \\
 &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(P \cup Q) \setminus \{y_j\}} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) \\
 &+ \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(P \cup Q) \setminus \{y_j\}}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(P \cup Q) \setminus \{y_j\}}} d_T(u,v)
 \end{aligned}$$

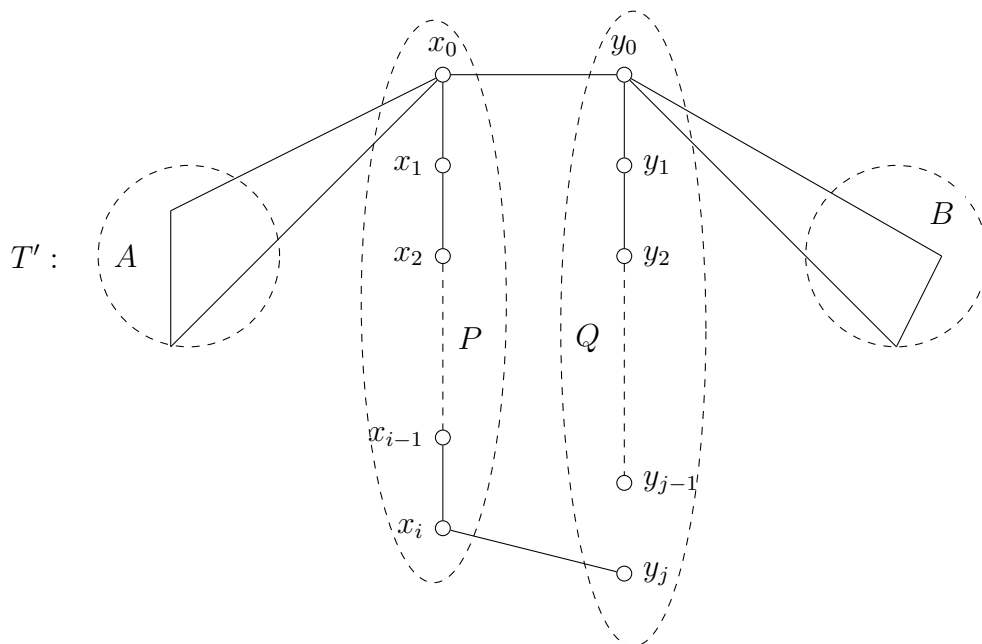


Figure 4.6: The tree T' in the proof of Lemma 4.2 (case (ii))

$$\begin{aligned}
 & + \sum_{u \in V(A)} [d_T(u, y_j) - r] + \sum_{u \in V(P \cup Q) \setminus \{y_j\}} d_T(u, y_j) \\
 & + \sum_{u \in V(B)} [d_T(u, y_j) - (r - 2)] \\
 & = W(T) - r|A| - (r - 2)|B|.
 \end{aligned}$$

Since $\deg_T(x_0) \geq 3$, we have $|A| \geq 1$, and since $\deg_T y_0 \geq 3$, we have $|B| \geq 1$. Furthermore, since $r \geq 2$, we have $r|A| \geq 2$ and $(r - 2)|B| \geq 0$. This implies that $r|A| + (r - 2)|B| \geq 2$, and so $W(T') < W(T)$. This, however, contradicts our assumption that T has the minimum Wiener index, and hence completing the proof of Lemma 4.2. \square

Next, we show that in a caterpillar-like tree with minimum Wiener index, the lengths of adjacent pendant segments are constrained by the sizes of the subtrees attached to them. More specifically, longer pendant segments must be attached to larger components.

Lemma 4.3 *Let T be a caterpillar-like tree of order n with maximum degree $\Delta \geq 3$ and let $S_1 : x_0, \dots, x_i$, and $S_2 : y_0, \dots, y_j$ be pendant segments of T such that $d_T(x_0, y_0) = 1$. Let $H = T - x_0y_0$ and let H_1 be the connected component of H that contains x_0 and H_2 be the connected component of H that contains y_0 . Lastly, let $A = H_1 - S_1$ and $B = H_2 - S_2$. If T has the minimum Wiener index and $|A| < |B|$, then $i \leq j$.*

Proof. Let T be a caterpillar-like tree of order n with maximum degree $\Delta \geq 3$ and let $S_1 : x_0, \dots, x_i$, and $S_2 : y_0, \dots, y_j$ be pendent segments of T such that $d_T(x_0, y_0) = 1$. Let A and B be as in the statement of the Lemma. Suppose, to the contrary, that T has minimum Wiener index, $|A| < |B|$ and $i > j$. We may assume that $i = j + r$, where $r \geq 1$.

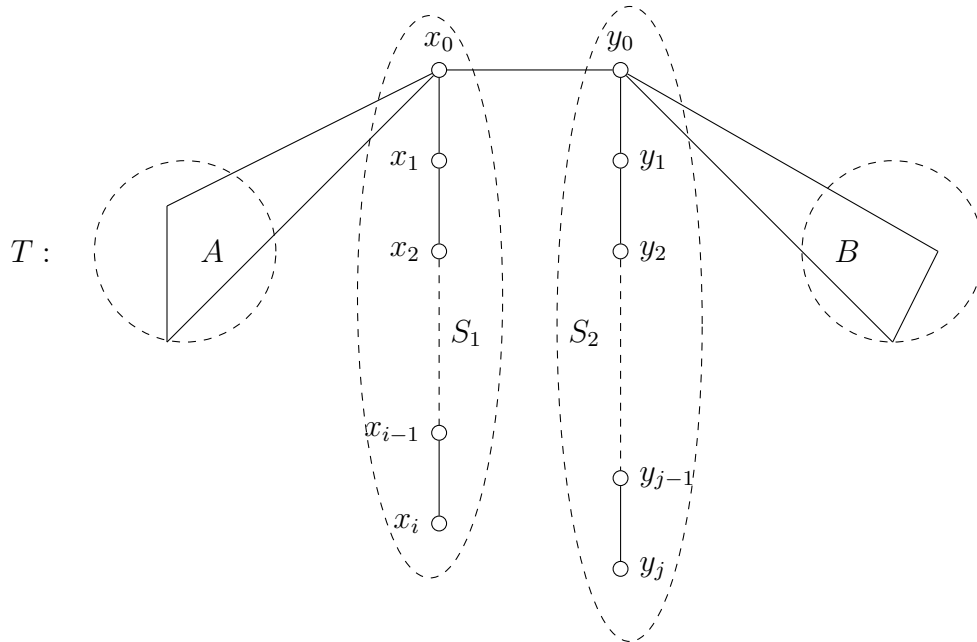


Figure 4.7: The tree T in the proof of Lemma 4.3

Then the Wiener index of T is given by

$$W(T) = \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(S_2 \cup S_1) \setminus \{x_i\}} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v)$$

$$\begin{aligned}
 & + \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_T(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(S_2 \cup S_1) \setminus \{x_i\}}} d_T(u, v) + \sum_{\substack{u \in V(B) \\ v \in V(S_2 \cup S_1) \setminus \{x_i\}}} d_T(u, v) \\
 & + \sum_{u \in V(A)} d_T(u, x_i) + \sum_{u \in V(S_2 \cup S_1) \setminus \{x_i\}} d_T(u, x_i) + \sum_{u \in V(B)} d_T(u, x_i).
 \end{aligned}$$

Let $T' = (T - x_i x_{i-1}) + \{y_j x_i\}$.

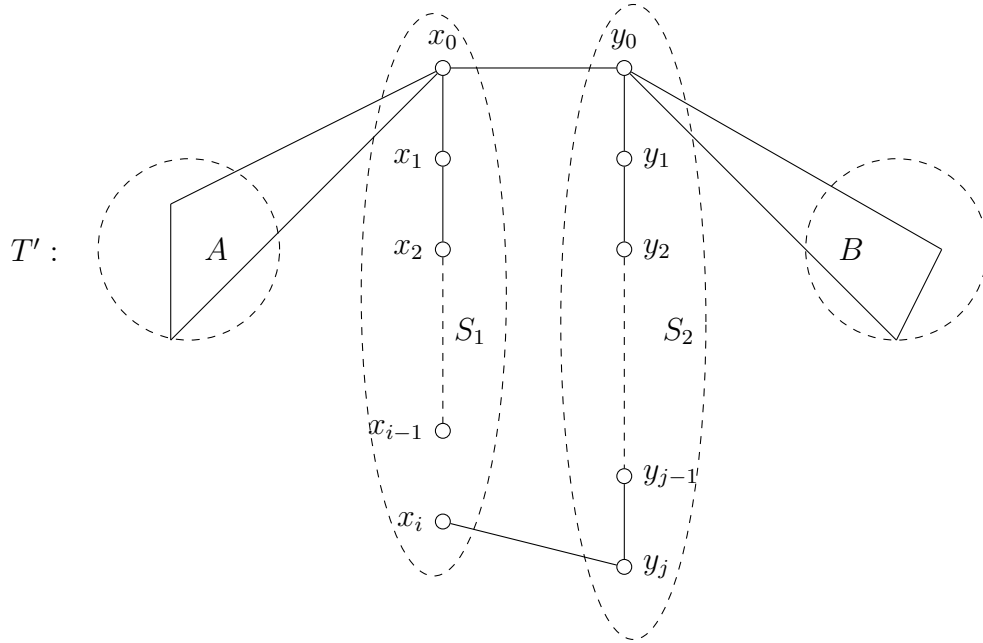


Figure 4.8: The tree T' in the proof of Lemma 4.3

Note that T' still has a maximum degree $\Delta \geq 3$. However, the Wiener index of T' is

$$\begin{aligned}
 W(T) = & \sum_{u, v \in V(A)} d_{T'}(u, v) + \sum_{u, v \in V(S_2 \cup S_1) \setminus \{x_i\}} d_{T'}(u, v) + \sum_{u, v \in V(B)} d_{T'}(u, v) \\
 & + \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_{T'}(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(S_2 \cup S_1) \setminus \{x_i\}}} d_{T'}(u, v) + \sum_{\substack{u \in V(B) \\ v \in V(S_2 \cup S_1) \setminus \{x_i\}}} d_{T'}(u, v) \\
 & + \sum_{u \in V(A)} d_{T'}(u, x_i) + \sum_{u \in V(S_2 \cup S_1) \setminus \{x_i\}} d_{T'}(u, x_i) + \sum_{u \in V(B)} d_{T'}(u, x_i)
 \end{aligned}$$

$$\begin{aligned}
&= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(S_2 \cup S_1) \setminus \{x_i\}} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) \\
&+ \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(S_2 \cup S_1) \setminus \{x_i\}}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(S_2 \cup S_1) \setminus \{x_i\}}} d_T(u,v) \\
&+ \sum_{u \in V(A)} [d_T(u, x_i) - (r - 2)] + \sum_{u \in V(S_2 \cup S_1) \setminus \{x_i\}} d_T(u, x_i) \\
&+ \sum_{u \in V(B)} [d_T(u, x_i) - r] \\
&= W(T) - |A|(r - 2) - r|B| \\
&= W(T) - r(|A| + |B|) + 2|A|, \text{ with } r \geq 1 \\
&\leq W(T) - (|B| + |A|) + 2|A| \\
&= W(T) - (|B| - |A|) \\
&< W(T).
\end{aligned}$$

Since $(|B| - |A|) > 0$, this contradicts the minimality of $W(T)$. \square

Lemma 4.4 *Let T be a caterpillar-like tree of order n with maximum degree $\Delta \geq 3$ and let $Q = u_0, u_1, \dots, u_r$ be the backbone. Furthermore, let A be the connected component of $T - u_i u_{i+1}$ that contains u_i , and B be the connected component of $T - u_i u_{i+1}$ that contains u_{i+1} . If T has minimum Wiener index, then the following conditions hold:*

- (i) *If $|A| < |B|$, then $\deg_T(u_i) \leq \deg(u_{i+1})$.*
- (ii) *There are at most two vertices of degree less than Δ in the backbone and they are end vertices of the backbone.*

Proof. Let T be a caterpillar-like tree of order n with maximum degree $\Delta \geq 3$ and let $Q = u_0, u_1, \dots, u_r$ be the backbone. Furthermore, let A and B be as in the statement of the Lemma.

First let us prove (i) Suppose, to the contrary, that T has minimum Wiener index, $|A| < |B|$ and $\deg_T(u_i) > \deg(u_{i+1})$. Let $v \in N_T(u_i) \setminus \{u_{i-1}, u_{i+1}\}$ and C be the connected component of $T - u_i v$ that contains v . Furthermore, let $A' = A - C$.

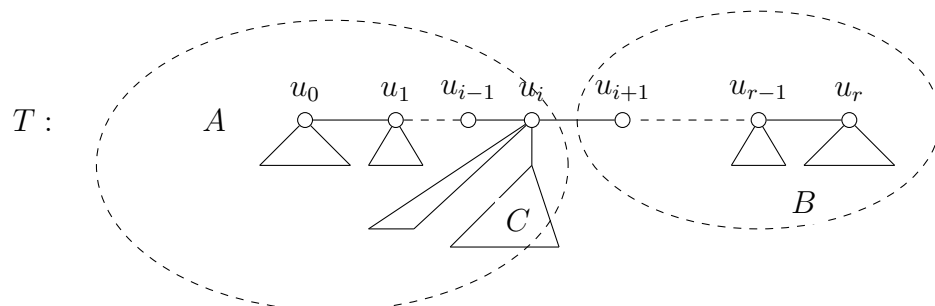


Figure 4.9: The tree T in the proof of Lemma 4.4 (i)

Thus, the Wiener index of T is given by

$$\begin{aligned}
 W(T) &= \sum_{u,v \in V(A')} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) + \sum_{u,v \in V(C)} d_T(u,v) \\
 &+ \sum_{\substack{u \in V(A') \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(C)}} d_T(u,v) + \sum_{\substack{u \in V(A') \\ v \in V(C)}} d_T(u,v).
 \end{aligned}$$

Let $T' = u_i v + u_{i+1} v$. Note that T' is still a caterpillar-like tree with maximum degree Δ . The Wiener index of T' is given by.

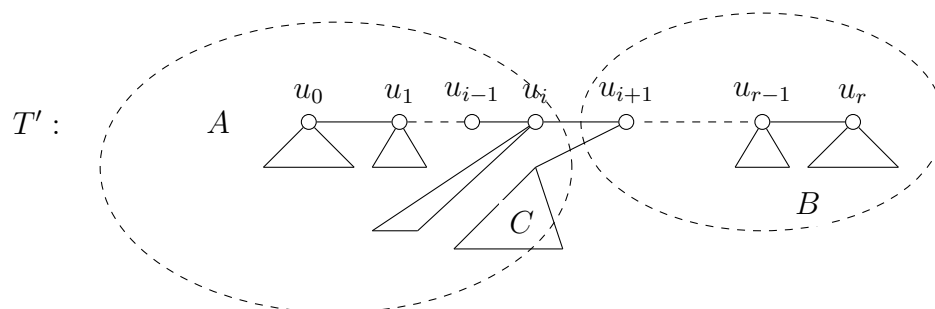


Figure 4.10: The tree T' in the proof of Lemma 4.4 (i)

$$\begin{aligned}
 W(T') &= \sum_{u,v \in V(A')} d_{T'}(u,v) + \sum_{u,v \in V(B)} d_{T'}(u,v) + \sum_{u,v \in V(C)} d_{T'}(u,v) \\
 &+ \sum_{\substack{u \in V(A') \\ v \in V(B)}} d_{T'}(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(C)}} d_{T'}(u,v) + \sum_{\substack{u \in V(A') \\ v \in V(C)}} d_{T'}(u,v)
 \end{aligned}$$

$$\begin{aligned}
 &= \sum_{u,v \in V(A')} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) + \sum_{u,v \in V(C)} d_T(u,v) \\
 &+ \sum_{\substack{u \in V(A') \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(C)}} [d_T(u,v) - 1] + \sum_{\substack{u \in V(A') \\ v \in V(C)}} [d_T(u,v) + 1] \\
 &= W(T) - |B||C| + |A'||C| \\
 &= W(T) - |C|(|B| - |A'|).
 \end{aligned}$$

Note that $|B| \geq |A| > |A'|$. Since $|A'| < |B|$ and $|C| > 0$, we have $W(T') < W(T)$. \square

We will need the following fact in the proof of II. Note that the proof of (i) also show that if $\deg(u_i) > \deg(u_{i+1})$, then we must have $|A| \geq |B|$.

Claim 4.1 *No small degree lies between large degrees in the backbone Q .*

Proof. Suppose, that $1 \leq s < k < h \leq r$ with $\deg_T(u_s) > \deg_T(u_k) < \deg_T(u_h)$. By choosing s and h so that $h - s$ is as small as possible, we can assume that $\deg_T(u_t) = \deg_T(u_k)$ for all $s < t < h$. Let C be a connected component of $T - u_s u_{s+1}$ that contains u_s and let D be a connected component of $T - u_{h-1} u_h$ that contains u_h . Similarly, let H be a connected component of $T - u_{k-1} u_k$ that contains u_{k-1} and F be a connected component of $T - u_k u_{k+1}$ that contains u_{k+1} . By construction, C is a subgraph of H and D is a subgraph of F , so

$$|C| \leq |H| \quad \text{and} \quad |D| \leq |F|. \quad (4.1)$$

Now, by applying Claim (i), to u_s and u_{s+1} and then to u_{h-1} and u_h we deduce that

$$|C| > |F| \quad \text{and} \quad |H| < |D|. \quad (4.2)$$

We have strict inequalities because $s + 1 < k + 1$ and $h - 1 > k - 1$. Combining (4.1) and (4.2), we have

$$|C| \leq |H| < |D|, \quad \text{implying} \quad |C| < |D|.$$

However, from $|C| > |F| \geq |D|$, we conclude $|C| > |D|$, which is a contradiction.

Now, we are in a good position to prove (ii).

Proof of (ii) By Claim 4.1, any vertex of degree less than Δ must be located at the end of the backbone. If there exists exactly one such vertex, then it is necessarily positioned at one of the two ends of the backbone, and the claim follows trivially. Suppose now that there are exactly two vertices within the backbone whose degrees are strictly less than Δ . Then these vertices must either be adjacent or be positioned at opposite ends of the backbone. In the case where more than two vertices in the backbone have degrees smaller than Δ , at least two of them must be contained within the same end of the backbone and must be adjacent. In the rest of this proof, we show that it is impossible to have two vertices of degree smaller than Δ on one end of the backbone and that are neighbours.

Now, suppose there exist two vertices u_{r-1} and u_r at the end of the backbone and are neighbors such that $\deg_T(u_{r-1}) < \Delta$ and $\deg_T(u_r) < \Delta$. Let A be the connected component of $T - u_{r-1}u_r$ that contains u_{r-1} , and B be the connected component of $T - u_{r-1}u_r$ that contains u_r . Let $S_1 : u_r, w_1, w_2, \dots, w_s$ be a pendant segment and let $B' = B - S_1$. By swapping the labels A and B if needed, we can assume that $|A| \geq |B|$.

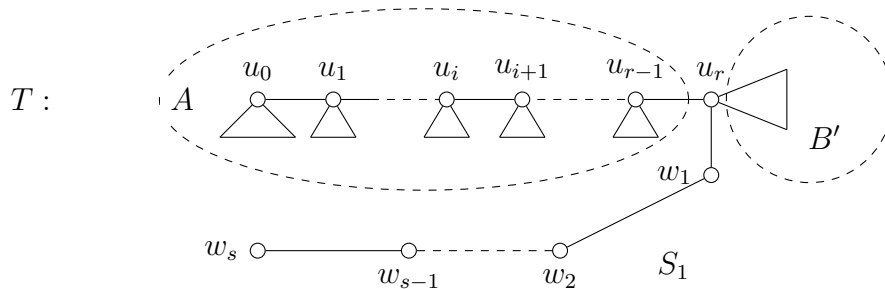


Figure 4.11: The tree T in the proof of Lemma 4.4 (ii)

The Wiener index of T is given by

$$\begin{aligned} W(T) &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(B')} d_T(u,v) + \sum_{u,v \in V(S_1)} d_T(u,v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(B')}} d_T(u,v) + \sum_{\substack{u \in V(B') \\ v \in V(S_1)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(S_1)}} d_T(u,v). \end{aligned}$$

Let $T' = T - u_r w_1 + w_1 u_{r-1}$.

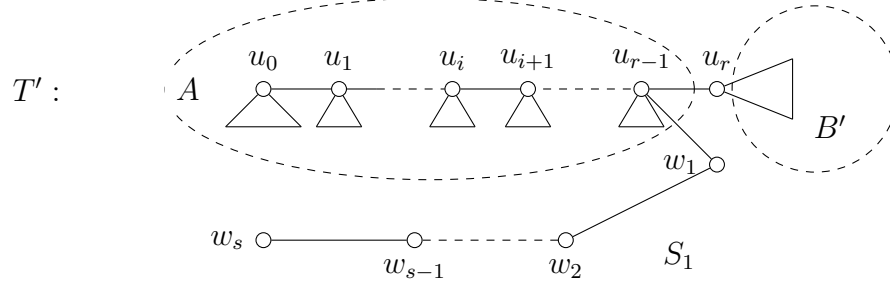


Figure 4.12: The tree T' in the proof of Lemma 4.4 (ii)

Since $\deg(u_{r-1}) < \Delta$, T' still has a maximum degree Δ . Thus, the Wiener index is given by

$$\begin{aligned} W(T') &= \sum_{u,v \in V(A)} d_{T'}(u,v) + \sum_{u,v \in V(B')} d_{T'}(u,v) + \sum_{u,v \in V(S_1)} d_{T'}(u,v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(B')}} d_{T'}(u,v) + \sum_{\substack{u \in V(B') \\ v \in V(S_1)}} d_{T'}(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(S_1)}} d_{T'}(u,v) \\ &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(B')} d_T(u,v) + \sum_{u,v \in V(S_1)} d_T(u,v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(B')}} d_T(u,v) + \sum_{\substack{u \in V(B') \\ v \in V(S_1)}} [d_T(u,v) + 1] + \sum_{\substack{u \in V(A) \\ v \in V(S_1)}} [d_T(u,v) - 1] \\ &= W(T) - |A||S_1| + |B'||S_1| \\ &= W(T) - |S_1|(|A| - |B'|) \\ &< W(T). \end{aligned}$$

Since B' is a proper subgraph of B , it follows that $|B'| < |B|$. Furthermore, by the above assumption $|A| \geq |B|$, it follows that $|A| > |B'|$, which implies that $W(T') < W(T)$. However, this contradicts the minimality of T . \square

Lemma 4.5 *Let T be a caterpillar-like tree of order n with maximum degree Δ , whose backbone is given by $Q = u_0, u_1, \dots, u_r$. If T has minimum Wiener index, then at most one vertex has degree less than Δ .*

Proof. By Lemma 4.4, we already know that the number of vertices of degree less than Δ it is at most 2. Thus, it remains to rigorously prove that it cannot be 2.

Suppose, to the contrary, that T has minimum Wiener index and the number of vertices in T with degree less than Δ is 2. That is, let u_0 and u_r be two such vertices satisfying $\deg_T(u_0) < \Delta$ and $\deg_T(u_r) < \Delta$. Let K be a pendent segment attached to u_r . Let B be the connected component of $T - u_r u_{r-1}$ that contain u_r and A the connected component of $T - u_0 u_1$ that contain u_0 . Furthermore, let $B' = B - K$ and $C = T - A - B$. Without loss of generality, we can assume that $|B| \leq |A|$ and hence $|B'| < |A|$.

Without any loss of generality, we may assume that $D_C(u_0) \leq D_C(u_r)$, where $D_C(x) = \sum_{v \in C} d_T(x, v)$. The Wiener index of T is given by,

$$\begin{aligned} W(T) &= \sum_{u,v \in V(A)} d_T(u, v) + \sum_{u,v \in V(B')} d_T(u, v) + \sum_{u,v \in V(C)} d_T(u, v) \\ &+ \sum_{u,v \in V(K)} d_T(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(B')}} d_T(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(C)}} d_T(u, v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(K)}} d_T(u, v) + \sum_{\substack{u \in V(B') \\ v \in V(C)}} d_T(u, v) + \sum_{\substack{u \in V(B') \\ v \in V(K)}} d_T(u, v) \end{aligned}$$

$$+ \sum_{\substack{u \in V(C) \\ v \in V(K)}} d_T(u, v).$$

Let T' be a tree obtained from T by removing K from u_r and adding it to u_0 . Note that T' is still a caterpillar-like tree with maximum degree Δ . The Wiener index is therefore given by

$$\begin{aligned} W(T') &= \sum_{u, v \in V(A)} d_{T'}(u, v) + \sum_{u, v \in V(B')} d_{T'}(u, v) + \sum_{u, v \in V(C)} d_{T'}(u, v) \\ &+ \sum_{u, v \in V(K)} d_{T'}(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(B')}} d_{T'}(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(C)}} d_{T'}(u, v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(K)}} d_{T'}(u, v) + \sum_{\substack{u \in V(B') \\ v \in V(C)}} d_{T'}(u, v) + \sum_{\substack{u \in V(B') \\ v \in V(K)}} d_{T'}(u, v) \\ &+ \sum_{\substack{u \in V(C) \\ v \in V(K)}} d_{T'}(u, v) \\ &= \sum_{u, v \in V(A)} d_T(u, v) + \sum_{u, v \in V(B')} d_T(u, v) + \sum_{u, v \in V(C)} d_T(u, v) \\ &+ \sum_{u, v \in V(K)} d_T(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(B')}} d_T(u, v) + \sum_{\substack{u \in V(A) \\ v \in V(C)}} d_T(u, v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(K)}} [d_T(u, v) + d_T(u, u_0) - d_T(u, u_r)] + \sum_{\substack{u \in V(B') \\ v \in V(C)}} d_T(u, v) \\ &+ \sum_{\substack{u \in V(B') \\ v \in V(K)}} [d_T(u, v) + d_T(u, u_0) - d_T(u, u_r)] \\ &+ \sum_{\substack{u \in V(C) \\ v \in V(K)}} [d_T(u, v) + d_T(u, u_0) - d_T(u, u_r)] \\ &= W(T) + |K|(D_A(u_0) - D_A(u_0) - r|A|) \\ &+ |K|(D_{B'}(u_r) + r|B'| - D_{B'}(u_r)) + |K|(D_C(u_0) - D_C(u_r)) \\ &= W(T) + |K|(-r|A| + r|B'| + D_C(u_0) - D_C(u_r)) \\ &\leq W(T) - r|K|(|A| - |B'|) \end{aligned}$$

$$< W(T).$$

Since $|K| > 0$, $|A| > |B'|$ and $D_C(u_0) \leq D_C(u_r)$. \square

Lemma 4.6 *Let T be a caterpillar-like tree with maximum degree $\Delta \geq 3$, and let $Q = u_0, u_1, \dots, u_{r-1}, u_r$ be the backbone of T . If T has minimum Wiener index, then the sequence of total lengths of pendant segments $s_{i,1}, \dots, s_{i,s_i}$ attached at each backbone vertex u_i , denoted*

$$L_i = \sum_{j=1}^{s_i} |S_{i,j}| \quad (0 \leq i \leq r)$$

forms a unimodal sequence. That is, there exists an index $m \in [0, r]$ such that

$$L_0 \leq L_1 \leq \dots \leq L_m \geq \dots \geq L_r.$$

Proof. Let T be a caterpillar-like tree with maximum degree $\Delta \geq 3$, and let $Q : u_0, u_1, \dots, u_r$ denote the backbone of T . Suppose, to the contrary, that the sequence (L_0, L_1, \dots, L_r) is not unimodal. Then there exist indices $0 \leq i_0 < i < i_1 \leq r$ such that

$$L_{i_0} > L_{i_0+1} \quad \text{and} \quad L_{i_1-1} < L_{i_1}. \quad \text{Note that } i_1 - 1 > i_0. \quad (4.3)$$

By Lemma 4.5, we know that $\deg_T(u_{i_0+1}) = \Delta = \deg_T(u_{i_1-1})$. So, condition (4.3) implies that there is a pendant segment S_{i_0} attached at u_{i_0} and a pendant segment at S_{i_0+1} at u_{i_0+1} with $l = |S_{i_0}| = |S_{i_0+1}| + 1$. Let x be a leaf end of the pendant segment S_{i_0} . Let A_{i_0} be a connected component of $T - u_{i_0}u_{i_0+1}$ that contains u_{i_0} and $B_{i_0} = T - A_{i_0}$. Furthermore, let $A'_{i_0} = A_{i_0} - S_{i_0}$ and $B'_{i_0} = B_{i_0} - S_{i_0+1}$. The Wiener index is given by

$$\begin{aligned} W(T) = & \sum_{u,v \in V(A'_{i_0})} d_T(u,v) + \sum_{u,v \in V(B'_{i_0})} d_T(u,v) + \sum_{u,v \in V(S_{i_0} \cup S_{i_0+1}) \setminus \{x\}} d_T(u,v) \\ & + \sum_{\substack{u \in V(A'_{i_0}) \\ v \in V(B'_{i_0})}} d_T(u,v) + \sum_{\substack{u \in V(A'_{i_0}) \\ v \in V(S_{i_0} \cup S_{i_0+1}) \setminus \{x\}}} d_T(u,v) \end{aligned}$$

$$\begin{aligned}
 & + \sum_{\substack{u \in V(B'_{i_0}) \\ v \in V(S_{i_0} \cup S_{i_0+1}) \setminus \{x\}}} d_T(u, v) + \sum_{u \in V(A_{i_0})} d_T(u, x) + \sum_{u \in V(B'_{i_0})} d_T(u, x) \\
 & + \sum_{u \in V(S_{i_0} \cup S_{i_0+1}) \setminus \{x\}} d_T(u, x).
 \end{aligned}$$

Let T' be a tree obtained by removing x from u_{i_0} and adding it to the leaf end of S_{i_0+1} . Note that T' is still a caterpillar-like tree with maximum degree. The Wiener index of T' , is therefore given by

$$\begin{aligned}
 W(T') &= \sum_{u, v \in V(A'_{i_0})} d_{T'}(u, v) + \sum_{u, v \in V(B'_{i_0})} d_{T'}(u, v) + \sum_{u, v \in V(S_{i_0} \cup S_{i_0+1}) \setminus \{x\}} d_{T'}(u, v) \\
 &+ \sum_{\substack{u \in V(A'_{i_0}) \\ v \in V(B'_{i_0})}} d_{T'}(u, v) + \sum_{\substack{u \in V(A'_{i_0}) \\ v \in V(S_{i_0} \cup S_{i_0+1}) \setminus \{x\}}} d_{T'}(u, v) \\
 &+ \sum_{\substack{u \in V(B'_{i_0}) \\ v \in V(S_{i_0} \cup S_{i_0+1}) \setminus \{x\}}} d_{T'}(u, v) + \sum_{u \in V(A'_{i_0})} d_{T'}(u, x) + \sum_{u \in V(B'_{i_0})} d_{T'}(u, x) \\
 &+ \sum_{u \in V(S_{i_0} \cup S_{i_0+1}) \setminus \{x\}} d_{T'}(u, x) \\
 &= \sum_{u, v \in V(A'_{i_0})} d_T(u, v) + \sum_{u, v \in V(B'_{i_0})} d_T(u, v) + \sum_{u, v \in V(S_{i_0} \cup S_{i_0+1}) \setminus \{x\}} d_T(u, v) \\
 &+ \sum_{\substack{u \in V(A'_{i_0}) \\ v \in V(B'_{i_0})}} d_T(u, v) + \sum_{\substack{u \in V(A_{i_0}) \\ v \in V(S_{i_0} \cup S_{i_0+1}) \setminus \{x\}}} d_T(u, v) \\
 &+ \sum_{\substack{u \in V(B'_{i_0}) \\ v \in V(S_{i_0} \cup S_{i_0+1}) \setminus \{x\}}} d_T(u, v) + \sum_{u \in V(A'_{i_0})} [d_T(u, x) + 1] \\
 &+ \sum_{u \in V(B'_{i_0})} [d_T(u, x) - 1] + \sum_{u \in V(S_{i_0} \cup S_{i_0+1}) \setminus \{x\}} d_T(u, x) \\
 &= W(T) - |B'_{i_0}| + |A'_{i_0}| \\
 &= W(T) + (|A'_{i_0}| - |B'_{i_0}|).
 \end{aligned}$$

If $|A'_{i_0}| < |B'_{i_0}|$, then $W(T') < W(T)$, contradicting the minimality of T . Therefore, we must have $|A'_{i_0}| \geq |B'_{i_0}|$.

Similarly, condition 4.3 implies that there is a pendant segment S_{i_1-1} attached at u_{i_1-1} and a pendant segment S_{i_1} at u_{i_1} with $|S_{i_1}| = |S_{i_1-1}| + 1$. Let y be a leaf end of the pendant segment S_{i_1} . Let A_{i_1-1} be a connected component of $T - u_{i_1-1}u_{i_1}$ that contains u_{i_1-1} and $B_{i_1-1} = T - A_{i_1-1}$. Furthermore, let $A'_{i_1-1} = A_{i_1-1} - S_{i_1-1}$ and $B'_{i_1-1} = B_{i_1-1} - S_{i_1}$. The Wiener index is given by

$$\begin{aligned}
 W(T) &= \sum_{u,v \in V(A'_{i_1-1})} d_T(u,v) + \sum_{u,v \in V(B'_{i_1-1})} d_T(u,v) \\
 &+ \sum_{u,v \in V(S_{i_1} \cup S_{i_1-1}) \setminus \{y\}} d_T(u,v) + \sum_{\substack{u \in V(A'_{i_1-1}) \\ v \in V(B'_{i_1-1})}} d_T(u,v) \\
 &+ \sum_{\substack{u \in V(A'_{i_1-1}) \\ v \in V(S_{i_1} \cup S_{i_1-1}) \setminus \{y\}}} d_T(u,v) + \sum_{\substack{u \in V(B_{i_1-1}) \\ v \in V(S_{i_1} \cup S_{i_1-1}) \setminus \{y\}}} d_T(u,v) \\
 &+ \sum_{u \in V(A'_{i_1-1})} d_T(u,y) + \sum_{u \in V(B'_{i_1-1})} d_T(u,y) \\
 &+ \sum_{u \in V(S_{i_1} \cup S_{i_1-1}) \setminus \{y\}} d_T(u,y).
 \end{aligned}$$

Let T'' be a tree obtained by removing y from u_{i_1} and adding it to the leaf end of S_{i_1-1} . Note that T'' is still a caterpillar-like tree with maximum degree. The Wiener index of T'' , is therefore given by

$$\begin{aligned}
 W(T'') &= \sum_{u,v \in V(A'_{i_1-1})} d_{T''}(u,v) + \sum_{u,v \in V(B'_{i_1-1})} d_{T''}(u,v) \\
 &+ \sum_{u,v \in V(S_{i_1} \cup S_{i_1-1}) \setminus \{y\}} d_{T''}(u,v) + \sum_{\substack{u \in V(A'_{i_1-1}) \\ v \in V(B'_{i_1-1})}} d_{T''}(u,v) \\
 &+ \sum_{\substack{u \in V(A'_{i_1-1}) \\ v \in V(S_{i_1} \cup S_{i_1-1}) \setminus \{y\}}} d_{T''}(u,v) + \sum_{\substack{u \in V(B_{i_1-1}) \\ v \in V(S_{i_1} \cup S_{i_1-1}) \setminus \{y\}}} d_{T''}(u,v) \\
 &+ \sum_{u \in V(A'_{i_1-1})} d_{T''}(u,y) + \sum_{u \in V(B'_{i_1-1})} d_{T''}(u,y) \\
 &+ \sum_{u \in V(S_{i_1} \cup S_{i_1-1}) \setminus \{y\}} d_{T''}(u,y)
 \end{aligned}$$

$$\begin{aligned}
&= \sum_{u,v \in V(A'_{i_1-1})} d_T(u,v) + \sum_{u,v \in V(B'_{i_1-1})} d_T(u,v) \\
&+ \sum_{u,v \in V(S_{i_1} \cup S_{i_1-1}) \setminus \{y\}} d_T(u,v) + \sum_{\substack{u \in V(A'_{i_1-1}) \\ v \in V(B'_{i_1-1})}} d_T(u,v) \\
&+ \sum_{\substack{u \in V(A'_{i_1-1}) \\ v \in V(S_{i_1} \cup S_{i_1-1}) \setminus \{y\}}} d_T(u,v) + \sum_{\substack{u \in V(B_{i_1-1}) \\ v \in V(S_{i_1} \cup S_{i_1-1}) \setminus \{y\}}} d_T(u,v) \\
&+ \sum_{u \in V(A'_{i_1-1})} [d_T(u,y) - 1] + \sum_{u \in V(B'_{i_1-1})} [d_T(u,y) + 1] \\
&+ \sum_{u \in V(S_{i_1} \cup S_{i_1-1}) \setminus \{y\}} d_T(u,y) \\
&= W(T) - |A'_{i_1-1}| + |B'_{i_1-1}| \\
&= W(T) + (|B'_{i_1-1}| - |A'_{i_1-1}|).
\end{aligned}$$

If $|B'_{i_1-1}| < |A'_{i_1-1}|$, then $W(T'') < W(T)$, contradicting the minimality of T . Therefore, we must have $|B'_{i_1-1}| \geq |A'_{i_1-1}|$.

However, since A'_{i_0} is a proper subgraph of A'_{i_1-1} and B'_{i_1-1} is a proper subgraph of B'_{i_0} , we have

$$|B'_{i_1-1}| \geq |A'_{i_1-1}| > |A'_{i_0}| \geq |B'_{i_0}| > |B'_{i_1-1}|$$

which is a contradiction. Therefore, our assumption that the sequence (L_0, L_1, \dots, L_r) is not unimodal is false. Hence, the sequence (L_0, L_1, \dots, L_r) is unimodal. \square

In the next lemma we show that in a minimum caterpillar-like tree, once the degree of an end of a backbone is less than Δ , then all segments attached to it has length at most 1.

Lemma 4.7 *Let T be a caterpillar-like tree of order n with maximum degree Δ , whose backbone is given by $Q = u_0, u_1, \dots, u_r$ and let $S_1 : u_1, w_1, w_2, \dots, w_s$ be a pendent segment attached to u_1 . If T has minimum Wiener index and $\deg_T(u_0) < \Delta$, then $s \leq 1$.*

Proof. Let T be a caterpillar-like tree of order n with maximum degree Δ , whose backbone is given by $Q = u_0, u_1, \dots, u_r$ and let $S_1 : u_1, w_1, w_2, \dots, w_s$ be a pendent segment attached to u_1 . Suppose, to the contrary, that T has minimum Wiener index, $\deg_T(u_0) < \Delta$ but u_1 has a pendent segment of length $s \geq 2$. Let A be a connected component of $T - u_0u_1$ containing u_1 and let B be a connected component of $T - u_0u_1$ containing u_0 . Furthermore, let $A' = A - S_1$.

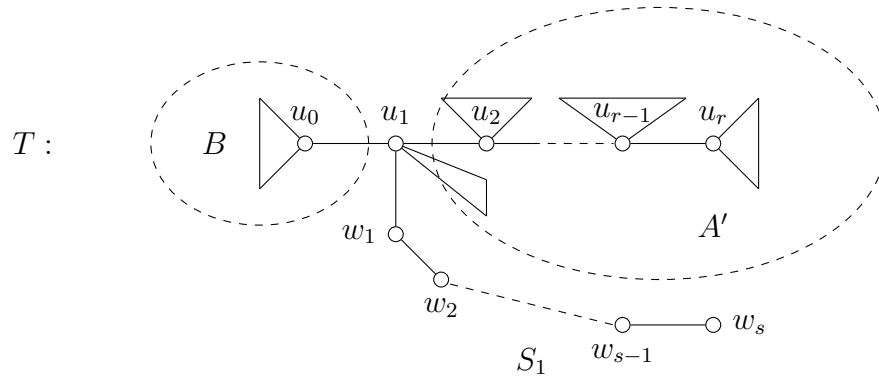


Figure 4.13: The tree T in the proof of Lemma 4.7

The Wiener index of T is given by

$$\begin{aligned}
 W(T) = & \sum_{u,v \in V(A')} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) + \sum_{u,v \in V(S_1) \setminus \{w_s\}} d_T(u,v) \\
 & + \sum_{\substack{u \in V(A') \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(A') \\ v \in V(S_1) \setminus \{w_s\}}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(S_1) \setminus \{w_s\}}} d_T(u,v) \\
 & + \sum_{u \in V(A')} d_T(u, w_s) + \sum_{u \in V(B)} d_T(u, w_s) + \sum_{u \in V(S_1) \setminus \{w_s\}} d_T(u, w_s).
 \end{aligned}$$

Let $T' = T - w_{s-1}w_s + w_su_0$.

Note that T' is a caterpillar-like tree with maximum degree Δ . Its Wiener index is given by,

$$W(T') = \sum_{u,v \in V(A')} d_{T'}(u,v) + \sum_{u,v \in V(B)} d_{T'}(u,v) + \sum_{u,v \in V(S_1) \setminus \{w_s\}} d_{T'}(u,v)$$

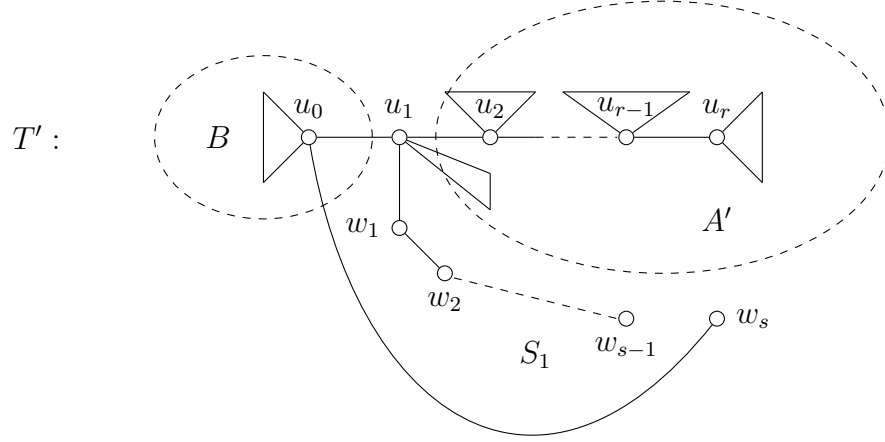


Figure 4.14: The tree T' in the proof of Lemma 4.7

$$\begin{aligned}
 & + \sum_{\substack{u \in V(A') \\ v \in V(B)}} d_{T'}(u, v) + \sum_{\substack{u \in V(A') \\ v \in V(S_1) \setminus \{w_s\}}} d_{T'}(u, v) + \sum_{\substack{u \in V(B) \\ v \in V(S_1) \setminus \{w_s\}}} d_{T'}(u, v) \\
 & + \sum_{u \in V(A')} d_{T'}(u, w_s) + \sum_{u \in V(B)} d_{T'}(u, w_s) + \sum_{u \in V(S_1) \setminus \{w_s\}} d_{T'}(u, w_s) \\
 & = \sum_{u, v \in V(A')} d_T(u, v) + \sum_{u, v \in V(B)} d_T(u, v) + \sum_{u, v \in V(S_1) \setminus \{w_s\}} d_T(u, v) \\
 & + \sum_{\substack{u \in V(A') \\ v \in V(B)}} d_T(u, v) + \sum_{\substack{u \in V(A') \\ v \in V(S_1) \setminus \{w_s\}}} d_T(u, v) + \sum_{\substack{u \in V(B) \\ v \in V(S_1) \setminus \{w_s\}}} d_T(u, v) \\
 & + \sum_{u \in V(A')} [d_T(u, w_s) - (s - 2)] + \sum_{u \in V(B)} [d_T(u, w_s) - s] \\
 & + \sum_{u \in V(S_1) \setminus \{w_s\}} [d_T(u, w_s) + 1] \\
 & = W(T) - [(s - 2)|A'| + s|B| - |S_1 \setminus \{w_s\}|].
 \end{aligned}$$

Since $s \geq 2$, then $(s - 2)|A'| + s|B| - |S_1 \setminus \{w_s\}| > 0$, implying that $W(T') < W(T)$. This contradicts the assumption that T has the minimum Wiener index. \square

Lemma 4.8 *Let T be a caterpillar-like tree of order n with maximum degree $\Delta \geq 3$, whose backbone is given by u_0, u_1, \dots, u_r . Let $S_1 = u_{s_0}, w_1, w_2, \dots, w_{t-1}, w_t$ be a pendant segment attached to u_{s_0} for some $s_0 < r$. Let A_{s_0} be the connected component of $T - u_{s_0}u_{s_0+1}$ that contains u_{s_0} . If T has minimum Wiener index, then $|A_{s_0} - S| + 1 \geq |S_1|$.*

Proof. Let T be a caterpillar-like tree of order n with maximum degree $\Delta \geq 3$, whose backbone is given by u_0, u_1, \dots, u_r . Let $S_1 = u_{s_0}, w_1, w_2, \dots, w_{t-1}, w_t$ be a pendant segment attached to u_{s_0} . Let A_{s_0} be the connected component of $T - u_{s_0}u_{s_0+1}$ that contains u_{s_0} . Let $A'_{s_0} = A_{s_0} - S_1$. We now consider two cases.

Case I: Suppose A'_{s_0} contains at least two segments of T , say Q and R , each contains the backbone vertex u_{s_0} . Now, assume for contradiction that $|A'_{s_0}| + 1 < |S_1|$. This implies

$$|Q| < |S_1| \quad \text{and} \quad |R| < |S_1|.$$

Thus, by Lemma 4.2, we have

$$|S_1| = |Q| + 1 \quad \text{and} \quad |S_1| = |R| + 1, \quad \text{thus } |Q| = |R|.$$

Since Q and R are pendant segments in A'_{s_0} , we have

$$|A'_{s_0}| \geq |Q| + |R| - 1.$$

Then,

$$|A'_{s_0}| + 1 \geq |Q| + |R| = 2|R|. \quad (4.4)$$

However, by our assumption, we have

$$|A'_{s_0}| + 1 < |S_1| = |R| + 1. \quad (4.5)$$

By combining (4.4) and (4.5), we get

$$2|R| \leq |A'_{s_0}| + 1 < |R| + 1,$$

which implies $2|R| < |R| + 1$. However we reach a contradiction since $|R| \geq 2$. Thus, the inequality must hold.

Case II: Suppose A'_{s_0} is a segment. By Lemma 4.2, we have

$$||A'_{s_0}| - |S_1|| \leq 1.$$

This implies

$$-1 \leq |A'_{s_0}| - |S_1| \quad \text{and thus} \quad |S_1| \leq |A'_{s_0}| + 1.$$

Hence

$$|A_{s_0} - S_1| + 1 = |A'_{s_0}| + 1 \geq |S_1|$$

as required. In both cases, the inequality holds. This completes the proof. \square

Lemma 4.9 *Let T be a caterpillar-like tree of order n with maximum degree $\Delta \geq 3$, whose backbone is given by $Q = u_0, u_1, \dots, u_r$. Let s_0 be an integer such that $0 < s_0 \leq r - 2$, and let $s_1 = s_0 - 1$. Let A_{s_0} be the connected component of $T - u_{s_0}u_{s_0+1}$ that contains u_{s_0} , and let B_{s_0+1} be the connected component of $T - \{u_{s_0}u_{s_0+1}, u_{s_0+1}u_{s_0+2}\}$ that contains u_{s_0+1} . Furthermore, let $C_{s_0+2} = T - A_{s_0} - B_{s_0+1}$.*

If T has minimum Wiener index, and the inequality

$$3|A_{s_0} - S_1| + |B_{s_0+1}| < |C_{s_0+2} - S_3|$$

holds for some pendant segments S_1 and S_3 attached to u_{s_0} and u_{s_0+2} , respectively, then it follows that

$$3|A_{s_1} - S'_1| + |B_{s_1+1}| < |C_{s_1+2} - S'_3|$$

for some pendant segments S'_1 and S'_3 attached to u_{s_1} and u_{s_1+2} , respectively.

Proof. Let T be a caterpillar-like tree with order n and maximum degree $\Delta \geq 3$, whose backbone is given by $Q = u_0, u_1, \dots, u_r$. Suppose, that T has minimum Wiener index and

$$3|A_{s_0} - S_1| + |B_{s_0+1}| < |C_{s_0+2} - S_3|$$

for some S_1 and S_3 attached to u_{s_0} and u_{s_0+2} respectively. We note that $|A_{s_0}| < 3|A_{s_0} - S_1| + |B_{s_0+1}|$, which implies, in particular, that

$|A_{s_0}| \leq |C_{s_0+2}|$. We are now going to prove this, in the following cases.

Case I: Suppose that $|S_1| \leq |B_{s_0+1}|$. Then,

$$\begin{aligned} 3|A_{s_0} - S_1| + |B_{s_0+1}| &= 3|A_{s_0}| - 3|S_1| + |B_{s_0+1}| \\ &= |A_{s_0}| + 2|A_{s_0}| - 3|S_1| + |B_{s_0+1}|. \end{aligned}$$

Since $|S_1| \leq |B_{s_0+1}|$, then it follows that

$$\begin{aligned} 3|A_{s_0} - S_1| + |B_{s_0+1}| &= |A_{s_0}| + 2|A_{s_0}| - 3|S_1| + |B_{s_0+1}| \\ &\geq |A_{s_0}| + 2|A_{s_0}| - 3|S_1| + |S_1| \\ &\geq |A_{s_0}| + 2|A_{s_0}| - 2|S_1| \\ &> 2(|A_{s_0}| - |S_1|) \\ &= |A_{s_0}| - |S_1| + |A_{s_0}| - |S_1|. \end{aligned}$$

From Lemma 4.8, we know that $|A_{s_0}| - |S_1| + 1 \geq |S_1|$, hence:

$$\begin{aligned} 3|A_{s_0} - S_1| + |B_{s_0+1}| &\geq |A_{s_0}| - |S_1| + |S_1| - 1 \\ &= |A_{s_0}| - 1. \end{aligned}$$

So,

$$|A_{s_0}| - 1 \leq 3|A_{s_0} - S_1| + |B_{s_0+1}| < |C_{s_0+2} - S_3|.$$

Thus

$$|A_{s_0}| \leq |C_{s_0+2} - S_3| < |C_{s_0+2}|.$$

Case II: Suppose that $|S_1| > |B_{s_0+1}|$. We will need the following claim.

Claim 4.2 B_{s_0+1} is a single segment.

Proof. If B_{s_0+1} has at least 2 segments, say Q and R , then $B_{s_0+1} \geq |Q| + |R| - 1$. Then by Lemma 4.2,

$$|S_1| - |Q| \leq 1 \quad \text{and} \quad |S_1| - |R| \leq 1.$$

Since $|Q|$ and $|R|$ are segments in B_{s_0+1} , and each contains at least one vertex, we have

$$\begin{aligned} 2S_1 - (|Q| + |R|) &\leq 2 && \Rightarrow 2S_1 \leq 2 + |Q| + |R| \\ & && \Rightarrow 2S_1 \leq B_{s_0+1} + 3 \\ & && \Rightarrow S_1 \leq \frac{B_{s_0+1} + 3}{2}. \end{aligned}$$

Since $|B_{s_0+1}| < |S_1|$,

$$\begin{aligned} S_1 + B_{s_0+1} &< S_1 + \frac{B_{s_0+1} + 3}{2} && \Rightarrow B_{s_0+1} < \frac{B_{s_0+1} + 3}{2} \\ & && \Rightarrow 2B_{s_0+1} < B_{s_0+1} + 3 \\ & && \Rightarrow 3B_{s_0+1} < 3 \\ & && \Rightarrow B_{s_0+1} < 1. \end{aligned}$$

Thus, we reach a contradiction since $B_{s_0+1} \geq |Q| + |R| - 1 \geq 3$. \square .

Now, we are proceeding proving the case. If $|S_1| > |B_{s_0+1}|$, then $|S_1| = |B_{s_0+1}| + 1$. So,

$$\begin{aligned} 3|A_{s_0} - S_1| + |B_{s_0+1}| &= 3|A_{s_0}| - 3|S_1| + |B_{s_0+1}| \\ &= 3|A_{s_0}| - 3(|B_{s_0+1}| + 1) + |B_{s_0+1}| \\ &= 3|A_{s_0}| - 2|B_{s_0+1}| - 3 \\ &= |A_{s_0}| + 2|A_{s_0}| - 2|B_{s_0+1}| - 3 \\ &= |A_{s_0}| + 2(|A_{s_0}| - |B_{s_0+1}|) - 3. \end{aligned}$$

Since S_1 is inside A_{s_0} ,

$$\begin{aligned} 3|A_{s_0} - S_1| + |B_{s_0+1}| &\geq |A_{s_0}| + 2(|S_1| - |B_{s_0+1}|) - 3 \\ &= |A_{s_0}| + 2(|B_{s_0+1}| + 1 - |B_{s_0+1}|) - 3 \\ &= |A_{s_0}| + 2 - 3 \\ &= |A_{s_0}| - 1. \end{aligned}$$

So,

$$|A_{s_0}| - 1 \leq 3|A_{s_0} - S_1| + |B_{s_0+1}| < |C_{s_0+2} - S_3|.$$

Thus,

$$|A_{s_0}| \leq |C_{s_0+2} - S_3| < |C_{s_0+2}|.$$

Now, let us continue with the lemma.

Since $A_{s_1} - S'_1$ is a subset of $A_{s_0} - S_1$, see Figure 4.15.

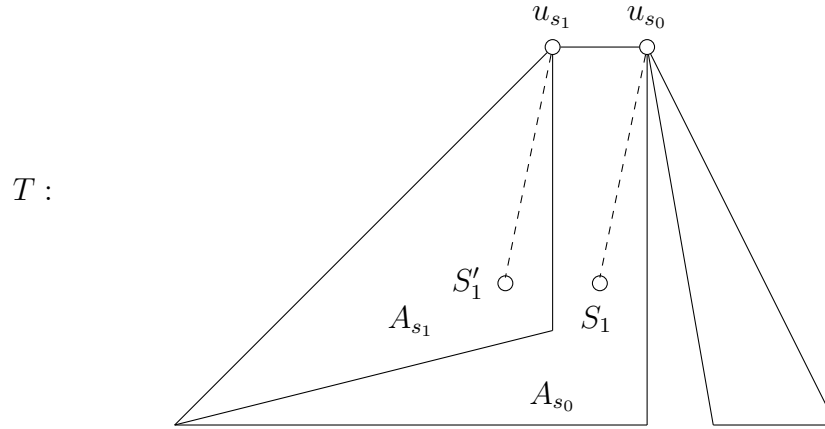


Figure 4.15: Decomposition of the tree T in the proof of Lemma 4.9

Then, it follows that

$$\begin{aligned} 3|A_{s_1} - S'_1| + |B_{s_1+1}| &< 3|A_{s_0} - S_1| + |B_{s_0+1}| \\ &< |C_{s_0+2} - S_3| \\ &< |C_{s_1+2} - S'_3|. \end{aligned}$$

Thus, we have

$$3|A_{s_1} - S'_1| + |B_{s_1+1}| < |C_{s_1+2} - S'_3|,$$

which completes the proof. \square

Lemma 4.10 *Let T be a caterpillar-like tree of order n with maximum degree $\Delta \geq 3$, whose backbone is given by $Q = u_0, u_1, \dots, u_r$ for some $s \leq r - 2$. Let A_s be the connected component of $T - u_s u_{s+1}$ that contains u_s , and let B_{s+1} be the connected component*

of $T - \{u_s u_{s+1}, u_{s+1} u_{s+2}\}$ that contains u_{s+1} . Furthermore, let $C_{s+2} = T - A_s - B_{s+1}$.

Let $S_s = \{u_s, u_{1,0}, u_{2,0}, \dots, u_{l,0}\}$ and $S_{s+2} = \{u_{s+2}, w_{1,0}, w_{2,0}, \dots, w_{l',0}\}$ be pendant segments attached to u_s and u_{s+2} , respectively. If T has minimum Wiener index, and s_0 is the largest integer, such that, the inequality

$$3|A_{s_0} - S_{s_0}| + |B_{s_0+1}| < |C_{s_0+2} - S_{s_0+2}|,$$

holds. Then it follows that

$$3|A_{s_0+2} - S_{s_0+2}| + |B_{s_0+3}| > |C_{s_0+4} - S_{s_0+4}|$$

for some pendant segments S_{s_0+2} and S_{s_0+4} .

Proof. Let T be a caterpillar-like tree of order n with maximum degree $\Delta \geq 3$, whose backbone is given by $Q = u_0, u_1, \dots, u_r$. Let A_s, B_{s+1} and C_{s+2} be as stated in the statement of the Lemma. Also, let the three pendent segments S_s and S_{s+2} be as stated in the statement of the Lemma. Now, suppose, to the contrary, that T has minimum Wiener index and $3|A_{s_0+2} - S_{s_0+2}| + |B_{s_0+3}| \leq |C_{s_0+4} - S_{s_0+4}|$ for some pendant segments S_{s_0+2} and S_{s_0+4} . Thus, the inequality also holds for $s_0 + 2$. However, this contradicts our assumption that s_0 is the largest integer for which the inequality holds and hence it must be of the case $3|A_{s_0+2} - S_{s_0+2}| + |B_{s_0+3}| > |C_{s_0+4} - S_{s_0+4}|$. \square

Lemma 4.11 *Let T be a caterpillar-like tree of order n with maximum degree $\Delta \geq 3$, with backbone $Q = u_0, u_1, \dots, u_r$ and some $s \leq r - 2$. Let A_s be the connected component of $T - u_s u_{s+1}$ that contains u_s , and let B_{s+1} be the connected component of $T - \{u_s u_{s+1}, u_{s+1} u_{s+2}\}$ that contains u_{s+1} . Furthermore, let $C_{s+2} = T - A_s - B_{s+1}$.*

Let $S_s = \{u_s, u_{1,0}, u_{2,0}, \dots, u_{l,0}\}$ and $S_{s+2} = \{u_{s+2}, w_{1,0}, w_{2,0}, \dots, w_{l',0}\}$ be pendant segments attached to u_s and u_{s+2} respectively. Suppose s_0 is the largest integer satisfying the structural condition

$$|C_{s_0+2} - S_{s_0+2}| > |B_{s_0+1}| + 3|A_{s_0} - S_{s_0}|.$$

Let l_0 be the smallest integer such that for some segments S_{l_0} and S_{l_0-2} attached to u_{l_0} and u_{l_0-2} we have

$$3|C_{l_0} - S_{l_0}| + |B_{l_0-1}| < |A_{l_0-2} - S_{l_0-2}|.$$

If T has minimum Wiener index among all caterpillar-like trees of order n and maximum degree Δ , then the following hold:

- (i) There do not exist three consecutive backbone vertices to which S_{s_0} , B_{s_0+1} , and S_{s_0+2} of equal length are attached within A_{s_0+2} or within $T - A_{l_0-3}$.
- (ii) There do not exist three consecutive backbone vertices to which segments S_{s_0} , B_{s_0+1} , and S_{s_0+2} have lengths $l - 1$, l , $l + 1$ in $T - A_{s_0+1} - C_{l_0-1}$.

Proof. Let T be an n -vertex caterpillar-like tree with maximum degree $\Delta \geq 3$, whose backbone is given by $Q = u_0, u_1, \dots, u_r$. Suppose, to the contrary, that T has minimum Wiener index. Furthermore, as shown in the proof of Lemma 4.9, $|C_{s_0+2} - S_{s_0+2}| > |B_{s_0+1}| + 3|A_{s_0} - S_{s_0}|$ imply that $|C_{s_0+2}| > |A_{s_0}|$, hence by Lemma 4.3 it follows that $l'' \geq l$. The Wiener index of T is therefore given by

$$\begin{aligned} W(T) = & \sum_{u,v \in V(A_{s_0} - S_{s_0})} d_T(u, v) + \sum_{u,v \in V(B_{s_0+1})} d_T(u, v) + \sum_{u,v \in V(C_{s_0+2} - S_{s_0+2})} d_T(u, v) \\ & + \sum_{u,v \in V(S_{s_0}) \setminus \{u_{l,0}\}} d_T(u, v) + \sum_{u,v \in V(S_{s_0+2})} d_T(u, v) + \sum_{\substack{u \in V(A_{s_0} - S_{s_0}) \\ v \in V(B_{s_0+1})}} d_T(u, v) \\ & + \sum_{\substack{u \in V(A_{s_0} - S_{s_0}) \\ v \in V(C_{s_0+2} - S_{s_0+2})}} d_T(u, v) + \sum_{\substack{u \in V(B_{s_0+1}) \\ v \in V(C_{s_0+2} - S_{s_0+2})}} d_T(u, v) \\ & + \sum_{\substack{u \in V(S_{s_0}) \setminus \{u_{l,0}\} \\ v \in V(S_{s_0+2})}} d_T(u, v) + \sum_{\substack{u \in V(A_{s_0} - S_{s_0}) \\ v \in V(S_{s_0}) \setminus \{u_{l,0}\}}} d_T(u, v) + \sum_{\substack{u \in V(A_{s_0} - S_{s_0}) \\ v \in V(S_{s_0+2})}} d_T(u, v) \\ & + \sum_{\substack{u \in V(B_{s_0+1}) \\ v \in V(S_{s_0}) \setminus \{u_{l,0}\}}} d_T(u, v) + \sum_{\substack{u \in V(B_{s_0+1}) \\ v \in V(S_{s_0+2})}} d_T(u, v) + \sum_{\substack{u \in V(C_{s_0+2} - S_{s_0+2}) \\ v \in V(S_{s_0}) \setminus \{u_{l,0}\}}} d_T(u, v) \end{aligned}$$

$$\begin{aligned}
 & + \sum_{\substack{u \in V(C_{s_0+2}-S_{s_0+2}) \\ v \in V(S_{s_0+2})}} d_T(u, v) + \sum_{u \in V(A_{s_0}-S_{s_0})} d_T(u, u_{l,0}) \\
 & + \sum_{u \in V(B_{s_0+1})} d_T(u, u_{l,0}) + \sum_{u \in V(C_{s_0+2}-S_{s_0+2})} d_T(u, u_{l,0}) \\
 & + \sum_{u \in V(S_{s_0}) \setminus \{u_{l,0}\}} d_T(u, u_{l,0}) + \sum_{u \in V(S_{s_0+2})} d_T(u, u_{l,0}).
 \end{aligned}$$

Let $T' = T - u_{l-1,0}u_{l,0} + w_{l',0}u_{l,0}$. The tree T' is still a caterpillar-like tree with maximum degree Δ . Its Wiener index is, therefore given by

$$\begin{aligned}
 W(T') & = \sum_{u, v \in V(A_{s_0}-S_{s_0})} d_{T'}(u, v) + \sum_{u, v \in V(B_{s_0+1})} d_{T'}(u, v) + \sum_{u, v \in V(C_{s_0+2}-S_{s_0+2})} d_{T'}(u, v) \\
 & + \sum_{u, v \in V(S_{s_0}) \setminus \{u_{l,0}\}} d_{T'}(u, v) + \sum_{u, v \in V(S_{s_0+2})} d_{T'}(u, v) + \sum_{\substack{u \in V(A_{s_0}-S_{s_0}) \\ v \in V(B_{s_0+1})}} d_{T'}(u, v) \\
 & + \sum_{\substack{u \in V(A_{s_0}-S_{s_0}) \\ v \in V(C_{s_0+2}-S_{s_0+2})}} d_{T'}(u, v) + \sum_{\substack{u \in V(B_{s_0+1}) \\ v \in V(C_{s_0+2}-S_{s_0+2})}} d_{T'}(u, v) \\
 & + \sum_{\substack{u \in V(S_{s_0}) \setminus \{u_{l,0}\} \\ v \in V(S_{s_0+2})}} d_{T'}(u, v) + \sum_{\substack{u \in V(A_{s_0}-S_{s_0}) \\ v \in V(S_{s_0}) \setminus \{u_{l,0}\}}} d_{T'}(u, v) + \sum_{\substack{u \in V(A_{s_0}-S_{s_0}) \\ v \in V(S_{s_0+2})}} d_{T'}(u, v) \\
 & + \sum_{\substack{u \in V(B_{s_0+1}) \\ v \in V(S_{s_0}) \setminus \{u_{l,0}\}}} d_{T'}(u, v) + \sum_{\substack{u \in V(B_{s_0+1}) \\ v \in V(S_{s_0+2})}} d_{T'}(u, v) + \sum_{\substack{u \in V(C_{s_0+2}-S_{s_0+2}) \\ v \in V(S_{s_0}) \setminus \{u_{l,0}\}}} d_{T'}(u, v) \\
 & + \sum_{\substack{u \in V(C_{s_0+2}-S_{s_0+2}) \\ v \in V(S_{s_0+2})}} d_{T'}(u, v) + \sum_{u \in V(A_{s_0}-S_{s_0})} d_{T'}(u, u_{l,0}) \\
 & + \sum_{u \in V(B_{s_0+1})} d_{T'}(u, u_{l,0}) + \sum_{u \in V(C_{s_0+2}-S_{s_0+2})} d_{T'}(u, u_{l,0}) \\
 & + \sum_{u \in V(S_{s_0}) \setminus \{u_{l,0}\}} d_{T'}(u, u_{l,0}) + \sum_{u \in V(S_{s_0+2})} d_{T'}(u, u_{l,0}) \\
 & = \sum_{u, v \in V(A_{s_0}-S_{s_0})} d_T(u, v) + \sum_{u, v \in V(B_{s_0+1})} d_T(u, v) + \sum_{u, v \in V(C_{s_0+2}-S_{s_0+2})} d_T(u, v)
 \end{aligned}$$

$$\begin{aligned}
& + \sum_{u,v \in V(S_{s_0}) \setminus \{u_{l,0}\}} d_T(u,v) + \sum_{u,v \in V(S_{s_0+2})} d_T(u,v) + \sum_{\substack{u \in V(A_{s_0} - S_{s_0}) \\ v \in V(B_{s_0+1})}} d_T(u,v) \\
& + \sum_{\substack{u \in V(A_{s_0} - S_{s_0}) \\ v \in V(C_{s_0+2} - S_{s_0+2})}} d_T(u,v) + \sum_{\substack{u \in V(B_{s_0+1}) \\ v \in V(C_{s_0+2} - S_{s_0+2})}} d_T(u,v) \\
& + \sum_{\substack{u \in V(S_{s_0}) \setminus \{u_{l,0}\} \\ v \in V(S_{s_0+2})}} d_T(u,v) + \sum_{\substack{u \in V(A_{s_0} - S_{s_0}) \\ v \in V(S_{s_0}) \setminus \{u_{l,0}\}}} d_T(u,v) + \sum_{\substack{u \in V(A_{s_0} - S_{s_0}) \\ v \in V(S_{s_0+2})}} d_T(u,v) \\
& + \sum_{\substack{u \in V(B_{s_0+1}) \\ v \in V(S_{s_0}) \setminus \{u_{l,0}\}}} d_T(u,v) + \sum_{\substack{u \in V(B_{s_0+1}) \\ v \in V(S_{s_0+2})}} d_T(u,v) + \sum_{\substack{u \in V(C_{s_0+2} - S_{s_0+2}) \\ v \in V(S_{s_0}) \setminus \{u_{l,0}\}}} d_T(u,v) \\
& + \sum_{\substack{u \in V(C_{s_0+2} - S_{s_0+2}) \\ v \in V(S_{s_0+2})}} d_T(u,v) + \sum_{u \in V(A_{s_0} - S_{s_0})} [d_T(u, u_{l,0}) + (l'' - l + 3)] \\
& + \sum_{u \in V(B_{s_0+1})} [d_T(u, u_{l,0}) + (l'' - l + 1)] \\
& + \sum_{u \in V(C_{s_0+2} - S_{s_0+2})} [d_T(u, u_{l,0}) + (l'' - l - 1)] + \sum_{u \in V(S_{s_0}) \setminus \{u_{l,0}\}} d_T(u, u_{l,0}) \\
& + \sum_{u \in V(S_{s_0+2})} d_T(u, u_{l,0}).
\end{aligned}$$

Note that the path induced by $(S_{s_0} \setminus \{u_{l,0}\}) \cup S_{s_0+2} \cup \{u_{l,0}\}$ in T and T' are isomorphic. That is,

$$\begin{aligned}
\sum_{u \in V(S_{s_0}) \setminus \{u_{l,0}\}} d_{T'}(u, u_{l,0}) + \sum_{u \in V(S_{s_0+2})} d_{T'}(u, u_{l,0}) &= \sum_{u \in V(S_{s_0}) \setminus \{u_{l,0}\}} d_T(u, u_{l,0}) \\
&+ \sum_{u \in V(S_{s_0+2})} d_T(u, u_{l,0}).
\end{aligned}$$

Proceeding with the calculations, we get

$$\begin{aligned}
W(T') &= W(T) + (l'' - l - 1) |C_{s_0+2} - S_{s_0+2}| + (l'' - l + 1) |B_{s_0+1}| \\
&\quad + (l'' - l + 3) |A_{s_0} - S_{s_0}| \\
&= W(T) + (l'' - l) (|C_{s_0+2} - S_{s_0+2}| + |B_{s_0+1}| + |A_{s_0} - S_{s_0}|) \\
&\quad + (-|C_{s_0+2} - S_{s_0+2}| + |B_{s_0+1}| + 3|A_{s_0} - S_{s_0}|).
\end{aligned}$$

Since $l'' \geq l$ and $|C_{s_0+2} - S_{s_0+2}| > |B_{s_0+1}| + 3|A_{s_0} - S_{s_0}|$, it follows that $-|C_{s_0+2} - S_{s_0+2}| + |B_{s_0+1}| + 3|A_{s_0} - S_{s_0}| < 0$, which implies $W(T') < W(T)$, contradicting minimality of T ,

Now, considering the two conditions,

- (i) Suppose there exist three consecutive segments S_{s_0} , B_{s_0+1} and S_{s_0+2} attached at u_{s_0} , u_{s_0+1} , and u_{s_0+2} respectively, having the same length, that is, $l'' = l$. Applying the transformation above, we have

$$\begin{aligned} W(T') &= W(T) + (l - l)(|C_{s_0+2} - S_{s_0+2}| + |B_{s_0+1}| + |A_{s_0} - S_{s_0}|) \\ &\quad + (-|C_{s_0+2} - S_{s_0+2}| + |B_{s_0+1}| + 3|A_{s_0} - S_{s_0}|) \\ &= W(T) - |C_{s_0+2} - S_{s_0+2}| + |B_{s_0+1}| + 3|A_{s_0} - S_{s_0}|. \end{aligned}$$

Since $|C_{s_0+2} - S_{s_0+2}| > |B_{s_0+1}| + 3|A_{s_0} - S_{s_0}|$, then $-|C_{s_0+2} - S_{s_0+2}| + |B_{s_0+1}| + 3|A_{s_0} - S_{s_0}| < 0$, implying $W(T') < W(T)$.

- (ii) Suppose there exist three consecutive segments having lengths $l - 1, l, l + 1$ within the specified region $T - (A_{s_0+1} \cup C_{l_0-1})$. In this case, we will apply the reverse transformation, where we will remove the final vertex of the right pendant segment whose length is $l + 1$ and attach it to the end of the left pendant segment whose length is $l - 1$. After applying the reverse transformation the three lengths become (l, l, l) , we obtain

$$\begin{aligned} W(T') &= W(T) + (l + 1 - (l - 1))(|C_{s_0+2} - S_{s_0+2}| + |B_{s_0+1}| \\ &\quad + |A_{s_0} - S_{s_0}|) + (-|C_{s_0+2} - S_{s_0+2}| + |B_{s_0+1}| + 3|A_{s_0} - S_{s_0}|) \\ &= W(T) + 2(|C_{s_0+2} - S_{s_0+2}| + |B_{s_0+1}| + |A_{s_0} - S_{s_0}|) \\ &\quad - |C_{s_0+2} - S_{s_0+2}| + |B_{s_0+1}| + 3|A_{s_0} - S_{s_0}| \\ &= W(T) + 2|C_{s_0+2} - S_{s_0+2}| + 2|B_{s_0+1}| + 2|A_{s_0} - S_{s_0}| \\ &\quad - |C_{s_0+2} - S_{s_0+2}| + |B_{s_0+1}| + 3|A_{s_0} - S_{s_0}| \\ &= W(T) + |C_{s_0+2} - S_{s_0+2}| + 3|B_{s_0+1}| + 5|A_{s_0} - S_{s_0}| \\ &> W(T). \end{aligned}$$

Thus, when we are moving from left to right the Wiener index increases by $|C_{s_0+2} - S_{s_0+2}| + 3|B_{s_0+1}| + 5|A_{s_0} - S_{s_0}|$.

Now, consider the inverse transformation, that is from right to left. Its effect on the Wiener index is the negative of the above, that is,

$$\begin{aligned} W(T') &= W(T) - (|C_{s_0+2} - S_{s_0+2} + 3|B_{s_0+1}| + 5|A_{s_0} - S_{s_0}|) \\ &< W(T). \end{aligned}$$

However, this contradicts the minimality of T .

Thus, the proof is complete. \square

Now we combine all the lemmas of this section to form the following theorem.

Theorem 4.12 *Let T be an n -vertex caterpillar-like tree with maximum degree $\Delta \geq 3$ whose backbone is given by $Q = u_0, u_1, \dots, u_{r-1}, u_r$. If T has minimum Wiener index then T must satisfy the following:*

(i) *Suppose a pendant segment $S = u_1, w_1, w_2, \dots, w_l$ is attached to vertex u_1 of the backbone. If $\deg_T(u_1) < \Delta$, then the segment S must have length at most 1.*

(ii)

$$\begin{cases} \deg(u_i) = \Delta, & \text{for all } 1 \leq i \leq r-1, \\ \deg(u_0), \deg(u_r) \leq \Delta, & \text{and at most one of them is strictly less} \\ & \text{than } \Delta. \end{cases}$$

This implies that all segments in the backbone have length 1.

(iii) *For each $i \in \{0, \dots, r\}$, let $S_{i,1}, S_{i,2}, \dots, S_{i,s_i}$ denote the pendant segments attached to u_i , where $s_i > 0$ is the number of pendant segments at u_i . Then:*

$$\begin{cases} ||S_{i,j}| - |S_{i,k}|| \leq 1, & \text{for all } 0 \leq i \leq r \text{ and } 1 \leq j, k \leq s_i, \\ ||S_{i,j}| - |S_{i+1,k}|| \leq 1, & \text{for all } 0 \leq i < r, 1 \leq j \leq s_i, 1 \leq k \leq s_{i+1}. \end{cases}$$

(iv) *The lengths of the segments attached along the backbone form a unimodal pattern. That is, if $L_i = \sum_{j=1}^{s_i} |S_{i,j}|$ denotes the total length of all pendant segments at vertex u_i , there exists an index m with $0 \leq m \leq r$ such that:*

$$L_0 \leq L_1 \leq \cdots \leq L_m \geq \cdots \geq L_{r-1} \geq L_r.$$

(v) *For any $0 \leq i < r$, let A_i be the connected component of $T - u_i u_{i+1}$ that contain u_i , and for $0 < i \leq r$, let B_i be the connected component of $T - u_i u_{i-1}$ that contain u_i . For $0 < i < r$, let C_i be the connected component of $T - u_i u_{i-1} - u_i u_{i+1}$ that contains u_i . Let s_0 be the largest integer such that*

$$3|A_{s_0} - S_{s_0,l}| + |B_{s_0+1}| < |C_{s_0+2} - S_{s_0+2,k}|$$

for some k and l . Let l_0 be the smallest integer such that

$$3|C_{l_0} - S_{s_0,t}| + |B_{l_0-1}| < |A_{l_0-2} - S_{l_0-2,s}|$$

for some t and s . Then,

1. *Attached within A_{s_0+2} , there do not exist three consecutive backbone vertices to which segments are of equal lengths.*
2. *There do not exist three consecutive backbone vertices to which pendant segment are of length $l - 1, l, l + 1$, respectively in $T - A_{s_0+1} - C_{l_0-1}$.*

(vi) *Neither u_0 nor u_r can have two pendant segments attached to them whose lengths are both greater than 1.*

Proof. We prove each item of the theorem by referring to the lemmas listed earlier.

(i) is exactly Lemma Lemma 4.7.

(ii) From Lemma 4.4 (Claim II.), we know that there are at most two vertices of degree less than Δ in the backbone and they are end vertices of the backbone. By Lemma 4.5, at most one of u_0 and u_r can have degree less than Δ .

(iii) is exactly Lemma 4.2.

(iv) is exactly Lemma 4.6.

(v) is exactly Lemma 4.11.

(vi) By symmetry, it is enough to only prove the claim for u_r . If one of u_0 or u_r have degree less than Δ , then Lemma 4.7 already covers the claim. Now, without any loss of generality, we may assume $\deg(u_r) = \Delta$. Suppose, to the contrary, that u_r has two pendant segment $S_1 = u_r, w_1, w_2, \dots, w_s$ and $S_2 = u_r, x_1, x_2, \dots, x_t$ with $t \geq s \geq 2$. Let A and B be two connected components of $T - u_{r-1}u_r$, such that A contains u_{r-1} and B contain u_r . Let $B' = B - S_1 - S_2$. The Wiener index of T is given by,

$$\begin{aligned} W(T) &= W(T - x_t) + \sum_{u \in V(A)} d_T(u, x_t) + \sum_{u \in V(S_1 \cup S_2) \setminus \{x_t, w_s\}} d_T(u, x_t) \\ &\quad + \sum_{u \in V(B')} d_T(u, x_t) + d_T(x_t, w_s). \end{aligned}$$

Let $T' = T - x_{t-1}x_t + x_t w_{s-1}$. Note that T' is still a caterpillar-like tree with maximum degree Δ .

$$\begin{aligned} W(T') &= W(T' - x_t) + \sum_{u \in V(A)} d_{T'}(u, x_t) + \sum_{u \in V(S_1 \cup S_2) \setminus \{x_t, w_s\}} d_{T'}(u, x_t) \\ &\quad + \sum_{u \in V(B')} d_{T'}(u, x_t) + d_{T'}(x_t, w_s) \\ &= W(T - x_t) + \sum_{u \in V(A)} [d_T(u, x_t) - (t - s)] + \sum_{u \in V(S_1 \cup S_2) \setminus \{x_t, w_s\}} d_T(u, x_t) \\ &\quad + \sum_{u \in V(B')} [d_T(u, x_t) - (t - s)] + [d_T(x_t, w_s) + 2 - (s + t)] \\ &= W(T) - (t - s) \cdot |V(A)| - (t - s)|V(B')| + 2 - (s + t) \\ &= W(T) - (t - s) \cdot [|V(A)| + |V(B')|] + 2 - (s + t). \end{aligned}$$

Since $s, t \geq 2$ and $s \leq t$, then $-(t - s) \cdot [|V(A)| + |V(B')|] + 2 - (s + t) < 0$, implying that $W(T') < W(T)$. However, this contradicts the minimality of T . Hence, neither u_0 nor u_r can have two pendant

segments attached to them whose lengths are both greater than 1. \square

While Theorem 4.12 does not always guarantee a full characterisation, we now present two corollaries where full characterisation is obtained.

Let $CL((d_0, h_0), (d_1, h_1), \dots, (d_r, h_r))$ be the caterpillar-like tree with backbone u_0, u_1, \dots, u_r such that d_i segments of length h_i are attached at u_i . See example in Figure 4.16.

Given a caterpillar-like tree T with backbone u_0, u_1, \dots, u_r , the *ex-*

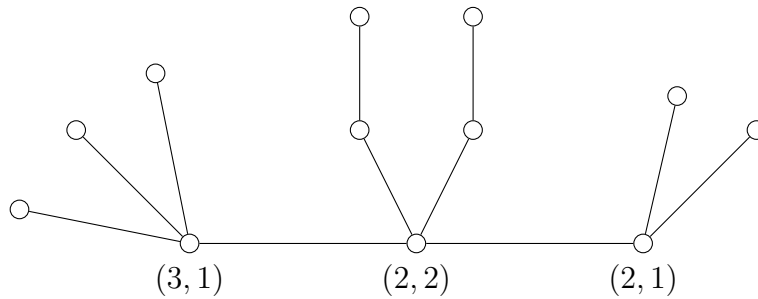


Figure 4.16: An example of $CL((3, 1), (2, 2), (2, 1))$

tended backbone of T is defined as the set consisting of all backbone vertices together with any vertex of degree 2 and is adjacent to either u_0 or u_r .

If $n = \Delta + 1$, then the only possible caterpillar-like tree with n vertices and maximum degree Δ is the star. In the next Corollary, we provide full characterisation of the n -vertex caterpillar-like tree with maximum degree Δ and minimum Wiener index for $\Delta + 1 < n \leq 2\Delta$.

Corollary 4.13 *Let Δ be a positive integer. For $\Delta + 1 < n \leq 2\Delta$, and any n -vertex caterpillar-like tree T with maximum degree Δ we have*

$$W(T) \leq W(CL((\Delta - 1, 1), (n - \Delta - 1, 1))).$$

Proof. Let Δ be a positive integer, and suppose that $\Delta + 1 < n \leq 2\Delta$. Let T be an n -vertex caterpillar-like tree with maximum degree Δ that minimizes the Wiener index among all such trees. By Theorem 4.12, T must satisfy the structural properties stated therein.

By (i) of the theorem, all internal vertices of the backbone of T have degree exactly Δ , and the two endpoints of the backbone have degree at most Δ , with at most one having degree strictly less than Δ . Suppose there are at least 3 vertices u_0, u_1, u_2 in the extended backbone. If none of these has degree 2, then the extended backbone coincides with the backbone, and we may apply item (i) of Theorem 4.12. In this case, u_1 must have degree Δ , and both u_0 and u_2 must have degree at least 3 and one of them has degree Δ . This gives at least

$$n \geq \Delta - 1 + \Delta - 2 + 2 + 3 = 2\Delta + 2$$

vertices. This contradicts the assumption that $n \leq 2\Delta$. Hence, the backbone cannot have more than two vertices.

Suppose that the extended backbone has a vertex of degree 2. Then it has to be u_0 or u_2 . Say, $\deg(u_0) = 2$. By (i), $\deg(u_1) = \Delta$. Suppose that $\deg(u_2) < \Delta$. Note that $\deg(u_2) \geq 2 = \deg(u_0)$. Now, let x be a leaf attached to u_0 , A be a connected component of $T - u_0u_1$ that contain u_0 , B be a connected component of $T - u_0u_1 - u_1u_2$ that contains u_1 and C be a connected component of $T - u_1u_2$ that contains u_2 . The Wiener index of T is, therefore given by

$$\begin{aligned} W(T) &= \sum_{u,v \in V(A) \setminus \{x\}} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) + \sum_{u,v \in V(C)} d_T(u,v) \\ &+ \sum_{v \in V(B)} d_T(u_0,v) + \sum_{u \in V(C)} d_T(u,u_0) + \sum_{\substack{u \in V(B) \\ v \in V(C)}} d_T(u,v) \\ &+ \sum_{u \in V(A) \setminus \{x\}} d_T(u,x) + \sum_{u \in V(B)} d_T(u,x) + \sum_{u \in V(C)} d_T(u,x). \end{aligned}$$

Let $T' = T - u_0x + u_2x$. Note that T is still a caterpillar-like tree with maximum degree Δ . The Wiener index of T' is given by,

$$\begin{aligned}
 W(T') &= \sum_{u,v \in V(A) \setminus \{x\}} d_{T'}(u,v) + \sum_{u,v \in V(B)} d_{T'}(u,v) + \sum_{u,v \in V(C)} d_{T'}(u,v) \\
 &+ \sum_{v \in V(B)} d_{T'}(u_0,v) + \sum_{u \in V(C)} d_{T'}(u,u_0) + \sum_{\substack{u \in V(B) \\ v \in V(C)}} d_{T'}(u,v) \\
 &+ \sum_{u \in V(A) \setminus \{x\}} d_{T'}(u,x) + \sum_{u \in V(B)} d_{T'}(u,x) + \sum_{u \in V(C)} d_{T'}(u,x) \\
 &= \sum_{u,v \in V(A) \setminus \{x\}} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) + \sum_{u,v \in V(C)} d_T(u,v) \\
 &+ \sum_{v \in V(B)} d_T(u_0,v) + \sum_{u \in V(C)} d_T(u,u_0) + \sum_{\substack{u \in V(B) \\ v \in V(C)}} d_T(u,v) \\
 &+ \sum_{u \in V(A) \setminus \{x\}} [d_T(u,x) + 2] + \sum_{u \in V(B)} d_T(u,x) + \sum_{u \in V(C)} [d_T(u,x) - 2]. \\
 &= W(T) - 2|C| + 2|V(A) \setminus \{x\}| \\
 &= W(T) - 2(|C| - |V(A) \setminus \{x\}|).
 \end{aligned}$$

Since $1 = |V(A) \setminus \{x\}| < |C|$, then $W(T') < W(T)$. However, this contradict the minimality of T , and hence both u_0 and u_2 cannot have degree 2.

Now, suppose the extended backbone consists of a single vertex. Then T is necessarily a star, with one central vertex of degree at most Δ and $n - 1$ leaves. In that case, the total number of vertices satisfies $n \leq \Delta + 1$, contradicting the assumption that $n > \Delta + 1$. Therefore, the extended backbone of T must consist of exactly two vertices, say u_0 and u_1 . If both of u_0 and u_1 has degree less than Δ , then T does not have maximum degree Δ , and hence

$$T = CL((\Delta - 1, 1), (n - \Delta - 1, 1)).$$

□

Corollary 4.14 *Let Δ be a positive integer. For $2\Delta + 1 \leq n \leq 3\Delta - 1$, and any n -vertex caterpillar-like tree T with maximum degree Δ we*

have

$$W(T) \leq W(CL(\Delta - 1, 1), (\Delta - 2, 1), (n - 2\Delta, 1)).$$

Proof. Suppose that $2\Delta + 1 \leq n \leq 3\Delta - 1$, and let T be an n -vertex caterpillar-like tree with maximum degree Δ that minimizes the Wiener index. Then, by Theorem 4.12, T satisfies all the stated structural properties stated therein.

Suppose, to the contrary, that the extended backbone of T has more than three vertices u_0, u_1, \dots, u_r with $r \geq 3$. If none of these has degree 2, then the extended backbone coincides with the backbone, and we may apply item (ii) of Theorem 4.12. Then, each one of u_1, \dots, u_{r-1} must have degree exactly Δ , and at most one endpoint (either u_0 or u_r) may have degree strictly less than Δ but at least 3. The total number of pendant segments is therefore at least

$$(\Delta - 1) + (r - 1)(\Delta - 2) + 2 = r\Delta - 2r + 3.$$

Including the $r + 1$ extended backbone vertices, the total number of vertices is at least

$$n \geq (r + 1) + r\Delta - 2r + 3 = r(\Delta - 1) + 4.$$

Setting $r = 3$ (the minimum for this case) gives:

$$n \geq 3(\Delta - 1) + 4 = 3\Delta + 1,$$

which contradicts the assumption that $n \leq 3\Delta - 1$.

Now, we are going to consider the following cases when the extended backbone has a vertex of degree 2.

Case I: Suppose, that the extended backbone has at least 5 vertices and at least one of them has degree 2.

Then u_0 and u_4 have degree at least 2. By (i) and (ii), u_1, u_2 and u_3 , they all have degree Δ . This gives at least

$$n \geq 2 + \Delta - 2 + 1 + \Delta - 2 + 1 + \Delta - 2 + 1 + 2 = 3\Delta + 1$$

however, this contradicts the assumption that $n \leq 3\Delta - 1$.

Case II: Suppose, that the extended backbone has vertices exactly 4 and at least one of them, say u_3 has degree 2.

Then, by (i) and (ii) of Theorem 4.12, u_1 and u_2 has degree Δ . We first show that u_0 cannot have degree Δ . Suppose, to the contrary, that $\deg(u_0) = \Delta$. Then u_0 has $\Delta - 1$ pendant vertices, while each of u_1 and u_2 has $\Delta - 2$ pendant vertices. Since u_3 has degree 2, it contributes one additional vertex. This gives at least

$$n \geq (\Delta - 1) + (\Delta - 2) + (\Delta - 2) + 4 = 3\Delta + 1$$

however, this contradicts the assumption that $n \leq 3\Delta - 1$. Hence, u_0 cannot have degree Δ , and so $\deg(u_0) = 2$.

Now, let x be a leaf attached to u_3 . Let A be a connected component of $T - u_0u_1$ that contain u_0 , B be a connected component of $T - u_0u_1 - u_1u_2$ that contains u_1 , C be a connected component of $T - u_1u_2 - u_2u_3$ that contains u_2 , and lastly let D be a connected component of $T - u_2u_3$ that contains u_3 . By (vi) of Theorem 4.12, $|C|$ cannot have two pendant segments attached whose lengths are both greater than 1. Hence $|C| + |D| \leq |A| + |B|$. The Wiener index of T is therefore given by,

$$\begin{aligned} W(T) &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) + \sum_{u,v \in V(C)} d_T(u,v) \\ &+ \sum_{u,v \in V(D) \setminus \{x\}} d_T(u,v) + \sum_{\substack{u \in V(D) \setminus \{x\} \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(D) \setminus \{x\} \\ v \in V(C)}} d_T(u,v) \\ &+ \sum_{\substack{u \in V(D) \setminus \{x\} \\ v \in V(A)}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(C)}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(A)}} d_T(u,v) \\ &+ \sum_{\substack{u \in V(C) \\ v \in V(A)}} d_T(u,v) + \sum_{u \in V(C)} d_T(u,x) + \sum_{u \in V(B)} d_T(u,x) \\ &+ \sum_{u \in V(D) \setminus \{x\}} d_T(u,x) + \sum_{u \in V(A)} d_T(u,x). \end{aligned}$$

Let $T' = T - u_3x + u_0x$. Note that T' is still a caterpillar-like tree. The Wiener index is, therefore, given by

$$W(T') = \sum_{u,v \in V(A)} d_{T'}(u,v) + \sum_{u,v \in V(B)} d_{T'}(u,v) + \sum_{u,v \in V(C)} d_{T'}(u,v)$$

$$\begin{aligned}
& + \sum_{u,v \in V(D) \setminus \{x\}} d_{T'}(u,v) + \sum_{\substack{u \in V(D) \setminus \{x\} \\ v \in V(B)}} d_{T'}(u,v) + \sum_{\substack{u \in V(D) \setminus \{x\} \\ v \in V(C)}} d_{T'}(u,v) \\
& + \sum_{\substack{u \in V(D) \setminus \{x\} \\ v \in V(A)}} d_{T'}(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(C)}} d_{T'}(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(A)}} d_{T'}(u,v) \\
& + \sum_{\substack{u \in V(C) \\ v \in V(A)}} d_{T'}(u,v) + \sum_{u \in V(C)} d_{T'}(u,x) + \sum_{u \in V(B)} d_{T'}(u,x) \\
& + \sum_{u \in V(D) \setminus \{x\}} d_{T'}(u,x) + \sum_{u \in V(A)} d_T(u,x) \\
& = \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) + \sum_{u,v \in V(C)} d_T(u,v) \\
& + \sum_{u,v \in V(D) \setminus \{x\}} d_T(u,v) + \sum_{\substack{u \in V(D) \setminus \{x\} \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(D) \setminus \{x\} \\ v \in V(C)}} d_T(u,v) \\
& + \sum_{\substack{u \in V(D) \setminus \{x\} \\ v \in V(A)}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(C)}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in V(A)}} d_T(u,v) \\
& + \sum_{\substack{u \in V(C) \\ v \in V(A)}} d_T(u,v) + \sum_{u \in V(C)} [d_T(u,x) + 1] + \sum_{u \in V(B)} [d_T(u,x) - 1] \\
& + \sum_{u \in V(D) \setminus \{x\}} [d_T(u,x) + 3] + \sum_{u \in V(A)} [d_T(u,x) - 3] \\
& = W(T) - 3|A| - |B| + |C| + 3|V(D) \setminus \{x\}| \\
& = W(T) - 3(|A| - |D \setminus \{x\}|) - (|B| - |C|).
\end{aligned}$$

Since $|C| + |D| \leq |A| + |B|$, we have $3(|A| - |D \setminus \{x\}|) + (|B| - |C|) > 0$, implying $W(T') < W(T)$. Therefore, the extended backbone cannot contain more than three vertices.

Suppose, to the contrary, that the extended backbone consists of only one vertex u_0 . Then all other $n - 1$ vertices must be attached directly to u_0 as pendant segments, implying that $\deg(u_0) = n - 1$. Since $\deg(u_0) \leq \Delta$ by assumption, it follows that

$$n - 1 \leq \Delta \quad \text{and} \quad n \leq \Delta + 1,$$

which contradicts the assumption that $n \geq 2\Delta + 1$.

Suppose that there are exactly 2 vertices u_0 and u_1 in the extended backbone. Then, by item (ii) of the theorem, both vertices must have degree at most Δ . Then all other $n - 2$ vertices are adjacent to either u_0 or u_1 . This gives at most

$$n \leq 2(\Delta - 1) + 2 = 2\Delta,$$

vertices, which contradicts the assumption that $n \geq 2\Delta + 1$. Hence, the extended backbone must consist of exactly three vertices, say u_0, u_1 and u_2 .

Now, suppose u_0 and u_2 have degree less than Δ . Then, by (ii), at least one of them has degree 2. This gives at most

$$n \leq 2 + \Delta - 1 + \Delta - 1 = 2\Delta,$$

this contradicts the assumption that $n \geq 2\Delta + 1$. So one of u_0 and u_2 has degree Δ , say it is u_2 .

Now, we are going to show that there's no pendant segment attached to u_1 has length longer than 2. Suppose that there is one of them that has length longer than 1 and u_0 and u_2 has degree exactly Δ . Then there's at least

$$n \geq \Delta + \Delta + \Delta - 1 + 1 = 3\Delta$$

vertices, contradicting the assumption that $n \leq 3\Delta - 1$.

Finally, suppose u_0 have degree less than Δ . Let $S_1 = u_1, w_1, w_2, \dots, w_{i-1}, w_i$ be a pendant segment attached to u_1 with $i \geq 2$. Let A be a connected component of $T - u_0u_1$ that contains u_0 , B be a connected component of $T - u_0u_1 - u_1u_2$ that contains u_1 and C be a connected component of $T - u_1u_2$ that contains u_2 . The Wiener index of T is, therefore given by

$$\begin{aligned} W(T) &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(B-S_1)} d_T(u,v) + d_T(u,v) + \sum_{u,v \in V(C)} d_T(u,v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(B-S_1)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(C)}} d_T(u,v) + \sum_{\substack{u \in V(B-S_1) \\ v \in V(C)}} d_T(u,v) \\ &+ \sum_{u \in V(A)} d_T(u, w_i) + \sum_{u \in V(B-S_1)} d_T(u, w_i) + \sum_{u \in V(C)} d_T(u, w_i) \end{aligned}$$

$$+ \sum_{u \in V(S_1) \setminus \{w_i\}} d_T(u, w_i).$$

Let $T' = T - w_{i-1}w_i + w_iu_0$. The Wiener index of T' , is

$$\begin{aligned} W(T') &= \sum_{u,v \in V(A)} d_{T'}(u,v) + \sum_{u,v \in V(B-S_1)} d_{T'}(u,v) + d_{T'}(u,v) + \sum_{u,v \in V(C)} d_T(u,v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(B-S_1)}} d_{T'}(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(C)}} d_{T'}(u,v) + \sum_{\substack{u \in V(B-S_1) \\ v \in V(C)}} d_{T'}(u,v) \\ &+ \sum_{u \in V(A)} d_{T'}(u, w_i) + \sum_{u \in V(B) \setminus S_1} d_{T'}(u, w_i) + \sum_{u \in V(C)} d_{T'}(u, w_i) \\ &+ \sum_{u \in V(S_1) \setminus \{w_i\}} d_{T'}(u, w_i) \\ &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(B-S_1)} d_T(u,v) + d_T(u,v) + \sum_{u,v \in V(C)} d_T(u,v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(B-S_1)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in V(C)}} d_T(u,v) + \sum_{\substack{u \in V(B-S_1) \\ v \in V(C)}} d_T(u,v) \\ &+ \sum_{u \in V(A)} [d_T(u, w_i) - i] + \sum_{u \in V(B-S_1)} [d_T(u, w_i) - (i-2)] \\ &+ \sum_{u \in V(C)} [d_T(u, w_i) - (i-2)] + \sum_{u \in V(S_1) \setminus \{w_i\}} [d_T(u, w_i) + 1] \\ &= W(T) - i|A| - (i-2)|B-S_1| - (i-2)|C| \\ &+ |S_1 \setminus \{w_i\}| \end{aligned}$$

Since $i \geq 2$ and $\deg(u_1) = \deg(u_2) = \Delta$, we have $|A| \geq 1$, $|B-S_1| \geq 1$, and $|C| \geq 1$, with $(i-2)|B-S_1| + (i-2)|C| > 0$. Furthermore, by Lemma 4.2, $|A| - |S_1| \leq 1$ which implies $|S_1 \setminus \{w_i\}| = |S_1| - 1$. Therefore $-i|A| + |S_1 - w_i| < -|A| + |S_1| - 1 \leq 1 - 1 = 0$, and as a result, $W(T') < W(T)$. However, this contradicts the minimality of T , and hence there's no pendant segment of length greater than 2 is attached to u_1 .

Let n_0, n_1, n_2 be the number of pendant segments of length 1 attached to u_0, u_1, u_2 , respectively. Then the total number of pendant vertices is

$$n_0 + n_1 + n_2 = n - 3,$$

with

$$n_0 \leq \Delta - 1, \quad n_1 \leq \Delta - 2, \quad n_2 \leq \Delta - 1.$$

This yields the caterpillar-like tree

$$CL((\Delta - 1, 1), (\Delta - 2, 1), (n - 2\Delta, 1)).$$

It remains to verify that $n - 2\Delta \leq \Delta - 1$, to ensure that the number of leaves attached to u_2 does not exceed the maximum degree Δ . This holds because $n \leq 3\Delta - 1$, and hence $n - 2\Delta \leq \Delta - 1$. \square

4.2 Maximal n -vertex caterpillar-like trees with given maximum degree

Recall that a *broom*, denoted $B_{n, \Delta-1}$, is a tree of order n obtained from a path $P_{n-\Delta+1}$ by adding $\Delta - 1$ new vertices and joining them to exactly one end of $P_{n-\Delta+1}$.

Theorem 4.15 ([13]) *If T is a tree in $\mathcal{T}(n, \Delta)$ with $\Delta \geq 3$, then*

$$W(T) \leq W(B_{n, \Delta-1}).$$

The equality holds if and only if $T \cong B_{n, \Delta-1}$.

Since a caterpillar-like tree is a special case of a tree in $\mathcal{T}(n, \Delta)$, we obtain the following corollary.

Corollary 4.16 *If T is a caterpillar-like tree of order n with given maximum degree Δ , then*

$$W(T) \leq W(B_{n, \Delta-1}),$$

with equality if and only if $T \cong B_{n, \Delta-1}$.

In the remainder of this section, we present a slightly different proof of this result. We need the following lemma, which follows directly from an iteration of the "Lengthening Lemma" in [8] and [13].

Lemma 4.17 (Lengthening Lemma) *Let T be a caterpillar-like tree whose backbone is given by $Q : u_{0,0}, u_{1,0}, \dots, u_{r,0}$. Let $S_1 : u_{i,0}, u_{i,1}, \dots, u_{i,s}$ and $S_2 = u_{i,0}, w_{i,1}, \dots, w_{i,t}$ be two segments rooted at $u_{i,0}$ for some i , where $0 \leq i \leq r$. If $T' = T - u_{i,0}u_{i,1} + u_{i,1}w_{i,t}$, then $W(T') > W(T)$.*

Proof. Let T be a caterpillar-like tree whose backbone is given by $Q : u_{0,0}, u_{1,0}, \dots, u_{r,0}$. Each of $u_{0,0}$ and $u_{r,0}$ have at least two pendant segments rooted at them. Let $u_{i,0}$ be a branching vertex of T such that there are at least two pendant segments $S_1 : u_{i,0}, u_{i,1}, \dots, u_{i,s}$ and $S_2 = u_{i,0}, w_{i,1}, \dots, w_{i,t}$ rooted at $u_{i,0}$ for some i , where $0 \leq i \leq r$. Without any loss of generality, we may assume that $s \leq t$. Let A be the connected component of $T - u_{i-1,0}u_{i,0}$ containing $u_{i-1,0}$ and B a connected component of $T - u_{i,0}u_{i+1,0}$ containing $u_{i+1,0}$. Furthermore, let $P_1 = V(S_1) \setminus \{u_{i,0}\}$ and $P_2 = V(S_2)$. The Wiener index of T is, therefore, given by

$$\begin{aligned} W(T) &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) + \sum_{u,v \in P_1} d_T(u,v) + \sum_{u,v \in P_2} d_T(u,v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in P_1}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in P_2}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in P_1}} d_T(u,v) \\ &+ \sum_{\substack{u \in V(B) \\ v \in P_2}} d_T(u,v) + \sum_{\substack{u \in P_1 \\ v \in P_2}} d_T(u,v). \end{aligned}$$

Let T' be the caterpillar-like tree obtained from T by removing the edge $u_{i,0}u_{i,1}$ and adding the edge $u_{i,1}u_{i,t}$; that is, $T' = T - u_{i,0}u_{i,1} + u_{i,1}u_{i,t}$. The Wiener index of T' is

$$\begin{aligned} W(T') &= \sum_{u,v \in V(A)} d_{T'}(u,v) + \sum_{u,v \in V(B)} d_{T'}(u,v) + \sum_{u,v \in P_1} d_{T'}(u,v) + \sum_{u,v \in P_2} d_{T'}(u,v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_{T'}(u,v) + \sum_{\substack{u \in V(A) \\ v \in P_1}} d_{T'}(u,v) + \sum_{\substack{u \in V(A) \\ v \in P_2}} d_{T'}(u,v) + \sum_{\substack{u \in V(B) \\ v \in P_1}} d_{T'}(u,v) \\ &+ \sum_{\substack{u \in V(B) \\ v \in P_2}} d_{T'}(u,v) + \sum_{\substack{u \in P_1 \\ v \in P_2}} d_{T'}(u,v) \\ &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) + \sum_{u,v \in P_1} d_T(u,v) + \sum_{u,v \in P_2} d_T(u,v) \end{aligned}$$

$$\begin{aligned}
 & + \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_T(u, v) + \sum_{\substack{u \in V(A) \\ v \in P_1}} [d_T(u, v) + t] + \sum_{\substack{u \in V(A) \\ v \in P_2}} d_T(u, v) \\
 & + \sum_{\substack{u \in V(B) \\ v \in P_1}} [d_T(u, v) + t] + \sum_{\substack{u \in V(B) \\ v \in P_2}} d_T(u, v) + \sum_{\substack{u \in P_1 \\ v \in P_2}} d_T(u, v) \\
 & = W(T) + t|V(A)||P_1| + t|V(B)||P_1| \\
 & = W(T) + t|P_1|(|V(A)| + |V(B)|).
 \end{aligned}$$

Since $t \geq 1$, we have $W(T') > W(T)$, and thus completing the proof. \square

Lemma 4.18 *Let T be an n -vertex caterpillar-like tree with maximum degree Δ . If T has maximum Wiener index, then T has exactly one branching vertex v and $\deg_T v = \Delta$.*

Proof. Suppose that T has maximum Wiener index among all caterpillar-like tree of order n and maximum degree Δ and T has at least two branching vertices. Let v be a vertex of maximum degree in T . Thus, $\deg_T v = \Delta$. Let u be an end vertex of the backbone apart from v . Let T' be the caterpillar-like tree obtained from T by applying the transformation in Lemma 4.17 with $u_{i,0}$ being u . Thus, by Lemma 4.17, we have $W(T') > W(T)$, which contradicts the maximality of T . Hence, the only branching vertex of T is v and $\deg_T v = \Delta$. \square

Lemma 4.19 *Let T be a caterpillar-like tree of order n with maximum degree Δ , and let v be the branching vertex. If T has maximum Wiener index, then among all the pendant segments rooted at v , there is at most one pendant segment whose length exceeds 1.*

Proof. Let T be a caterpillar-like tree of order n with maximum degree Δ , and let v be the branching vertex. Then there exists at least one pendant segment in T rooted at $v = u_{i,0}$. Let $S_1 : v, u_{i,1}, \dots, u_{i,s}$ and $S_2 : v, w_{i,1}, \dots, w_{i,t}$ be two pendant segments in T rooted at $v = u_{i,0}$. Without any loss of generality, we may assume that $s \leq t$.

Suppose, to the contrary, that T has maximum Wiener index and both s and t are at least 2. Let A be a connected component

of $T - u_{i-1,0}v$ containing $u_{i-1,0}$ and B a connected component of $T - vu_{i+1,0}$ containing $u_{i+1,0}$. Furthermore, let $P_1 = V(S_1) \setminus \{v, u_{i,1}\}$ and $P_2 = V(S_2) \cup \{u_{i,1}\}$. The Wiener index of T is, therefore, given by

$$\begin{aligned} W(T) &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) + \sum_{u,v \in P_1} d_T(u,v) + \sum_{u,v \in P_2} d_T(u,v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in P_1}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in P_2}} d_T(u,v) + \sum_{\substack{u \in V(B) \\ v \in P_1}} d_T(u,v) \\ &+ \sum_{\substack{u \in V(B) \\ v \in P_2}} d_T(u,v) + \sum_{\substack{u \in P_1 \\ v \in P_2}} d_T(u,v). \end{aligned}$$

Let T' be the caterpillar-like tree obtained from T by removing the edge $u_{i,1}u_{i,2}$ and adding the edge $u_{i,2}w_{i,t}$; that is, $T' = T - u_{i,1}u_{i,2} + u_{i,2}w_{i,t}$. Note that $\deg_{T'}(v) = \deg_T(v)$. The Wiener index of T' is

$$\begin{aligned} W(T') &= \sum_{u,v \in V(A)} d_{T'}(u,v) + \sum_{u,v \in V(B)} d_{T'}(u,v) + \sum_{u,v \in P_1} d_{T'}(u,v) + \sum_{u,v \in P_2} d_{T'}(u,v) \\ &+ \sum_{\substack{u \in V(B) \\ v \in P_2}} d_{T'}(u,v) + \sum_{\substack{u \in P_1 \\ v \in P_2}} d_{T'}(u,v) \\ &= \sum_{u,v \in V(A)} d_T(u,v) + \sum_{u,v \in V(B)} d_T(u,v) + \sum_{u,v \in P_1} d_T(u,v) + \sum_{u,v \in P_2} d_T(u,v) \\ &+ \sum_{\substack{u \in V(A) \\ v \in V(B)}} d_T(u,v) + \sum_{\substack{u \in V(A) \\ v \in P_1}} [d_T(u,v) + (t-1)] + \sum_{\substack{u \in V(A) \\ v \in P_2}} d_T(u,v) \\ &+ \sum_{\substack{u \in V(B) \\ v \in P_1}} [d_T(u,v) + (t-1)] + \sum_{\substack{u \in V(B) \\ v \in P_2}} d_T(u,v) + \sum_{\substack{u \in P_1 \\ v \in P_2}} d_T(u,v) \\ &= W(T) + (t-1)|V(A)||P_1| + (t-1)|V(B)||P_1| \\ &= W(T) + (t-1)|P_1|(|V(A)| + |V(B)|). \end{aligned}$$

Since $t \geq 2$, we have $W(T') > W(T)$, which contradicts the maximality of T . \square

Lemma 4.17, Lemma 4.18 and Lemma 4.19 imply the characterisation of an n -vertex caterpillar-like tree with given maximum degree and largest Wiener index provided in Corollary 4.16.

5 | Conclusion

In this thesis, we studied extremal caterpillar-like trees under certain restrictions relative to the Wiener index. In particular, we characterised caterpillar-like trees with given number of leaves as well as caterpillar-like trees with given maximum degree that achieve the minimum (resp. maximum) Wiener index.

In Chapter 2, we presented the explicit formulas for the Wiener index of some classes of graphs. Furthermore, we presented some known bounds on the Wiener index of some classes of graphs.

In Chapter 3, we showed that the caterpillar-like tree with given number of leaves and minimum Wiener index is the star-like tree $S_{n,\ell}$, where each pendant segment of $S_{n,\ell}$ has length either $\lfloor \frac{n-1}{\ell} \rfloor$ or $\lceil \frac{n-1}{\ell} \rceil$. We also showed that the caterpillar-like tree with given number of leaves and maximum Wiener index is the double broom $B_{n, \lceil \frac{\ell}{2} \rceil, \lfloor \frac{\ell}{2} \rfloor}$, where ℓ is the number of leaves on the ends of $B_{n, \lceil \frac{\ell}{2} \rceil, \lfloor \frac{\ell}{2} \rfloor}$ and $|\ell_2 - \ell_1| \leq 1$.

In Chapter 4, although the caterpillar-like tree with given maximum degree and minimum Wiener index was difficult to uniquely characterize, we established several necessary structural conditions that must be satisfied by such a caterpillar-like tree. We provided corollaries that fully characterise the n -vertex caterpillar-like tree with minimum Wiener index for $\Delta + 1 < n \leq 2\Delta$ and $2\Delta + 1 \leq n \leq 3\Delta - 1$, respectively. We closed this chapter by providing that among all n -vertex caterpillar-like tree with given maximum degree Δ , the Wiener index is maximized by $B_{n, \Delta-1}$.

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A



Appendix

Date: **RESEARCH ETHICS DECLARATION**

To be included in the Appendices of research papers/dissertations/theses submitted for postgraduate examination where research did not involve interaction with human participants, or the use of animal subjects, and therefore did not require research ethics approval.

Candidates whose research did require ethics clearance must include their ethics approval letter in the Appendix of their examination submission.

Name of Candidate: Ndimphiwe

Name of Supervisor: Prof. Eric Andriantiana (and co-supervisor Dr. Zekhaya Shozi)

Degree: Master of Science (Mathematics)

Title of research: Extremal caterpillar-like trees relative to the Wiener index

DECLARATION

I declare that my research did not require ethical clearance because (tick all that apply):

I did not collect data from human participants or animal subjects	<input checked="" type="checkbox"/>
I used previously collected data that had already received ethics clearance.	<input type="checkbox"/>
I analysed documents / open-access digital texts that are freely available in the public domain.	<input type="checkbox"/>
I did a literature review/analysis of theoretical or secondary material only.	<input type="checkbox"/>
I used human datasets of non-sensitive information that are either anonymous (identifiers were never collected) or have been deidentified (identifiers have been completely removed).	<input type="checkbox"/>
I used commercially produced human biological material (e.g. established human cell lines).	<input type="checkbox"/>
I observed people in public spaces and natural environments where they had no reasonable expectation of privacy and I did not interact with them or intervene in any way.	<input type="checkbox"/>
I used non-living animal materials (eg bones of already deceased organisms or fossils) while complying with any custody and/or jurisdiction requirements.	<input type="checkbox"/>
I did a content analysis of public media (newspapers, advertisements, and social media posts).	<input type="checkbox"/>
I did a simulation study with no real-world consequences and does not involve disturbing or distressing content.	<input type="checkbox"/>
I observed flora, fauna, and ecosystems without interfering with or disturbing their natural state while complying with any jurisdiction requirements.	<input type="checkbox"/>
Other (Please provide details):	<input type="checkbox"/>

Signature of Candidate:

Date:

29/10/2025

Signature of Supervisor: