On the Second Smallest Eigenvalue of
The Laplacain

by

Waleed Ebrahim Al-Jasem

A Thesis Presented to the

FACULTY OF THE COLLEGE OF GRADUATE STUDIES
KING FAHD UNIVERSITY OF PETROLEUM & MINERALS
DHAHRAN, SAUDI ARABIA

In Partial Fulfillment of the
Requirements for the Degree of

MASTER OF SCIENCE

In

MATHEMATICS

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On the second smallest eigenvalue of the Laplacian

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King Fahd University of Petroleum and Minerals (Saudi Arabia), 1993
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WALEED EBRAHIM AL-JASEM

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Waleed Ebrahim Al-Jasem

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has been presented to and accepted by the Dean, College of Graduate Studies, in
partial fulfillment of the requirements for the degree of

Master of Science in Mathematics

Dean, College of Graduate Studies
Date: 4-7-93

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خلاصة الرسالة

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THESIS ABSTRACT

Full Name of Student: Waleed Ebrahim Al-Jasem

Title of Study: On the second smallest eigenvalue of the Laplacian

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The eigenvalues of a graph in this thesis are the eigenvalues of its Laplacian matrix. Let \( \lambda_{n-1} \) and \( f \) denote the second smallest eigenvalue and its corresponding eigenvector, respectively. A tree is said to be of type I if \( f \) has one or more zeros. A certain class of family having three pendant vertices is characterized to be of type I. Various properties in this class are investigated. Furthermore, centers and centroids are defined and characterized on that family. Centers, centroids and characteristic vertices of certain classes of caterpillars are investigated.

MASTER OF SCIENCE DEGREE
KING FAHD UNIVERSITY OF PETROLEUM & MINERALS
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INTRODUCTION

Let $G$ be a graph with vertex set $V = \{v_1, \ldots, v_n\}$ and edge set $E$. Denote by $L(G)$ the $n$-by-$n$ matrix $(a_{ij})$, where $a_{ij}$ is the degree of the vertex $i$ when $j = i$; $a_{ij} = -1$ when $j \neq i$ and $ij$ is an edge of $E$; and $a_{ij} = 0$. otherwise. While $L(G)$ depends on the labeling of $V$, its characteristic polynomial does not. If $\lambda_n \leq \lambda_{n-1} \leq \cdots \lambda_1$ are the eigenvalues of $L(G)$, then $\lambda_n = 0$ and $\lambda_{n-1} > 0$ if and only if $G$ is connected. For connected graphs, the eigenvectors of $L(G)$ corresponding to $\lambda_2$ afford “characteristic valuation” of $G$, a concept introduced by M Fiedler [9].

Chapters II and III explore the “characteristic vertices” arising from characteristic valuations of trees belonging to a family with specified properties. Trees with three end-vertices together with caterpillars are investigated. The location of a characteristic vertex is also compared with that of a center or a centroid of the tree.
Chapter 1

Basic Properties of the Laplacian Matrix of a Graph

We begin the thesis with an introductory chapter which consists of the basic definitions and concepts of graph theory and the Laplacian matrix. The origin of the problem with a historical background is given in the second section. Some of the known results about the Laplacian matrix are also presented. In the last section, we give the types of trees, introducing the characteristic edge and the characteristic vertex together with some examples.

1.1 Basic Definitions

A graph $G = (V, E)$ consists of two sets: a finite set $V$ of elements called vertices and a finite set $E$ of elements called edges. Each edge is identified with a pair of vertices. The vertices $v_i$ and $v_j$ associated with an edge $e$ are called the end vertices of $e$. The edge $e$ is then denoted as $e = v_i v_j$. If the edges of a graph
G are identified with ordered pairs of vertices, then G is called a directed graph. Otherwise, G is called an undirected graph. All edges having the same pair of end vertices are called parallel edges. If e = v_i v_i, then e is called a self-loop at vertex v_i. A graph is called a simple graph if it has no parallel edges or self loops. A graph G has order n if its vertex set has n elements. A graph with no edges is called an empty graph. A graph with no vertices (and hence no edges) is called a null graph.

An edge is said to be incident on its end vertices. Two vertices are adjacent if they are end vertices of some edge. If two edges have a common end vertex, then these edges are said to be adjacent. The number of edges incident on a vertex v_i is called the degree (valency) of the vertex. and it is denoted by d(v_i). A vertex of degree 1 is called a pendant vertex. A vertex of degree 0 is called an isolated vertex. δ(G) and Δ(G) denote, respectively, the minimum and maximum degrees in G.

A graph G' = (V', E') is a subgraph of the graph G = (V, E) if V' and E' are, respectively, subsets of V and E. The graph $\overline{G} = (V, E')$ is called the complement of a simple graph G = (V, E) if the edge v_i v_j is in E' if and only if it is not in E.

A walk in a graph G = (V, E) is a finite alternating sequence of vertices and edges $v_0, e_1, v_1, e_2, \ldots, v_{k-1}, e_k, v_k$ beginning and ending with vertices such that $v_{i-1}$ and $v_i$ are the end vertices of the edge $e_i, \quad 1 \leq i \leq k$. A walk is open if its end
vertices are distinct: otherwise it is closed. A walk is a trail if all its edges are distinct. An open trail is a path if all its vertices are distinct. A closed trail is a circuit if all its vertices except the end vertices are distinct. The number of edges in a path (circuit) is called the length of the path (circuit). A graph \(G\) is connected if there exists a path between every pair of vertices in \(G\).

Two graphs \(G_1\) and \(G_2\) are said to be isomorphic if there exists a one-to-one correspondence between their vertex sets and a one-to-one correspondence between their edge sets so that the corresponding edges of \(G_1\) and \(G_2\) are incident on the corresponding vertices of \(G_1\) and \(G_2\). A graph is said to be acyclic if it has no circuits. A tree is a connected acyclic graph.

The Laplacian matrix \(L(G)\) (also known as the degree matrix.) of a graph \(G\) with \(V(G) = \{v_1, v_2, \ldots, v_n\}\) is the \(n \times n\) matrix \(L(G) = (a_{ij})\), where

\[
a_{ij} = \begin{cases} 
\text{degree of } v_i, & \text{if } i = j, \\
-1, & \text{if there is an edge between vertex } v_i \text{ and vertex } v_j, \\
0, & \text{otherwise}.
\end{cases}
\]

The characteristic polynomial of \(G\) is defined to be the characteristic polynomial of the Laplacian matrix; i.e. the characteristic polynomial of \(G = \phi(G, \lambda) = |L(G) - \lambda I|\). The eigenvalues of a graph \(G\) of order \(n\) are defined to be the roots of the characteristic polynomial of \(G\). Since \(L(G)\) is a real symmetric matrix, the
eigenvalues of $G$ are real, and so can be ordered as follows:

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} \geq \lambda_n.$$  

The sequence of the $n$ eigenvalues is called the spectrum of $G$. The second smallest eigenvalue $\lambda_{n-1}$ is denoted by $\alpha(G)$; and it is called the algebraic connectivity of $G$. The family of all eigenvectors that correspond to $\alpha(G)$ is denoted by $\mathcal{E}(G)$.

The cartesian product $G_1 \times G_2$ of the graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is defined as $G_1 \times G_2 = (V_1 \times V_2, E)$ where $((u_1, u_2), (v_1, v_2)) \in E$ if and only if either $u_1 = v_1$ and $(u_2, v_2) \in E_2$ or $u_2 = v_2$ and $(u_1, v_1) \in E_1$.

As an example, see figure 1.1.1.

![Figure 1.1.1](image)

Let us mention two concepts related to the algebraic connectivity $\alpha(G)$ of a graph $G$.

The edge-connectivity of $G$, denoted by $\kappa(G)$ is the minimal number of edges whose removal disconnects $G$. Similarly, the minimal number of vertices of $G$
whose removal would result in losing connectivity of the graph $G$ is the vertex-connectivity of $G$, denoted by $\nu(G)$.

### 1.2 Historical Background and Applications of the Laplace Matrix of a Graph

There are several matrices which may be associated with a finite simple graph $G = (V, E)$. If $V = \{1, \ldots, n\}$, then perhaps the most commonly associated matrix is the $n \times n$ adjacency matrix, $A = A(G)$, defined by

$$
a_{ij} = \begin{cases} 
1, & \text{if } (i, j) \in E. \\
0, & \text{otherwise}.
\end{cases}
$$

Since $G$ is simple, $A$ is a symmetric $(0, 1)$ matrix with zero diagonal. The term "algebraic graph theory" may be defined as the theory which relates the geometric structure of $G$ with the spectral properties of $A$. Some excellent general references are the books by N. Biggs [3]; Cvetković, Doob, and Sachs [5]; and Cvetković, Doob, Gutman, and Torgasev [7]. An explosion of graph theory began in the 1950's with such people as Coollatz and Singowitz [4] and A.J. Hoffman [12].

Let the edge set of $G$ be $\{e_1, \ldots, e_m\}$. For each edge $e_j = v_i v_k$, choose one of the end vertices to be the positive end of $e_j$ and the other to be the negative end. We refer to this procedure by saying that $G$ has been given an orientation. The vertex-edge incidence matrix afforded by an orientation of $G$ is the $n \times m$ matrix.
\[ Q = (q_{ij}), \text{ where} \]

\[
q_{ij} = \begin{cases} 
+1, & \text{if } v_i \text{ is the positive end of } e_j, \\
-1, & \text{if it is the negative end} \\
0, & \text{otherwise} 
\end{cases}
\]

This matrix \( Q \) has been studied by Poincaré [14], among others.

The matrix that this thesis is concerned with is the matrix defined as

\[ L(G) = D(G) - A(G), \]

where \( D(G) \) is the diagonal matrix of vertex degrees.

This matrix is variously referred to as the Laplacian matrix, Kirchoff matrix, or matrix of Admittance. The term Laplacian comes from the fact that such matrices arise when using discretizations in looking for nontrivial solutions to \( \Delta \phi = \lambda \phi \) on a region \( \Omega \).

The origin of the Laplacian matrix can be dated back to Kirchoff [13] in an 1847 paper concerned with electrical networks through the well known matrix-tree theorem: if \( L = L(G) \), where \( G \) is a graph on \( n \) vertices, then:

\[ k(G) = (-1)^{i+j} \det L(i|j) \quad \text{for all } i, j = 1, \ldots, n \]

where \( k(G) \) is the number of spanning trees of \( G \) and \( L(i|j) \) is the matrix obtained from \( L(G) \) by deleting the \( i \)-th row and \( j \)-th column.
Forsman [10] and Gutman [11] have shown how the connection between \( L(G) = QQ^t \) and \( K(G) = Q^tQ \) simultaneously explain the statistical and the dynamic properties of flexible branched polymer molecules. Indeed, since \( L(G) \) and \( K(G) \) share the same nonzero eigenvalues, it follows that for bipartite graphs the smallest eigenvalue of \( A(G^*) \geq -2 \), where \( G^* \) is the line graph of \( G \). This observation, first made by Hoffman, has led to a new direction in spectral theory [6], [7]. Eichinger [8] has shown how the spectrum of \( L(G) \) may be used to calculate the radius of gyration of a Gaussian molecule. Due to its importance in physical and chemical properties, the spectrum of \( L(G) \) is more natural and important than the more widely studied adjacency spectrum. In [2], Bier uses the smallest positive eigenvalue of \( L(G) \) to estimate the “magnifying coefficient” of \( G \).

Another application within mathematics is in the problem of decomposition of graphs. The second smallest eigenvalue of \( L(G) \) is used in characterizing reducibility. It was proved [7] that a connected graph can be decomposed into two subgraphs by the signs of the eigenvector belonging to the second smallest eigenvalue.

### 1.3 Known Results on the Laplacian Matrix

In this section, known results about the Laplacian matrix are given.

**Theorem 1.3.1.** The number 0 is an eigenvalue of every tree.
Proof: Let $T$ be a tree of order $n$, and $L$ is the Laplacian matrix of $T$. If

$$\bar{u} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

is a vector of dimension $n$, then $L\bar{u} = \vec{0} = 0\bar{u}$. So, 0 is an eigenvalue of $L$.

Theorem 1.3.2 [16]. Let $\lambda > 1$ be an integer. If $\lambda$ is an eigenvalue of $L$, then $\lambda$ must divide $n$.

Theorem 1.3.3 [6]. If $K_n$ is the complete graph of order $n$, then $L(K_n) = nI - J$, where $J$ is the $n \times n$ matrix all of whose entries are ones.

Theorem 1.3.4 [6]. If $\overline{G}$ is the complement of $G$, then

$$L(G) + L(\overline{G}) = nI - J.$$ 

Theorem 1.3.5 [6]. The edge connectivity $e(G)$, the vertex connectivity $\nu(G)$ and the algebraic connectivity $\alpha(T)$ of any graph $G$ of order $n$ satisfy

$$e(G) \geq \nu(G) \geq \alpha(G).$$

Theorem 1.3.6 [14]. If $\mathbb{R}_n$ is the space of all real column vectors with $n$ coordinates, and

$$S = \left\{ x = (x_1, \ldots, x_n)^T \in \mathbb{R}_n; \quad \sum_{i=1}^{n} x_i = 0, \quad \sum_{i=1}^{n} x_i^2 = 1 \right\}.$$
then the algebraic connectivity of $G = (V, E)$ satisfies

$$a(G) = \min_{x \in S} \sum_{i < k} (x_i - x_k)^2,$$

or

$$a(G) = \min_{x \in S} x^T L(G)x.$$

**Theorem 1.3.7 [1].** The algebraic connectivity $a(G)$ satisfies the following properties:

1. $a(G) \geq 0$, $a(G) = 0 \iff G$ is not connected.

2. If $G_1 = (V, E_1)$ and $G_2 = (V, E_2)$ and $E_1 \subset E_2$, then $a(G_1) \leq a(G_2)$.

3. If $G_1 = (V, E_1)$, $G_2 = (V, E_2)$ and $E_1 \cap E_2 = \emptyset$, then $a(G_1) + a(G_2) \leq a(G_3)$ where $G_3 = (V, E_1 \cup E_2)$.

4. If $G_1$ is obtained from $G$ by removing $k$ vertices (and incident edges), then

$$a(G_1) \geq a(G) - k.$$

**Theorem 1.3.8 [1].** Let $G_1$ and $G_2$ be graphs. Then

$$a(G_1 \times G_2) = \min(a(G_1), a(G_2)).$$

**Theorem 1.3.9.** For the complete graph $K_n$, the spectrum of $K_n$ is:

$$\begin{pmatrix}
0 & n \\
1 & n - 1
\end{pmatrix}$$
Proof: If $L(K_n)$ is the Laplacian matrix of $K_n$, then:

$$
|L(K_n) - \lambda I| = \begin{vmatrix}
  n - 1 - \lambda & -1 & -1 & \cdots & -1 \\
  -1 & n - 1 - \lambda & -1 & \cdots & -1 \\
  -1 & -1 & n - 1 - \lambda & \cdots & -1 \\
  \cdot & \cdot & \cdot & \ddots & \cdot \\
  -1 & -1 & -1 & \cdots & n - 1 - \lambda \\
\end{vmatrix}
$$

Subtract the first column of $|L(K_n) - \lambda I|$ from all the other columns of $|L(K_n) - \lambda I|$. Then we get:

$$
|L(K_n) - \lambda I| = \begin{vmatrix}
  n - 1 - \lambda & -n + \lambda & -n + \lambda & \cdots & -n + \lambda \\
  -1 & n - \lambda & 0 & \cdots & 0 \\
  -1 & 0 & n - \lambda & \cdots & 0 \\
  \cdot & \cdot & \cdot & \ddots & \cdot \\
  -1 & 0 & 0 & \cdots & n - \lambda \\
\end{vmatrix}
$$

Now adding to the first row of the above matrix every one of the other rows,
we get:

$$|L(K_n) - \lambda I| = \begin{vmatrix} -\lambda & 0 & 0 & \cdots & 0 \\ -1 & n - \lambda & 0 & \cdots & 0 \\ -1 & 0 & n - \lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & 0 & \cdots & n - \lambda \end{vmatrix} = -\lambda(n - \lambda)^{n-1}.$$ 

Therefore, the spectrum of $K_n$ is:

$$\begin{pmatrix} 0 & n \\ 1 & n-1 \end{pmatrix}.$$

**Theorem 1.3.10** [7]. Let $G$ be a graph of order $n$. Let $\overline{G}$ be its complement. If $\lambda_1 = 0 \leq \lambda_2 \leq \cdots \leq \lambda_n$ are the eigenvalues of $L(G)$, then $\lambda' = \lambda'_2 \leq \cdots \leq \lambda'_n$ are the eigenvalues of $L(\overline{G})$ where

$$\lambda'_k = n - \lambda_{n+2-k}, \quad k = 2, \ldots, n.$$ 

In addition, the eigenvectors of $L(\overline{G})$ corresponding to $\lambda'_k$ and those of $L(G)$ corresponding to $\lambda_{n+2-k}$ coincide.

**Theorem 1.3.11.** If $m$ is the minimum valency of a noncomplete graph $G$, then $a(G) \leq m$.

The star $S_n$ is a tree of order $n$, having $n - 1$ pendant vertices and one vertex of degree $n - 1$. Figure 1.2.1 shows the general shape of $S_n$. 
Theorem 1.3.12. If $S_n$ is a star of order $n$, then the spectrum of $S_n$ is:

$$
\begin{pmatrix}
0 & n & 1 \\
1 & 1 & n-2
\end{pmatrix}.
$$

Proof: If $L(S_n)$ is the Laplacian matrix of $S_n$, then:

$$
|L(S_n) - \lambda I| =
\begin{vmatrix}
1 - \lambda & 0 & 0 & \cdots & -1 \\
0 & 1 - \lambda & 0 & \cdots & -1 \\
0 & 0 & 1 - \lambda & \cdots & -1 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
-1 & -1 & -1 & \cdots & n - 1 - \lambda
\end{vmatrix}
$$

Add to the last row of $|L(S_n) - \lambda I|$ every other row multiplied by $\left(\frac{1}{1-\lambda}\right)$. Then we get:

$$
|L(S_n) - \lambda I| =
\begin{vmatrix}
1 - \lambda & 0 & 0 & \cdots & -1 \\
0 & 1 - \lambda & 0 & \cdots & -1 \\
0 & 0 & 1 - \lambda & \cdots & -1 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & n - 1 - \lambda - \frac{(n-1)}{1-\lambda}
\end{vmatrix}
$$
\[
= \left[ n - 1 - \lambda - \left( \frac{n - 1}{1 - \lambda} \right) \right] (1 - \lambda)^{n - 1} \\
= \lambda(\lambda - n)(1 - \lambda)^{n - 2}
\]

Therefore, the spectrum of \( S_n \) is:

\[
\begin{pmatrix}
0 & n & 1 \\
1 & 1 & n - 2
\end{pmatrix}
\]

**Theorem 1.3.13** [1]. If \( C_n \) is a circuit of order \( n \), then

\[
a(C_n) = 2 \left( 1 - \cos \frac{2\pi}{n} \right)
\]

**Theorem 1.3.14** [5]. (Interlacing Theorem). Let \( G \) be a graph with spectrum \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \) and let the spectrum of \( G - v_1 \) be \( \mu_1 \geq \mu_2 \geq \cdots \geq \mu_{p-1} \). Then the spectrum of \( G - v_1 \) is "interlaced" with the spectrum of \( G \); that is,

\[
\lambda_1 \geq \mu_1 \geq \lambda_2 \geq \mu_2 \geq \cdots \geq \mu_{p-1} \geq \lambda_p.
\]

**Theorem 1.3.15.** Let \( T \) be a tree of order \( n \), and \( \bar{f} = (x_1, \ldots, x_n)^t \in E(T) \), then:

\[
\sum_{i=1}^{n} x_i = 0.
\]

**Proof.** Since the vector \( \bar{u} = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \) is an eigenvector of \( L \) corresponding to zero,
i.e., \( L \vec{u} = 0 \vec{u} \), then each \( \vec{x} \in \mathcal{E}(T) \) must be perpendicular to it, i.e.

\[
\vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \quad \text{and} \quad \vec{x} \cdot \vec{u} = 0 \quad \text{or} \quad \sum_{i=1}^{n} x_i = 0.
\]

Theorem 1.3.16. Let \( T \) be a tree of order \( n \). Then, \( a(T) \) is bounded as follows:

\[
0 = \lambda_n < \lambda_{n-1} = a(T) \leq 1.
\]

Proof. Since \( T \) is connected, \( a(G) = \lambda_{n-1} \neq 0 \) (Theorem 1.3.7(1)). Also, using Theorem 1.3.11, \( a(T) \leq 1 \).

1.4 Types of Trees

We will discuss two types of trees according to the corresponding eigenvectors of \( a(T) \). Type I and type II trees will be defined and some results will be obtained based on type I trees.

Theorem 1.4.1 [9]. Let \( T \) be a tree. Suppose \( \vec{z} = (z_1, \ldots, z_n)^t \) is an eigenvector of \( L(T) \) corresponding to \( a(T) \). Then two cases can occur:

1. \( \vec{V} = \{ i \in V | z_i = 0 \} \neq \phi \), then the graph \( \tilde{T} = (\vec{V}, \tilde{E}) \) induced by \( T \) on \( \vec{V} \) is connected and there exists exactly one vertex \( j \in \vec{V} \) which is adjacent (in
$T$) to a vertex not belonging to $\bar{V}$. Moreover, the values of $\bar{z}$ along any path starting at $j$ are increasing, decreasing, or identically zero.

2. If $z_i \neq 0$ for all $i \in V$, then $T$ contains exactly one edge $jk$ such that $z_j$ and $z_k$ have different signs, say $z_j > 0$ and $z_k < 0$. Moreover, the values of $\bar{z}$ along any path that starts at $j$ and does not contain $k$ increase while the values of $\bar{z}$ along any path that starts at $k$ and does not contain $j$ decrease.

If a tree satisfies the first case of the previous theorem then it is called a type I tree, and if it satisfies the second case, then it is a type II tree.

The vertex described in the first part of the above theorem is referred to as the characteristic vertex of $T$, and the edge described in the second part of that theorem is called the characteristic edge of $T$.

Theorem 1.4.2. Let $T = (V, E)$ be a tree. Let $g, h \in \mathcal{E}(T)$. Then $u \in V$ is a characteristic vertex of $T$ afforded by $g$, if and only if $u$ is a characteristic vertex of $T$ afforded by $h$.

Proof: If $a(T)$ is a simple eigenvalue, then $g$ is a nonzero multiple of $h$ and the result is immediate from the definitions. So, we assume $a(T)$ is a multiple root. Let $V_0 = \{v \in V|z(v) = 0 \text{ for all eigenvectors } z \text{ corresponding to } a(T)\}$. If $V_0$ were empty, we could find some $z$ such that $z(v) \neq 0$ for all $v \in V$. This contradicts Theorem 1.4.1.
Theorem 1.4.3 [1]. If \( T \) is a tree, and \( a(T) \) is multiple, then \( T \) is of type \( I \).

Theorem 1.4.4 [16]. (A Reduction Theorem for Type I Trees). Let \( T = (V, E) \) be a tree on \( n \geq 4 \) vertices. Suppose there is an eigenvector \( \vec{X} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \) belonging to \( a(T) \) and a pendant vertex \( v \in V \) such that \( x_v = 0 \). Let \( u \) be the vertex adjacent to \( v \). Denote by \( T_1 = (V_1, E_1) \) the subgraph obtained from \( T \) by deleting \( v \) from \( V \) and \( \{u, v\} \) from \( E \). Then

(i) \( x_u = 0 \)

(ii) \( a(T_1) = a(T_2) \)

(iii) \( \vec{X}|_{V_1} \) is an eigenvector belonging to \( a(T_1) \), where \( \vec{X}|_{V_1} \) is the restriction of \( \vec{X} \) to \( V_1 \).

(iv) \( F(T_1) = F(T_2) \) where \( F(T) \) denotes the set of characteristic vertices of \( T \).

Example 1.4.1. Let \( T \) be the tree shown below in Figure 1.4.1.

![Figure 1.4.1](image)

Then the characteristic polynomial of \( T \) is

\[
x(x^2 - 3x + 1)^2(x^2 - 6x + 7)
\]
and $a(T) = \frac{3 - \sqrt{5}}{2} \approx 0.382$ has multiplicity 2. One eigenvector belonging to $a(T)$ is shown in Figure 1.4.1.

If vertex $v$ and its edge are erased, the result is $T_1$, as shown in Figure 1.4.2.

![Figure 1.4.2]

Not only that, but the numbers which remain constitute an eigenvector belonging to $a(T_1)$. Indeed, the characteristic polynomial of $T_1$ is

$$x(x - 2)(x^2 - 3x + 1)(x^2 - 5x + 3)$$

and one can check that $a(T_1) = a(T)$. (In the case of $T_1$, $\frac{3 - \sqrt{5}}{2}$ is a simple eigenvalue). We may apply the theorem again by removing vertex $u$ from $T_1$, obtaining the eigenvectors of $a(T_2)$ as shown in Figure 1.4.3. The characteristic polynomial of $T_2$ is

$$x(x^2 - 3x + 1)(x^2 - 5x + 5).$$

One can check that $a(T_2) = a(T)$, too. Since there is no longer a pendant vertex of value 0, the reduction process stops.

![Figure 1.4.3]
Example 1.4.2. The reduction process described in Theorem 1.4.4 and in Example 1.4.1 is not entirely reversible. If we increase the degree of vertex \( v \) in Figure 1.4.1 by attaching a new pendant vertex to it, we obtain a tree \( T' \) of type II.

\[
\begin{align*}
-0.61 & -1.4 & -1.84 \\
1 & .76 & .33 & .76 & 1
\end{align*}
\]

Figure 1.4.4

The characteristic polynomial for \( T' \) is

\[ q(x) = x(x - 2)(x^2 - 3x + 1)(x^4 - 4x^3 + 25x^2 - 22x + 4). \]

While it is true that \( \lambda = \frac{3 - \sqrt{5}}{2} \) is an eigenvalue of \( L(T') \), \( \lambda \) is greater than the simple eigenvalue of \( a(T') = 0.2434 \). An approximate valuation of \( T' \) is shown in Figure 1.4.4.

Theorem 1.4.5. (A Partial Converse to the Reduction Theorem).

Let \( T = (V, E) \) be a type I tree. Choose an eigenvector \( f \) belonging to \( a(T) \) and choose \( w \in V \) such that \( f(w) = 0 \). Let \( T' = (V', E') \) be a tree obtained from \( T \) by adjoining a new pendant vertex \( u \) at \( w \). (So, \( V' = V \cup \{u\} \) and \( E' = E \cup \{(u, v)\} \)).

Then \( a(T) \) is an eigenvalue of \( L(T') \). If \( a(T') = a(T') \), then \( F(T) = F(T') \) and \( f' \) is an eigenvector belonging to \( a(T') \), where \( f'(v) = f(v), \quad v \in V, \) and \( f'(u) = 0 \).
Chapter 2

Trees With Three End-Vertices

Let $T$ be the family of trees with three end vertices. If $T \in T$, and $T$ is a type I tree, then what is the general shape of $T$? In this chapter we will partially answer this question by introducing the basic definitions and concepts of passive and active branches. Furthermore, automorphism of graphs is given together with two important theorems. Also, some basic and important theorems for the tree $T \in T$ are given together with the proofs.

In the last section, we give a list of theorems characterizing a class of type I trees $T \in T$, together with the general form of the characteristic eigenvector of $a(T)$. Furthermore, the characteristic vertices of these trees are determined and the values of $a(T)$ are given.
2.1 Passive and Active Branches; Automorphism

Suppose \( v \) is a vertex of a tree \( T \). Denote by \( T_v \) the subgraph of \( T \) obtained by deleting \( v \) and all edges incident with it. A branch (of \( T \)) at \( v \) is a connected component of \( T_v \). If \( T \) is a type I tree, \( v = w_T \), the characteristic vertex of \( T \), \( \vec{f} \in \mathcal{E}(T) \), and \( B \) is a branch at \( w_T \), then \( f \) is uniformly +, uniformly −, or identically zero on the vertices of \( B \). Of course, every \( \vec{f} \in \mathcal{E}(T) \) is orthogonal to the vector each of whose component is 1, i.e. an eigenvector afforded by 0. Thus there will always be a positive branch and a negative branch at \( w_T \) for any characteristic valuation.

If \( B \) is a branch at \( v \), we denote by \( r(B) \) the vertex of \( B \) which is adjacent (in \( T \)) to \( v \). It will frequently be convenient to view \( B \) as a rooted tree. In such a situation, we always take \( r(B) \) as the root. If \( v = w_T \) and \( f \in \mathcal{E}(T) \), then \( f(r(B)) \) determines the sign of \( f \) throughout \( B \).

Let \( T \) be a type I tree. Let \( B \) be a branch at \( w_T \). We call \( B \) passive if \( f(r(B)) = 0 \) for every \( f \in \mathcal{E}(T) \). A branch at \( w_T \) is active if it is not passive.

Theorem 2.1.1 (15) Let \( T \) be a type I tree with characteristic vertex \( w \) and algebraic connectivity \( a(T) \). Let \( m \) be the multiplicity of \( a(T) \) as an eigenvalue of \( L(T) \). Then exactly \( m + 1 \) of the branches at \( w \) are active.
Theorem 2.1.2 (15) Let \( w \) be a vertex of the tree \( T = (V, E) \). Suppose \( B_1 = (V_1, E_1) \) and \( B_2 = (V_2, E_2) \) are two (different) branches of \( T \) rooted at \( w \). Let \( \alpha : V_1 \to V_2 \) be an isomorphism of the rooted trees \( B_1 \) and \( B_2 \). (Then, in particular, \( \alpha(w) = w \).) Let \( f \in \mathcal{E}(T) \) be fixed but arbitrary, then either

(i) \( f(\alpha(v)) = f(v) \), \( v \in V_1 \), or

(ii) \( F(T) = \{w\} \) and there is a \( g \in \mathcal{E}(T) \) such that \( g(v) = -g(\alpha(v)) > 0 \), \( w \neq v \in V_1 \); and \( g(v) = 0 \), \( v \notin V_1 \cup V_2 \).

Let \( w \) be a vertex of the tree \( T = (V, E) \). Suppose \( B_1 = (V_1, E_1) \) and \( B_2 = (V_2, E_2) \) are two branches of \( T \) rooted at \( w \). Assume the rooted trees \( B_1 \) and \( B_2 \) are isomorphic. We say that \( f \in \mathcal{E}(T) \) distinguishes \( B_1 \) from \( B_2 \) if there is an isomorphism

\[ \alpha : V_1 \to V_2 \]

such that \( f(\alpha(v)) \neq f(v) \) for some \( v \in V_1 \).

Theorem 2.1.3 (15) Let \( T = (V, E) \) be a tree. Choose \( w \in V \). Suppose there are \( k > 2 \) branches \( B_1 = (V_1, E_1), \ldots, B_k = (V_k, E_k) \) rooted at \( w \). If these branches are all isomorphic as rooted trees, and if there is a characteristic valuation of \( T \) which distinguishes \( B_1 \) from \( B_2 \), then the multiplicity of \( a(T) \) is at least \( k - 1 \).

Theorem 2.1.4 (15) Let \( T = (V, E) \) be a type I tree with characteristic vertex \( w \) and algebraic connectivity \( a(T) \). Let \( f \in \mathcal{E}(T) \). Suppose \( T' = (V', E') \) is the
tree obtained from $T$ by adjoining a new pendant vertex $p$, to $w$. [So, $V' = V \cup \{p\}, \ E' = E \cup \{(p,w)\}.$] Extend $f$ to a function $f'$ on $V'$ by defining $f'(p) = 0$. Then $a(T') = a(T)$ and $f' \in \mathcal{E}(T')$. [In particular, $T'$ is a type I tree with the characteristic vertex $w$.]

2.2 Basic Results on the Laplacian Matrix of a Tree

The next few theorems are just basic results on arbitrary trees of type I. Some of the proofs are presented to simplify the restriction to $T$. They will be used in the next section.

Theorem 2.2.1 Let $\{i,j\} \in E$ and $z_i > 0, \ z_j > 0$. Suppose also that vertex $i$ is on the unique path from vertex $j$ to either the characteristic vertex of $T$ (Case 1) or the characteristic edge of $T$ (Case 2). If the degree of vertex $j$ is $k+1$, let vertices $i_1, i_2, \ldots, i_k$ be the other neighbors of $j$ besides $i$. Then

1. $z_i < z_j < z_s, \ s = 1, \ldots, k$

and

2. $z_j - z_i = a \cdot z_j + \sum_{s=1}^{k} (z_{i_s} - z_j)$ where $a = a(T)$.
Proof:

1. Assume that \( \tilde{V} = \{ i \in V | z_i = 0 \} \neq \emptyset \), then call the characteristic vertex of \( T \), \( c \). Then any path from \( c \) to \( i_s \) will be either increasing or decreasing. (The values of \( z \) along this path cannot be identically zero, since otherwise \( z_i \) and \( z_j \) will be zero.) If the values of \( z \) along this path are decreasing, then \( z_i < 0, \ z_j < 0 \) (contradiction). So the values of \( z \) along this path is increasing, and so \( z_i < z_j < z_{i_s} \).

Assume that \( \tilde{V} = \emptyset \), then the characteristic edge of \( T \) is say \( \ell, k \) such that \( z_\ell > 0, \ z_k < 0 \). Consider the path from \( \ell \) to \( i_s \); if the path contains \( k \), then the path from \( k \) to \( i_s \) is decreasing, but \( z_k < 0 \); so \( z_s, z_j, z_i < 0 \) (contradiction). So the path does not contain \( k \), so the path must be increasing for the values of \( z \). Therefore, \( z_i < z_j < z_{i_s} \).

2. Since \( a \) is the smallest eigenvalue for \( L \), then

\[
L \vec{z} = a \vec{z} \quad \text{where} \ \vec{z} \ \text{is the corresponding eigenvector.}
\]

Then by considering the \( j \)-th element of this equality we have:

\[
-z_i + (k + 1)z_j - z_i - z_{i_2} - \cdots - z_{i_s} = az_j
\]

\[
\Rightarrow -z_i + kz_j + z_j - \sum_{i=1}^{k} z_{i_s} = az_j
\]

\[
\Rightarrow z_j - z_i = az_j + \sum_{i=1}^{k} (z_{i_s} - z_j)
\]
Remark 2.2.1 Let $T$ be a tree with $\lambda_{n-1} = a$. If $i$ is a vertex with degree $d$, then for any eigenvector $\bar{X} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$ belonging to $a$, we have:

$$\sum_{(ij) \in E} x_j = (d - a) x_i.$$

Proof: By the definition of the eigenvalue $a$, we have:

$$L \bar{X} = a \bar{X}.$$

By the definition of the Laplacian matrix, we will get:

$$- \sum_{(ij) \in E} x_j + dx_i = ax_i \quad \text{for the } x_i \text{ element in } x$$

$$\Rightarrow \sum_{(ij) \in E} x_j = (d - a) x_i$$

Remark 2.2.2 Suppose $v$ is a pendant vertex with $(u, v) \in E$. If $\bar{X} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$, then $x_u = (1 - a)x_v$. In particular, if $a = 1$, then $x_u = 0$ for every $u$ adjacent to a pendant vertex. In addition, if $x_u = 0$, then $x_u = 0$, i.e., a pendant vertex is never an isolated zero of an eigenvector belonging to $a$. 
Theorem 2.2.2 Let $T$ be a tree as shown in Figure 2.2.1 which has a path of order $k$ as a subtree of $T$. If $g = (a_1, \ldots, a_n)' \in \mathcal{E}(T)$, then:

$$a_i = a_1 f_i(a); \quad i = 2, \ldots, k$$

where $f_i(a)$ is a polynomial in $a$.

Proof: By Remark 2.2.2

$$\Rightarrow a_2 = (1-a)a_1 = a_1 f_2(a) \text{ where } f_2(a) = (1-a).$$

Again,

$$a_1 \div a_3 = (2-a)a_2$$

$$\Rightarrow a_3 = (2-a)a_2 - a_1$$

$$= (2-a)(1-a)a_1 - a_1 = [(2-a)(1-a) - 1]a_1$$

$$= a_1 f_3(a) \text{ where } f_3(a) = (2-a)(1-a) - 1$$

$$a_i + a_{i-2} = (2-a)a_{i-1}$$

$$\Rightarrow a_i = (2-a)a_{i-1} - a_{i-2}.$$
Assume that the statement is true for $a_1, a_2, \ldots, a_{i-1}$.

\[ a_i = (2 - a) a_{i-1}(a) - a_{i-2}(a) \]

\[ = a_1 [(2 - a) f_{i-1}(a) - f_{i-2}(a)] \]

\[ a_i = a_i f_i(a). \]

**Theorem 2.2.3** If $T$ is a tree of order $n$, and the diameter of $T$ is $d$, then $a(T) \leq 2 \left(1 - \cos \frac{\pi}{d+1}\right)$.

**Proof:** Let $n = d + k + 1$ and let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} > \lambda_n = 0$ be the eigenvalues of $T$. If we have more than one longest path, then specify one of them, say $P_1$. Remove one pendant vertex which is not belonging to $P_1$ (say $v_1$). Let $T_1$ be the tree obtained after removing $v_1$, having the spectrum:

\[ \mu_1^{(1)} \geq \mu_2^{(1)} \geq \cdots \geq \mu_{n-2}^{(1)} > \mu_{n-1}^{(1)} = 0. \]

By using the Interlacing Theorem 1.3.14, we have:

\[ \lambda_1 \geq \mu_1^{(1)} \geq \lambda_2 \geq \mu_2^{(1)} \geq \cdots \geq \mu_{n-2}^{(1)} \geq \lambda_{n-1} > \mu_{n-1}^{(1)} = \lambda_n = 0. \]

Again, remove one pendant vertex $v_2$ which is not belonging to $P_1$ to get the tree $T_2$. Let the spectrum of $T_2$ be:

\[ \mu_1^{(2)} \geq \mu_2^{(2)} \geq \cdots \geq \mu_{n-3}^{(2)} > \mu_{n-2}^{(2)} = 0. \]
Using the Interlacing Theorem, we get:

\[ \mu_1^{(1)} \geq \mu_1^{(2)} \geq \mu_2^{(1)} \geq \mu_2^{(2)} \geq \cdots \geq \mu_{n-3}^{(2)} \geq \mu_{n-2}^{(1)} > \mu_{n-2}^{(2)} = \mu_{n-1}^{(1)} = 0. \]

We remove pendant vertices which are not belonging to \( P_1 k \)-times so that we get a path of order \( d + 1 \). Let \( \mu_1^{(i)} \geq \mu_2^{(i)} \geq \cdots \geq \mu_{n-i}^{(i)} = 0 \) be the eigenvalues of the tree \( T_i \) after removing the vertex \( r_i \). Again, applying the Interlacing Theorem we get:

\[ \mu_{n-k}^{(k)} \geq \mu_{n-k}^{(k-1)} \geq \mu_{n-k-2}^{(k-2)} \geq \cdots \geq \mu_{n-2}^{(1)} \geq \lambda_{n-1} \]

but by Theorem 2.3.3 \( \mu_{n-k-1}^{(k)} = a(P_{n-1}) = 2 \left( 1 - \cos \frac{\pi}{d+1} \right) \), \( \lambda_{n-1} = a(T) \Rightarrow a(T) \leq 2 \left( 1 - \cos \frac{\pi}{d+1} \right) \).

### 2.3 Towards a Characterization of Type I Trees with Three End-Vertices

In this section, we will study all trees \( T \in T \) which are of type I, giving their general shape. We will also locate the characteristic vertices of these trees. Furthermore, we will give the general formulas for \( a(T) \) with the corresponding eigenvector(s).

**Theorem 2.3.1** If \( T \in T \) is a tree of type I, then the multiplicity of \( a(T) \) is not more than 2.

**Proof:** If the multiplicity is more than 2, then by Theorem 2.1.1, the active branches are at least 4. But we could only have 2 or 3 branches.
Theorem 2.3.2 If $T$ is of order $n = 3k + 1$, having the shape shown in Figure 2.3.1, then:

1. $T$ is of type I.

2. The only characteristic vertex is $v_3$.

3. There exists $f \in \mathcal{E}(T)$ such that $|\tilde{V}| = 1$ where $\tilde{V} = \{v_i : \tilde{f}(v_i) = 0\}$.

Proof: The three branches rooted at $v_3$ are all isomorphic as rooted trees. Call them $B_1, B_2$ and $B_3$. Assume that there is no characteristic valuation of $T$ which distinguishes $B_1$ from $B_2$, $B_2$ from $B_3$, or $B_1$ from $B_3$. If we have $f(v), \quad v \in B_1$ is somewhere positive and somewhere negative, then according to our first assumption $f(B_2)$ and $f(B_3)$ will be so, and this contradicts Theorem 1.4.1. So, $f(B_1), f(B_2)$ and $f(B_3)$ are either all positive or all negative.

By Theorem 1.3.15, $\tilde{f}(v_3) = - \sum_{\substack{\gamma \in \mathcal{U} \setminus \{v_3\} \in \mathcal{E}(T)}} f(v_i)$. This result again contradicts Theorem 1.4.1. Therefore, this is a contradiction to our first assumption. As a result, there exists a characteristic valuation of $T$ which distinguishes two of the branches.

According to Theorem 2.1.3, the multiplicity of $a(T)$ is at least 2. By Theorem 1.4.3 the graph is of type I. Also, by Theorem 2.3.1, the multiplicity of $a(T)$ is 2.
Now, if the characteristic vertex $w_T \neq v_3$, then we will have at most 2 active branches, but by Theorem 2.1.1, we should have 3 active branches at $w_T$, and we have a contradiction. Therefore, $w_T = v_3$. Now, since we have 3 active branches at $w_T = v_3$, $\bar{V} = \{v_3\}$.

**Theorem 2.3.3** [6] If $P_n$ is a path of order $n$, then the eigenvalues of $L(P_n)$ are

$$\lambda_1 = 4 \sin^2 \left( \frac{\pi k}{2n} \right), \quad k = 0, 1, 2, \ldots, n - 1.$$ 
$$a(P_n) = \lambda_1 = 4 \sin^2 \left( \frac{\pi}{2n} \right).$$

![Figure 2.3.2](image)

**Theorem 2.3.4** If $P_{2k+1}$ is a path of order $2k + 1$, labelled as shown in figure (2.3.2), then:

1. The path is of type I.

2. The only characteristic vertex is $w_T = v_{k+1}$. 
3. The multiplicity of $a(T)$ is one, and if $\vec{f} \in E(P_{2k+1})$, then

$$\vec{f} = \left( \begin{array}{c}
  a_1 \\
  a_1f_2(a) \\
  a_1f_3(a) \\
  \vdots \\
  a_1f_k(a) \\
  \vdots \\
  -a_1f_k(a) \\
  -a_1f_{k-1}(a) \\
  \vdots \\
  -a_1f_3(a) \\
  -a_1f_2(a) \\
  -a_1
\end{array} \right)$$

where $a_1$ is a nonzero real number, and $f_i(a)$ are polynomials in $a$.

Proof: Let $\vec{f} \in E(P_{2k+1})$ and $\vec{f}(v_i) = a_i$. By using Theorem 2.2.4,

$$\vec{f}(v_{k+1}) = a_1f_{k+1}(a) = a_{2k+1}f_{k+1}(a)$$

$$\Rightarrow (a_1 - a_{2k+1})f_{k+1}(a) = 0.$$

If $a_1 = a_{2k+1}$ then either $\sum_{i=1}^{2k+1} \vec{f}(v_i) \neq 0$ which contradicts Theorem 1.3.15, or we will have more than 2 characteristic vertices which contradicts Theorem 1.4.1.

Therefore, $f_{k+1}(a) = 0$ and $f(v_{k+1}) = 0$. So, the path is a type I tree. Since we don't have more than 2 branches, then by using Theorem 2.1.1, the multiplicity
of \( a(T) \) is one. Again, by Theorem 2.2.4,

\[
\bar{f} = \begin{pmatrix}
    a_1 \\
    a_1 f_2(a) \\
    a_1 f_3(a) \\
    \vdots \\
    a_k f_k(a) \\
    \quad \ddots \\
    a_{2k+1} f_{2k}(a) \\
    \vdots \\
    a_{2k+1} f_{2k+1}(a) \\
    a_{2k+1}
\end{pmatrix}
\]

By using Remark 2.2.2:

\[ a_k + a_{k+2} = 0 \Rightarrow a_k = -a_{k+2}. \]
So \( a_1 f_k(a) = -a_{2k+1} f_k(a) \). Since \( f_k(a) \neq 0 \), \( a_1 = -a_{2k+1} \), and so

\[
\begin{pmatrix}
a_1 \\
a_1 f_2(a) \\
a_1 f_3(a) \\
\vdots \\
a_1 f_k(a) \\
o \\
a_1 f_k(a) \\
\vdots \\
a_1 f_3(a) \\
a_1 f_2(a) \\
a_1 \\
\end{pmatrix}
\]

Figure 2.3.3

**Theorem 2.3.5** If \( T \) is of order \( n = 2k + 2 \), having the shape shown in figure 2.3.3, then:

1. \( T \) is of type I.
2. The only characteristic vertex is $w_T = v_{k+1}$.

3. $\hat{V} = \{v_{2k+1}, v_{2k+2}\}$.

4. $a(T) = 4 \sin^2 \left( \frac{\pi}{2(2k+1)} \right)$.

5. If $B_1 = (V_1, E_1)$ and $B_2 = (V_2, E_2)$ are the two (different) isomorphic branches of $T$ rooted at $v_{k+1}$, and $\alpha : V_1 \to V_2$ is an isomorphism of the rooted trees $B_1$ and $B_2$, then there exists $\bar{f} \in \mathcal{E}(T)$ such that $\bar{f}(v) = -\bar{f}(\alpha(v)) > 0, \ v \notin \{v_{2k+1}, v_{2k+3}\}$, and $f(v_{k+1}) = f(v_{2k+2}) = 0$.

Proof: Let $P_{2k+1}$ be a path of order $2k + 1$, then adjoin the vertex $v_{2k+2}$ to the vertex $v_{k+1}$, obtaining the tree $T$ shown in figure 2.3.3. By Theorems 2.1.4 and 2.3.4 $a(T) = a(P_{2k+1}) = 4 \sin^2 \left( \frac{\pi}{2(2k+1)} \right)$ and if $\bar{g} \in \mathcal{E}(P_{2k+1})$ such that $\bar{g}(v) = -\bar{g}(\alpha(v)) > 0, \ v_{k+1} \neq w \in V_1$, and $\bar{g}(v_{k+1}) = 0$, and $\bar{f}$ is the extension of $\bar{g}$ by defining $\bar{f}(v_{2k+2}) = 0$, then $\bar{f} \in \mathcal{E}(T)$ and so $T$ is type I tree with characteristic vertex $w_T = v_{k+1}$. Therefore all parts of the theorem are proved.

Theorem 2.3.6 Let $T$ be as shown in figure 2.3.1. Then $a(T) = 4 \sin^2 \left( \frac{\pi}{2(2k+1)} \right)$.

Proof: By Theorem 2.1.2, we will have two cases:

1. there exists $\bar{f} \in \mathcal{E}(T)$ s.t. $\bar{f}(\alpha(v)) = f(v), \ v \in V_1$, or

2. $F(T) = \{w\}$ and there is a $\bar{g} \in \mathcal{E}(T)$ such that $\bar{g}(v) = \bar{g}(\alpha(v)) > 0, \ w \neq v \in V_1$, and $\bar{g}(v) = 0, \ v \notin V_1 \cup V_2$. 
The first case is illustrated in figure 2.3.4 and the second one is illustrated in figure 2.3.5. Both cases could be proved by the same technique used in proving Theorem 2.3.5.

Figure 2.3.4

Figure 2.3.5
In Theorem 2.3.3, we have proved that there exists $\bar{f} \in E(T)$ such that the first case is satisfied. Since the multiplicity of $a(T)$ is 2, there exists two linearly independent vectors $\bar{g}_1, \bar{g}_2 \in E(T)$. If $\bar{g}_1 \in E(T)$ satisfies the first case, then

$$
\bar{g}_1 = \begin{pmatrix}
  b_1 \\
  b_2 \\
  \vdots \\
  b_k \\
  0 \\
  b_k \\
  \vdots \\
  b_1 \\
  -2b_k \\
  \vdots \\
  -2b_1
\end{pmatrix}
$$

Now, if $\bar{g}_2$ also satisfies the first case, then

$$
\bar{g}_2 = \begin{pmatrix}
  a_1 \\
  a_2 \\
  \vdots \\
  a_k \\
  0 \\
  a_k \\
  \vdots \\
  a_1 \\
  -2a_k \\
  \vdots \\
  -2a_1
\end{pmatrix}
$$
and by Theorem 2.2.2 we have

\[
\begin{pmatrix}
a_1 \\
a_1 f_2(a) \\
a_1 f_3(a) \\
\vdots \\
a_1 f_k(a) \\
0 \\
a_1 f_1(a) \\
\vdots \\
a_1 f_1(a) \\
a_1 \\
-2a_1 \\
-2a_1 f_2(a) \\
\vdots \\
-2a_1 f_k(a)
\end{pmatrix}
= a_1
\begin{pmatrix}
1 \\
f_2(a) \\
f_3(a) \\
\vdots \\
f_k(a) \\
f_k(a) \\
f_2(a) \\
1 \\
-2 \\
-2f_2(a) \\
\vdots \\
-2f_k(a)
\end{pmatrix}
\]

So,

\[
\Rightarrow \frac{1}{a_1} g_2 - \frac{1}{b_1} g_1 = 0
\]

This implies that

\( g_1 \) and \( g_2 \) are linearly dependent (contradiction).

Therefore,

\( g_2 \) cannot satisfy the first condition

So,

\( g_2 \) satisfies the second condition.

Remove the pendant vertex \( v \) with \( \tilde{g}_2(v) = 0 \). By Theorem 1.4.4 (Reduction Theorem), we have the tree \( T_{k-1} \) with \( a(T_{k-1}) = a(T) \) and \( \tilde{g}_2|_{k-1} \) is the eigenvector
belonging to $a(T_{k-1})$, where $g_2|_{k-1}$ is the restriction of $g_2$ to $V_{k-1} = V - \{v\}$. Repeat this technique $(k - 1)$ times until you get the path $P_{2k+1}$ with $a(P_{2k+1}) = a(T)$ and $g_2|_{V_0}$ is the restriction of $g_2$ to $V_0 = V - \bigcup_{i=1}^{k} \{v_i\}$ (where $g_2(v_i) = 0$). Therefore, by Theorem 2.3.4, $a(T) = 4 \sin^2 \left( \frac{\pi}{2(2k+1)} \right)$.

![Figure 2.3.6](image)

**Theorem 2.3.7** If $T \in T$ is of order $n = 2k + s + 1$, having the shape shown in figure 2.3.6, where $1 \leq s < k$, then

1. $T$ is of type I.

2. The characteristic vertex $w_T = v_{k+1}$.

3. $a(T) = 4 \sin^2 \left( \frac{\pi}{2(2k+1)} \right)$.

4. If $B_1 = (V_1, E_1)$ and $B_2 = (V_2, E_2)$ are two (different) isomorphic branches of $T$ rooted at $v_{k+1}$ and $\alpha : V_1 \to V_2$ is the isomorphism of the rooted trees $B_1$ and $B_2$, then $\exists g \in E(T)$ such that $g(v) = -g(\alpha(v)) > 0$, $v_{k+1} \neq v \in V_1$ and $g(v) = 0$, $v \notin V_1 \cup V_2$. 
Proof: Consider all the trees $T_i$ such that $1 \leq i \leq k$ as shown in Figure 2.3.7.

We have, $T = T_2$, and by The Interlacing Theorem 1.3.14. we have:

$$a(T_1) \geq a(T_2) \geq \cdots \geq a(T_s) \geq \cdots \geq a(T_k).$$

Since $a(T_1) = a(T_k)$, then:

$$a(T_1) = a(T_2) = \cdots = a(T_s) = \cdots = a(T_k).$$

Now, for the tree $T_1$, there exists $g_1 \in \mathcal{E}(T_1)$ such that $g_1(v) = -g_1(\alpha(v)) > 0$, $v_{k+1} \neq v \in V_1$, $g_1(v_{k+1}) = g_1(v_{2k+2}) = 0$ where $\alpha : V_1 \rightarrow V_2$ is the isomorphism of the two different isomorphic branches of $T$, $B_1 = (V_1, E_1)$ and $B_2 = (V_2, E_2)$ rooted at $v_{k+1}$. Adjoin a vertex $v_{2k+3}$ to the vertex $v_{2k+2}$. Since $a(T_1) = a(T_2)$, then by Theorem 1.4.5, $F(T_1) = F(T_2)$ and $g_2 \in \mathcal{E}(T_2)$, $g_2(v) = g_1(v), \ v \in V(T_1)$ and $g_2(v_{2k+2}) = 0$. If $S = 2$, then it's done. Otherwise, in the same way we can prove that, for the tree $T_3$, $\exists \ g_3 \in \mathcal{E}(T_3)$ such that...
\[ \tilde{g}_3(v) = \tilde{g}_2(v), \quad v \in V(T_2) \] and \[ \tilde{g}_3(v_{\omega+3}) = 0. \] Continuing in the same manner, we conclude the existence of the \( \tilde{g}_s \in \mathcal{E}(T_s) \) such that \[ \tilde{g}(v) = -\tilde{g}(\alpha(v)) > 0 \] \( v_{k+1} \neq v \in V_1 \) and \( \tilde{g}(v) = 0, \quad v \in V_1 \cup V_2. \) Therefore, all parts of the theorem have been proved.
Chapter 3

Centers, Centroids and Characteristic Vertices of A Caterpillar

In this chapter, we will introduce centers and centroids of a graph $G$. If $T \in \mathcal{T}$ and $F(T)$ is the set of characteristic vertices of $T$, then should the center and centroid overlap the characteristic vertices of $T$? We will see that the answer is no. Furthermore, we study type I caterpillars together with their centers and centroids.

3.1 Center and Centroid

Let $T$ be a tree. A branch rooted at $v \in V$ is a maximal subtree containing $v$ as a pendant vertex. (The number of branches of $v$ is $d(v)$). The weight, $w(v)$, of $v$ is the maximum number of edges in any branch at $v$. A vertex $v$ is a centroid
point of T if

\[ w(v) = \min_{u \in V} w(u). \]

\[ u \quad v \quad w \]

uv: characteristic edge
w: centroid

Figure 3.1.1

Example 3.1.1 Let T be the tree shown in Figure 3.1.1. Then the characteristic polynomial is \( x(x - 1)^4(x^6 - 16x^5 + 91x^4 - 232x^3 + 266x^2 - 16x - 11) \) and \( a(T) = 0.1288129 \) is a simple eigenvalue. Moreover, T is of type II and \( F(T) = \{u, v\} \).

But w is the unique centroid point of T.

The eccentricity \( e(v) \) of a vertex \( v \) of a connected graph \( G \) is the number

\[ \max_{u \in V(G)} d(u, v). \]

The radius \( \text{rad} \) \( G \) is defined as \( \min_{v \in V(G)} e(v) \) while the diameter \( \text{diam} \) \( G \) is \( \max_{v \in V(G)} e(v) \). A vertex \( v \) is a center point of \( T \) if

\[ e(v) = \min_{u \in V} e(u) \]
Example 3.1.2 Let $T$ be the tree shown in Figure 3.1.2. Its characteristic polynomial is $x(x - 1)^6(x^6 - 18x^5 + 109x^4 - 288x^3 + 336x^2 - 146x + 13)$ and $a(T) = 0.1179743$. In this case, $F(T) = \{v, w\}$, but $u$ is the unique center point.

If $T \in T$, then we label the vertices as shown in Figure 3.1.3

![Diagram of a tree with vertices labeled $v_1, v_2, \ldots, v_k, v_{k+1}, v_{k+2}$, and so on.]

Figure 3.1.3

Theorem 3.1.1 If $T \in T$ such that $T$ is a type I tree then the only center (centroid) in the tree $T$ is the characteristic vertex $v_{k+1}$.

Proof: If the centroid $o$ is not $v_{k+1}$, then $w(o) \geq k + s + 1 > w(v_{k+1}) = k$ which contradicts the definition of a centroid, so $v_{k+1}$ is the centroid. If the center $C$ is not $v_{k+1}$, then

$$e(c) \geq k + 1 > e(v_{k+1}) = k$$
which also contradicts the definition of a center of \( T \), so \( v_{k+1} \) is the center.

**Theorem 3.1.2** If \( T \in T \) such that \( T \) is of order \( n = k + \ell + s + 1 \) where \( k > \ell \geq s \geq 1 \), \( k, \ell \) and \( s \) are the orders of the branches of \( T \) at \( v_{k+1} \), then if \( k + \ell \) is even then the only center is \( \frac{k + \ell + 2}{2} \), and if \( k + \ell \) is odd, then the only centers are \( \frac{k + \ell + 1}{2} \) and \( \frac{k + \ell + 3}{2} \).

**Proof:** Assume that \( k + \ell \) is even

\[
e \left( \frac{k + \ell + 2}{2} \right) = \frac{k + \ell}{2}
\]

\[
e(i) = i - 1 \quad \left( \frac{k + \ell + 2}{2} < i \leq k + \ell + 1 \right)
\]

\[
> \frac{k + \ell}{2}
\]

\[
e(j) = k + \ell - j + 1 \quad \left( 1 \leq j < \frac{k + \ell + 2}{2} \right)
\]

\[
\geq k + \ell - \frac{k + \ell}{2} + 1
\]

\[
= \frac{k + \ell}{2} + 1 > \frac{k + \ell}{2}
\]

\[
e(m) = m - 1 \quad \left( k + \ell + 2 \leq m \leq k + \ell + s + 1 \right)
\]

\[
\geq (k + \ell + 2) - 1 = k + \ell + 1 > \frac{k + \ell}{2}
\]

\[
\Rightarrow \text{The only center is} \quad \frac{k + \ell + 2}{2}
\]

Assume that \( k + \ell \) is odd

\[
e \left( \frac{k + \ell + 1}{2} \right) = \max \left\{ \frac{k + \ell - 1}{2}, \frac{k + \ell}{2}, \frac{k + \ell - 1}{2} \right\}
\]
\[
\begin{align*}
\ &= \max \left\{ \frac{k + \ell - 1}{2}, \frac{k + \ell - 1}{2} \right\} \\
\ &= \frac{k + \ell + 1}{2} \\
\ &= \max \left\{ \frac{k + \ell + 1}{2}, \frac{k - \ell - 1}{2} \right\} \\
\ &= \frac{k + \ell + 1}{2} \\
\end{align*}
\]

\[
e(i) = i - 1 \quad \left( \frac{k + \ell + 3}{2} < i < k + \ell - 1 \right)
\]

\[
> \frac{k + \ell + 3}{2} - 1 = \frac{k + \ell + 1}{2}
\]

\[
e(j) = k + \ell - (j - 1) \quad \left( 1 \leq j \leq \frac{k - \ell + 1}{2} \right)
\]

\[
= k + \ell - j + 1
\]

\[
> k + \ell - \frac{k + \ell + 1}{2} + 1 = \frac{k + \ell + 1}{2}
\]

\[
e(m) = m - 1 \quad \left( k + \ell + 2 \leq m \leq k + \ell - s + 1 \right)
\]

\[
\geq (k + \ell + 2) - 1 = k + \ell + 1 > \frac{k + \ell + 1}{2}
\]

\[
\Rightarrow \text{The only centers are } \frac{k + \ell + 1}{2} \text{ and } \frac{k + \ell + 3}{2}
\]

Theorem 3.1.3 If \( T \in T \) is a tree of order \( n = k + \ell + s + 1 \) where \( k > \ell \geq s \geq 1 \), \( k, \ell \) and \( s \) are the orders of the branches of \( T \) at \( v_{k+1} \). Let \( i = \frac{k - \ell - s + 2}{2} \).

Then:

1. If \( i < 1 \) then the only centroid is \( \ell + 1 \).
2. If $i \geq 1$ then if $n$ is odd, then the only centroid is $\ell + i$, and if $n$ is even, then the only centroids are $\ell + [i]$ and $\ell + [i] + 1$.

Proof:

1. Assume that $i = \frac{k - (\ell + s - 2)}{2} < 1$:

   $\Rightarrow k < \ell + s$

   $w(\ell + 1) = k$

   $w(\ell + j) = \ell + s + (j - 1)$ \quad $(2 \leq j \leq k + 1)$

   $\geq \ell + s + 1 > k + 1 > k = w(\ell + 1)$

   $w(n) = k + \ell - n + 1 + s$ \quad $(1 \leq n \leq \ell)$

   $\geq k + \ell + 1 + s = k + 1 + s > k = w(\ell + 1)$

   $w(m) = m - 1$ \quad $(k + \ell + 2 \leq m \leq k + \ell + s + 1)$

   $\geq k + \ell + 2 - 1 = k + \ell + 1 > k = w(\ell + 1)$

   $\Rightarrow \ell + 1$ is the centroid.

2. Assume that $i \geq 1$ and $n$ is odd:

   If $i = 1$ then $k = \ell + s$ and

   $w(\ell + i) = \ell + s = k$

   $w(\ell + j) = \ell + s + (j - 1)$ \quad $(2 \leq j \leq k + 1)$
\[ \geq \ell + s + (2 - 1) = \ell + s + 1 > k = w(\ell + 1) \]

\[ w(n) = k + \ell - n + s + 1 \quad (1 \leq n \leq \ell) \]

\[ \geq k + \ell - \ell + 1 + s = k + 1 + s > k = w(\ell + 1) \]

\[ w(m) = m - 1 \quad (k + \ell + 2 \leq m \leq k + \ell + s + 1) \]

\[ \geq (k + \ell + 2) - 1 = k + \ell + 1 > k = w(\ell + 1) \]

\[ \Rightarrow \ell + 1 \text{ is the centroid } . \]

If \( i > 1 \) then \( k > \ell + s \), and

\[ w(\ell + i) = w \left( \frac{k + \ell - s + 2}{2} \right) \]

\[ = \max \left\{ \frac{k + \ell - s + 2}{2} - 1 \div s, \quad k + \ell - \frac{k + \ell - s + 2}{2} + 1 \right\} \]

\[ = \frac{k + \ell + s}{2} \]

\[ w(\ell + i + j) = w \left( \frac{k + \ell - s + 2}{2} + j \right) \quad \left( 1 \leq j \leq \frac{k + \ell + s}{2} \right) \]

\[ = \frac{k + \ell + s}{2} + j \]

\[ \geq \frac{k + \ell + s}{2} + 1 > \frac{k + \ell + s}{2} = w(\ell + i) \]

\[ w(n) = k + \ell - n + 1 + s \quad (1 \leq n \leq \ell) \]

\[ \geq k + \ell - \ell + 1 + s = k + 1 + s > \frac{k + \ell + s}{2} = w(\ell + i) \]

\[ w(m) = m - 1 \quad (k + \ell + 2 \leq m \leq k + \ell + s + 1) \]

\[ \geq (k + \ell + 2) - 1 = k + \ell + 1 > \frac{k + \ell + s}{2} = w(\ell + i) \]

\[ w(\ell + 1) = k \quad \text{but} \quad k > \ell + s \Rightarrow 2k > k + \ell + s \]

\[ \Rightarrow k > \frac{k + \ell + s}{2} \Rightarrow w(\ell + 1) > w(\ell + i) . \]
\[ w(\ell + f) = \max\{\ell + f - 1 + s, \ k + \ell - (\ell + f) + 1\}(\ell + 2 \leq \ell + f \leq \frac{k + \ell - s}{2}) \]

If \( \ell + f = \frac{k + \ell - s}{2} \), then:

\[
w(\ell \div f) = \max\left\{\frac{k + \ell - s}{2} - 1 + s, \ \frac{k + \ell - s}{2} + 1\right\}
\]

\[
= \max\left\{\frac{k + \ell + s}{2} - 1, \ \frac{k + \ell + s}{2} + 1\right\}
\]

\[
= \frac{k + \ell + s}{2} + 1
\]

So, if \( \ell + 2 \leq \ell + f \leq \frac{k + \ell - s}{2} \), then

\[
w(\ell + f) = k + \ell - (\ell + f) + 1
\]

\[
\geq k + \ell - \frac{k + \ell - s}{2} + 1 = \frac{k + \ell + s}{2} + 1
\]

\[
> \frac{k + \ell + s}{2} = w(\ell + i)
\]

Assume that \( i \geq 1 \) and \( n \) is even. Since \( n \) is even, \( i = \frac{k - \ell - s + 2}{2} \) is not an integer. So, if

\[ i = \frac{3}{2} \Rightarrow k = \ell + s + 1 \]

\[ w(\ell + 1) = k \]

\[ w(\ell + 2) = \ell + s + 1 = k \]

\[ w(\ell + j) = \ell + s + (j - 1) \quad (3 \leq j \leq k + 1) \]

\[ \geq \ell + s + (3 - 1) = \ell + s + 2 = k + 1 > k \]

\[ w(n) = k + \ell - n + 1 + s \quad (1 \leq n \leq \ell) \]

\[ \geq k + \ell - \ell + 1 + s = k + 1 + s > k \]
\[ w(m) = m - 1 \quad (k + \ell + 2 \leq m \leq k + \ell + s + 1) \]
\[ \geq (k + \ell + 2) - 1 = k + \ell + 1 > k \]
\[ \Rightarrow \ell + 1 \text{ and } \ell + 2 \text{ are the only centroids in this case.} \]

Assume that \( i > \frac{3}{2}, \) then

\[ k > \ell + s + 1 \]
\[ w(\ell + [i]) = w \left( \frac{k + \ell - s + 1}{2} \right) = \max \left\{ \frac{k + \ell - s + 1}{2} - 1 + s, \ k + \ell - \frac{k + \ell - s + 1}{2} + 1 \right\} = \max \left\{ \frac{k + \ell + s - 1}{2}, \frac{k + \ell + s + 1}{2} \right\} = \frac{k + \ell + s + 1}{2} \]
\[ w(\ell + [i] + 1) = w \left( \frac{k + \ell - s - 3}{2} \right) = \max \left\{ \frac{k + \ell - s + 3}{2} - 1 + s, \ k + \ell - \frac{k + \ell - s + 3}{2} + 1 \right\} = \max \left\{ \frac{k + \ell + s + 1}{2}, \frac{k + \ell + s - 1}{2} \right\} = \frac{k + \ell + s + 1}{2} \]
\[ w(q) = k + \ell - q + 1 + s \quad (1 \leq q \leq \ell) \]
\[ \geq k + \ell - \ell + 1 + s = k + 1 + s > \frac{k + \ell + s + 1}{2} \]
\[ w(m) = m - 1 \quad (k + \ell + 2 \leq m \leq k + \ell + s + 1) \]
\[ \geq (k + \ell + 2) - 1 = k + \ell + 1 > \frac{k + \ell + s + 1}{2} \]
\[ w(\ell + [i] + j) = \frac{k + \ell - s + 1}{2} + j - 1 + s \quad (2 \leq j \leq \frac{k + \ell + s + 1}{2}) \]
\[ = \frac{k + \ell + s - 1}{2} + j \geq \frac{k + \ell + s - 1}{2} + 2 \]
\[ = \frac{k + \ell + s + 3}{2} > \frac{k + \ell + s + 1}{2} \]
\[ \Rightarrow \ell + [i] \text{ and } \ell + [i] + 1 \text{ are the only centroids.} \]
3.2 Center and Centroid of a Caterpillar

A caterpillar $C$ is a tree such that if we remove all pendant vertices, we get a path. A list of caterpillars showing the location of the characteristic vertices, centers and centroids is given in the next page.

The circle $\bigcirc$ indicates that the vertex is a center. The square $\square$ indicates that the vertex is a centroid. The triangle $\triangle$ indicates that the vertex is a characteristic vertex.
A list of caterpillars of order $n$, $3 \leq n \leq 9$ is given in Appendix 4.

**Theorem 3.2.4** If a caterpillar is of the shape shown below, where $n = i + j + \ell + 1$ and $j \geq i$, then:

1. If $j < i + \ell + 1$ then the only centroid is $i + 1$.

2. If $j = i + \ell + 2s$ (where $s$ is a natural number) then the only centroid is $i + s + 1$.

3. If $j = i + \ell + 2s + 1$ (where $s$ is a whole number), then the only centroids are $i + s + 1$ and $i + s + 2$.

![Figure 3.2.1](image)

**Proof:**

1. Assume that $j < i + \ell + 1$, then:

$$w(i + 1) = j$$

$$w(n) = (i - n + 1) + j + \ell \quad (1 \leq n \leq i)$$

$$\geq (i - i) + 1 + j + \ell = 1 + j + \ell > w(i + 1)$$
\[ w(m) = n - 1 > w(i + 1) \quad (i + j + 2 \leq m \leq i + j + \ell + 1) \]
\[ w(p) = (p - 1) + \ell \quad (i + 2 \leq p \leq i + j + 1) \]
\[ \geq ((i + 2) - 1) + \ell = i + \ell + 1 > w(i + 1) \]

So \( i + 1 \) is the only centroid.

2. Assume that \( j = i + \ell + 2s \)

\[ w(i + s \div 1) = \max\{i + s + \ell, j - s\} \]
\[ = \max\{i + s + \ell, (i + \ell + 2s) - s\} \]
\[ = \max\{i + s + \ell, i + \ell + s\} \]
\[ = i + s + \ell \]

\[ w(m) = (i + j + 1) - m + \ell \quad (1 \leq m \leq i) \]
\[ \geq (i + j + 1) - i + \ell = j + \ell + 1 \]
\[ = i + \ell + 2s + \ell + 1 = i + 2\ell + 2s + 1 > w(i + s + 1) \]

\[ w(i + 1) = j = i + \ell + 2s > w(i + s + 1) \]

\[ w(n) = i + j + 1 - n \quad (i + 2 \leq n \leq i + s) \]
\[ = 2i + \ell + 2s + 1 - n \]
\[ \geq 2i + \ell + 2s + 1 - (i + s) = i + \ell + s + 1 > w(i + s + 1) \]

\[ w(p) = p - 1 + \ell \quad (i + s + 2 \leq p \leq i + j + 1) \]
\[ \geq (i + s + 2) - 1 + \ell = i + s + \ell + 1 > w(i + s + 1) \]

\[ w(q) = i + j + \ell \quad (i + j + 2 \leq q \leq i + j + \ell + 1) \]
\[= i + (i + \ell + 2s) \div \ell = 2i + 2\ell + 2s > w(i + s + 1)\]

So, \(i + s + 1\) is the only centroid.

3. Assume that \(j = i + \ell + 2s + 1\)

\[w(i + s + 1) = \max\{i + s + \ell, j - s\} = \max\{i + s + \ell, i + \ell + 2s + 1 - s\}\]
\[= \max\{i + s + \ell, i + s - \ell + 1\} = i + s + \ell + 1\]

\[w(i + s + 2) = \max\{i + s + 1 + \ell, j - s - 1\}\]
\[= \max\{i + s + 1 + \ell, i - \ell + 2s + 1 - s - 1\} = \max\{i + s + 1 + \ell, i + \ell + s\}\]
\[= i + s + \ell + 1\]

\[w(m) = (i + j + 1) - m \div \ell \quad (1 \leq m \leq i)\]
\[= (i + i + \ell + 2s + 1) - m \div \ell\]
\[= 2i + 2\ell + 2s + 1 - m \geq 2i + 2\ell + 2s + 1 - i\]
\[= i + 2\ell + 2s + 1 > w(i + s + 1) = w(i + s + 2)\]

\[w(i + 1) = i + \ell + 2s > w(i + s + 1) = w(i + s + 2)\]

\[w(r) = i + j + 1 - r \quad (i + 2 \leq r \leq i + s)\]
\[= 2i + j + 2s + 2 - r \geq 2i + j + 2s + 2 - (i + s)\]
\[= i + j + s + 2 > w(i + s + 1) = w(i + s + 2)\]

\[w(p) = p - 1 + \ell \geq i + s + 3 - 1 + \ell \quad (i + s + 3 \leq p \leq i + j + 1)\]
\[= i + s + \ell + 2 > w(i + s + 1) = w(i + s + 2)\]

\[w(q) = i + j + \ell \quad (i + j + 2 \leq q \leq i + j + \ell + 1)\]
\[ i + (i + \ell + 2s + 1) + \ell = 2i + 2\ell - 2s - 1 > w(i + s + 1) = w(i + s + 2) \]

So, \( i + s + 1 \) and \( i + s + 2 \) are the only centroids.

Corollary 3.2.1 If the caterpillar is of the shape shown below, where \( n = k + \ell \), then:

1. If \( k < \ell + 1 \), then the only centroid is 2.

2. If \( k = \ell + 2s + 1 \) (\( s \) is a natural number), then the only centroid is \( s + 1 \).

3. If \( k = \ell + 2s \) (\( s \) is a natural number), then the only centroids are \( s \) and \( s + 1 \).

![Diagram of a caterpillar graph]

Figure 3.2.2

Proof: This is a direct consequence of the last theorem by putting \( i = 1 \) and \( j + 2 = k \).

Theorem 3.2.5 Let \( C = (V, E) \) be a caterpillar of order \( n \), and let \( B_1 = (V_1, E_1) \) and \( B_2 = (V_2, E_2) \), \( V_1 \cap V_2 = \phi \), be two isomorphic (but different) branches rooted at \( v \in V \) such that any vertex of a longest path of \( C \) belongs to \( V_1 \cup V_2 \), then \( v \) is the centroid of \( C \).
Proof: Let $B'_1$ arise from $B_1$ by removing the vertex $v$ and the adjacent edge. Also, let $B'_2$ arise from $B_2$ by removing the vertex $v$ and the adjacent edge. We have:

$$V'_1 = V_1 - \{v\} \quad \text{and} \quad V'_2 = V_2 - \{v\}$$

where $V'_1$ and $V'_2$ are the sets of vertices of $B'_1$ and $B'_2$ respectively. Let $V_3$ be the set of vertices which are adjacent to $v$ and not included in $V_1 \cup V_2$.

$$w(v) = |V'_1| - 1 = |V'_2| - 1$$

$$w(u) = (|V_1| - 1) + |V_3| + r \quad \quad u \in V'_1 \cup V'_2$$

where $r$ is the length of the path between $v$ and $u$. Since $|V_3| \geq 0$ and $r \geq 1$, $w(u) > w(v)$. Also, if $p \in V_2$, then:

$$w(p) = n - 1 > w(v).$$

So, $v$ is the only centroid of $C$. 
Theorem 3.2.6 Let $C = (V, E)$ be a caterpillar of order $n$ and let $B_1 = (V_1, E_1)$ and $B_2 = (V_2, E_2)$ be two isomorphic branches rooted at $v_1$ and $v_2$ respectively, where $v_1$ and $v_2$ are adjacent and $\text{deg}(v_1) = \text{deg}(v_2)$ in $C$. Suppose also, that any vertex belonging to a longest path in $C$ must also belong to $V_1 \cup V_2$. Then, both $v_1$ and $v_2$ are the only centroids of $C$.

![Figure 3.2.4](image)

**Figure 3.2.4**

**Proof:** Let $B'_i$ arise from $B_i$ by removing the vertex $v_i$ and the adjacent edges. We have:

$$V'_i = V_i - \{v_i\}$$

where $V'_i$ is the set of vertices of $B'_i$, $(i = 1, 2)$. Let $V''_i$ be the set of vertices which are adjacent to $v_i$ and not included in $V_1$ or $V_2$.

$$w(v_1) = |V''_1| + |V''_2| + 1$$

$$w(v_2) = |V''_1| + |V''_2| + 1$$
since $|V'_1| = |V'_2|$ and $|V'_1| = |V'_2|$, we have:

$$w(v_1) = w(v_2) = |V'_1| + |V'_2| + 1.$$  

If $p \in V'_1 \cup V'_2$, then:

$$w(p) = |V'_1| + |V'_2| + 1 + |V'_2| + r$$

where $r = \min_{i=1,2} \{ \text{length of the path between } v_i \text{ and } p \}$. Since $|V'_1| \geq 0$, $|V'_2| \geq 0$ and $r \geq 1$, then:

$$w(p) > w(v_1) = w(v_2).$$

If $q \in V'_1 \cup V'_2$, then

$$w(q) = n - 1 > w(v_1) = w(v_2).$$

So, $v_1$ and $v_2$ are the only centroids of $C$.

### 3.3 Type I Caterpillars

In this section, a characterization of a class of caterpillars of type I is given.

**Theorem 3.3.7** Let $C = (V, E)$ be a caterpillar of order $n$, and let $B_1 = (V_1, E_1)$ and $B_2 = (V_2, E_2), V_1 \cap V_2 = \emptyset$ be two isomorphic (but different) branches rooted at $w \in V$ such that any vertex of a longest path of $C$ belongs to $V_1 \cup V_2$, then

$F(C) = \{w\}$ and there is a $g \in \mathcal{E}(C)$ such that $g(v) = -g(v') > 0, w \neq v \in V_1$ and $g(v) = 0, v \notin V_1 \cup V_2$. 
Proof: Let \( C^* = (V^*, E^*) \) be the caterpillar obtained from \( C = (V, E) \) by removing all pendant vertices incident with \( w \) and all corresponding edges (see figure 3.2.3). Let \( \alpha : V_1 \rightarrow V_2 \) be an isomorphism of the rooted trees \( B_1 \) and \( B_2 \). Let \( f \in E(C^*) \) be fixed but arbitrary. We need to prove that \( f(\alpha(v)) = f(v), \quad v \in V_1 \) is not satisfied. Assume that \( f(\alpha(v)) = f(v) \), \( v \in V_1 \). If \( C^* \) is a type II caterpillar, then one of the following conditions should happen:

1. \( f(v) > 0, w \neq v \in C^* \) and \( f(w) < 0 \).

2. \( f(v) < 0, w \neq v \in C^* \) and \( f(w) > 0 \).

3. \( \exists v_1, v_2 \in V_1 \) and \( v_3, v_4 \in V_2 \) such that \( f(v_3) = f(v_1) > 0 \) and \( f(v_4) = f(v_2) < 0 \).

In (1) or (2) we will get 3 characteristic vertices (2 characteristic edges) which contradicts Theorem 1.4.1. In (3), we will get either 2 or 4 characteristic edges which again contradicts Theorem 1.4.1.

If \( C^* \) is a type I caterpillar, then:

If \( v_1 \in V_1(V_2) \) is the characteristic vertex of \( C^* \) (\( f(v_1) = 0 \)) then \( \exists v_2 \in V_2(V_1) \) such that \( f(v_2) = 0 \). In this case, we will have two characteristic vertices which contradicts Theorem 1.4.1. If \( w \) is the characteristic vertex (\( f(w) = 0 \)), then \( \sum_{v_i \in E^* \atop v_i \neq w} f(v_i) < 0 \) or \( \sum_{v_i \in E^* \atop v_i \neq w} f(v_i) > 0 \) which contradicts Theorem 1.3.15. So, we have proved that \( f(\alpha(v)) = f(v), \quad v \in V_1 \) is not satisfied for \( C^* \). By Theorem 2.1.2,
applied to \( w \). we have \( F(C^\sim) = \{w\} \) and there is a \( g \in \mathcal{E}(C^\sim) \) such that

\[
g(v) = -g(\alpha(v)) > 0, \quad w \neq v \in V_1 \text{ and } g(v) = 0, \quad v \notin V_1 \cup V_2.\]

Now, adjoin a new pendant vertex \( p_1 \) to \( w \), so \( V^{(1)} = V^\sim \cup \{p_1\} E^{(1)} = E^\sim \cup \{\{p_1, w\}\} \). Extend \( f \) to a function \( f^{(1)} \) on \( V^{(1)} \) by defining \( f^{(1)}(p_1) = 0 \), and then applying Theorem 2.1.4, the new caterpillar \( C^{(1)} \) is a type I tree, \( f'' \in \mathcal{E}(C^{(1)}) \) and \( a(C^{(1)}) = a(C^{(\sim)}) \). Apply the same technique to \( C^{(1)} \) to get \( C^{(2)} \) with \( f'' \in \mathcal{E}(C^{(2)}) \) where \( f^{(2)} \) is the extension of \( f^{(1)} \) on \( V^{(2)} \) by defining \( f^{(2)}(p_2) = 0 \) where \( V^{(2)} = V^{(1)} \cup \{p_2\} \). We continue applying the same technique until we get \( C = C^{(q)} \) where \( q \) is the number of times the technique is used.

**Remark:** Actually, it is found that this theorem is true not only for caterpillars, but also for any tree \( T \). The same proof is used.
Appendices

The results below were obtained with the help of Mathematica.

Appendix 1: The eigenvalues of all trees with three end vertices; $4 \leq n \leq 14$.

Appendix 2: The second smallest eigenvalue with the corresponding eigenvector for all trees with three end vertices; $4 \leq n \leq 14$.

Appendix 3: The eigenvalues of all paths of order $n$ with the eigenvector for the second smallest eigenvalue; $1 \leq n \leq 14$.

Appendix 4: The second smallest eigenvalue with the corresponding eigenvector for all Caterpillars of order $n$; $3 \leq n \leq 8$. 
### Appendix I:
The eigenvalues of all trees with three end vertices, $4 \leq n \leq 14$

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Note: The table assumes that the eigenvalues are listed in ascending order.
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**Appendix 2:** The second smallest eigenvalue with the corresponding eigenvector for all trees with three end vertices; $4 \leq n \leq 14$.

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Appendix 3:

The smallest eigenvalue with the corresponding eigenvector of $L(P_n)$ where $P_n$ is a path on $n$ vertices:

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Appendix 4: The second smallest eigenvalue with the corresponding eigenvector for all Caterpillars of order $n$; $3 \leq n \leq 8$. 

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