CENTRALITY IN CONNECTED GRAPHS AND SOME RELATED INDICES

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Dinesh Pandey

Dinesh Pandey

Dedicated to...

my father ***Shree Ramdhyan Pandey***

&

my mother ***Smt. Ashtama Devi***

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SUMMARY

This thesis is a study about different central parts of connected graphs and some graphical indices related to them. The center, centroid, characteristic set and the subtree core are four different central parts of a tree. There are many central parts defined for a graph but when restricted to trees, most of them coincide with the centroid. The center, median and the security center are three known different central parts of a graph. Related to these central parts, there are different topological indices associated with a graph. The Wiener index and the total eccentricity index are two such topological indices related to the median and the center, respectively.

We define the subgraph core and the characteristic center as two new central parts of a graph and study their centrality behaviour. It is shown that the subgraph core and the characteristic center are different from the center, median and the security center. We obtain the tree which maximizes the distance between the characteristic center and the subtree core among all trees on n vertices. The asymptotic nature of the distances between different central parts are also studied. We continue this study to obtain the trees which maximize the distances between different central parts over trees with fixed diameter and over binary trees on n vertices. A new graphical index associated with the subgraph core of a graph is introduced. We define the *subgraph index* of a graph and obtain the graphs which extremize the subgraph index over unicyclic graphs and over graphs with fixed number of pendant vertices. We further continue this study for the Wiener index and the total eccentricity index. We study the extremization problems on the Wiener index and the total eccentricity index over graphs with fixed number of pendant vertices and over graphs with fixed number of cut vertices.

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List of Symbols

$C(G)$	:	Center of the graph G.
$C_d(T)$	:	Centroid of the tree T
$D_G(v)$	:	Sum of distances between v and every other vertex of G
$e_G(v)$	:	Eccentricity of G in v.
$M(G)$	:	Median of G
$\mathbb{S}(G)$	:	Security center of G
$S_c(T)$	:	Subtree core of T
$S_c(G)$	:	Subgraph core of G
$\chi(G, Y)$	:	Characteristic set of G w.r.t. the Fiedler vector Y
$\chi(G)$	:	Characteristic center of G
h_k	:	The number of connected labelled graphs on k vertices
$F(G)$	:	Subgraph index of G
$W(G)$	:	Wiener index of G
$\varepsilon(G)$	:	Total eccentricity index of G
$f_G(v)$	:	Number of connected subgraphs of G containing v
$\mathfrak{H}_{n,k}$	:	Set of all connected graphs on n vertices with k pendant vertices
$\mathfrak{T}_{n,k}$	:	Set of all trees on n vertices with k pendant vertices
γ_n^d	:	Set of all trees on n vertices with diameter d
$\mathfrak{C}_{n,s}$	:	Set of all connected graphs on n vertices with s cut vertices
$\mathfrak{C}_{n,k}^t$	:	Set of all trees on n vertices with s cut vertices
$\mathcal{U}_n$	:	Set of all unicyclic graphs on n vertices
$\mathcal{U}_{n,g}$	:	Set of all unicyclic graphs on n vertices with girth g
P_n	:	Path on n vertices
$K_{1,n-1}$	:	Star on n vertices

$P_{n-g,g}$	: The path-star tree on n vertices
$T(l,m,d)$	: The tree of order n obtained by taking the path $P_d : v_1 v_2 \cdots v_d$ and adding l pendant vertices adjacent to v_1 and m pendant vertices adjacent to v_d
T_{rg}^{n}	: rgood binary tree on n vertices
$T_{rg}^{n,l}$	: crg tree on n vertices
C_n	: Cycle on n vertices
K_n	: Complete graph on n vertices
$U_{n,g}^{p}$	: The graph obtained by adding $n-g$ pendant vertices at one vertex of C_g.
$U_{n,g}^{p}$	: The graph obtained by adding an edge between a pendant vertex of P_{n-g} and a vertex of C_g.
P_n^k	: The graph obtained by adding k pendant vertices at one vertex of K_{n-k}
$T_e(u)$	: The component of $T-e$ containing the vertex u where $e=\{u,v\}$

Chapter 1

Introduction and preliminaries

In this chapter, we give a brief literature survey on the study of different central parts of connected graphs and some associated indices. We also define two new central parts for connected graphs and discuss the motivation for our study.

1.1 Introduction

Throughout the thesis, all graphs are finite, simple, connected and undirected. The vertex set and the edge set of a graph G are denoted by $V(G)$ and $E(G)$, respectively. We denote an edge with end vertices u and v by $\{u, v\}$. The distance between two vertices u and v of G is denoted by $d_G(u, v)$ (or simply $d(u, v)$ when the context is clear) and defined as the number of edges in a shortest path joining u and v. The diameter of G is defined as $diam(G) = \max\{d(u, v) : u, v \in V(G)\}$. For two subsets X and Y of $V(G)$, the distance between X and Y is defined as $d_G(X, Y) = \min\{d(x, y) : x \in X, y \in Y\}$.

The degree of a vertex $v \in V(G)$ is the number of edges incident with v and we denote it by $deg(v)$. By $N_G(v)$, we mean the set of vertices adjacent to v. A vertex of degree one is called a *pendant vertex*. A vertex v of G is called a *cut vertex* of G if $G - v$ is disconnected. A graph G with $|V(G)| \geqslant 2$ is called a *2-connected graph* if it has no cut vertex. A maximal two connected subgraph of G is called a *block* of G. An edge e of G is called a *bridge* if $G - e$ is disconnected. A complete graph on n vertices is denoted by K_n. A graph G is called *bipartite* if $V(G)$ can be partitioned into two parts V_1 and V_2 such that for any edge $\{u, v\} \in E(G)$, $u \in V_1$ and $v \in V_2$. A *complete bipartite graph* is a bipartite graph with bipartition V_1 and V_2 such that for every $u \in V_1$ and $v \in V_2$, $\{u, v\} \in E(G)$. A complete bipartite graph with $|V_1| = m$ and $|V_2| = n$ is denoted by $K_{m,n}$. A tree is a connected acyclic graph. A *path* on n vertices is denoted by P_n and we denote the *star* on n vertices by $K_{1,n-1}$.

By specifying a vertex r of a tree T, we say T is a rooted tree with root r. A *binary tree* is a tree in which every non-pendant vertex has degree 3. A *rooted binary tree* is a tree in which the root has degree two and any other vertex is either a pendant vertex or a vertex of degree 3. Note that the number of vertices in a binary tree is always even and every binary tree on n vertices has $\frac{n+2}{2}$ pendant vertices. The number of vertices in a rooted binary tree is always odd.

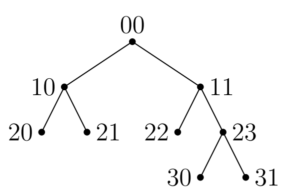
Let T be a rooted binary tree with root r. The *height* of a vertex v in T is denoted by $ht(v)$ and defined as $ht(v) = d(v, r)$. The height of T is denoted by $ht(T)$ and defined as $ht(T) = \max\{ht(v) : v \in V(T)\}$. We say a vertex v of T is at level l if $ht(v) = l$. Let $P(r, v)$ denotes the path joining r and v. For $u, v \in V(T)$, v is called a successor of u if $P(r, v)$ contains $P(r, u)$. If v is a successor of u and u is adjacent to v, then we call v is a child of u and u is the parent of v. We call a rooted binary tree to be ordered, if for $l \geqslant 1$, the vertices at level l are put in a linear order such that if u and v are vertices at level $l + 1$ with different parents then the orders of u and v at level $l + 1$ are same as the order of their parents at level l.

Definition 1.1.1 ([38]). *A rooted binary tree is called an rgood binary tree if*

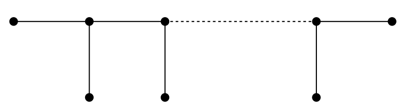
(*i*) *the heights of any two of it's pendant vertices differ by at most 1 and*

(*ii*) *the vertices of the tree can be ordered such that the parents of the pendant vertices at the highest level make a final segment in the ordering of the vertices at next to highest level.*

A single vertex rooted binary tree is also rgood. All rgood binary trees on n vertices are isomorphic and we denote it by T_{rg}^n. A *caterpillar* is a tree which has a path such that every vertex not on the path is adjacent to some vertex on the path. A *binary caterpillar* is a caterpillar which is also a binary tree. Note that a binary caterpillar on n vertices has diameter $\frac{n}{2}$.



(a)



(b)

Figure 1.1: (a) Structure of an rgood binary tree (b) Structure of a binary caterpillar

If G and H are two isomorphic graphs, we write $G \cong H$. A cycle on n vertices is denoted by C_n. The *girth* of a graph is the length of a smallest cycle contained in it. A *unicyclic graph* is a graph containing exactly one cycle. For $3 \leqslant g < n$, let $U_{n,g}^p$ be the unicyclic graph obtained by attaching $n-g$ pendant vertices at one vertex of the cycle C_g and $U_{n,g}^l$ be the unicyclic graph obtained by joining an edge between a pendant vertex of the path P_{n-g} and a vertex of C_g. Note that $U_{n,n-1}^p \cong U_{n,n-1}^l$.

A real matrix A is said to be *nonnegative* if all its entries are nonnegative. If all the entries of A are positive, we say A is a *positive matrix*. Similarly we can define

Figure 1.2: The graphs $U^p_{n,g}$ and $U^l_{n,g}$

positive and nonnegative vectors. We write $A \geqslant 0$, if A is nonnegative and $A > 0$ if A is positive. If A and B are matrices of same order, then $A \geqslant B$ and $A > B$ means $A - B \geqslant 0$ and $A - B > 0$, respectively.

A *permutation matrix* is a square matrix in which exactly one entry in each row and each column is 1 and all other entries are 0. For a matrix A, by A^T we mean the transpose of A. A square matrix A of order $n \geqslant 2$ is said to be *reducible* if there exists a permutation matrix P such that

$$P^T AP = \begin{pmatrix} B & C \\ \mathbf{0} & D \end{pmatrix}$$

where B and D are square matrices of order r and $n - r$, respectively with $1 \leqslant r \leqslant n - 1$. A square matrix is called *irreducible* if it is not reducible. For a square matrix A, $\rho(A) = \max\{|\lambda_i| : \lambda_i \text{ is an eigenvalue of A}\}$ is called the spectral radius of A. The following is the well known Perron-Frobenius theorem which has many applications.

Theorem 1.1.2 ([15])**.** *Let $A \geqslant 0$ be an irreducible square matrix of order $n \geqslant 2$. Then $\rho(A)$ is a simple eigenvalue of A, and there is a positive eigenvector corresponding to the eigenvalue $\rho(A)$. There are no nonnegative eigenvector corresponding to any other eigenvalue of A.*

For nonnegative square matrices A and B (order of B is greater than or equal to order of A), by the notation $A \ll B$, we mean there exist permutation matrices P and Q such that P^TAP is entry wise dominated by a principal submatrix of Q^TBQ, with strict inequality in at least one place, in case A and B have same order. A useful fact from the Perron-Frobenius theory is that if B is irreducible and $A \ll B$ then $\rho(A) < \rho(B)$. For more on nonnegative matrix theory, we refer to [15] and [17].

1.2 Different central parts of graphs

It was Jordan in 1869 who first introduced the notion of centrality in graphs by defining the two central parts of trees, the *center* and the *centroid*. This definition of center by Jordan was given for trees which was later adopted for graphs.

Let G be a graph. The *eccentricity* $e(v)$ of v in G is defined as $e(v) = \max\{d(v,u) : u \in V(G)\}$. The $\min\{e(v) : v \in V(G)\}$ is called the *radius* of G and denoted by $rad(G)$. Clearly $diam(G) = \max\{e(v) : v \in V(G)\}$. A vertex v is a *central vertex* if $e(v) = rad(G)$. The *center* of G is the set of all central vertices and we denote it by $C(G)$. The following result is due to Jordan [19] which tells about the center of a tree.

Proposition 1.2.1 ([6], Theorem 2.1)**.** *The center of a tree consists of either a single vertex or two adjacent vertices.*

The above result is generalised by Harary and Norman for graphs in [16].

Proposition 1.2.2 ([16], Lemma 1)**.** *The center of a graph G is contained in a block of G.*

Let T be a tree. A *branch* at $v \in V(T)$ is a maximal subtree of T containing v as a pendant vertex. The *weight* $\omega(v)$ of v is the maximum number of edges in a branch at v. A vertex of minimum weight in T is called a *centroid vertex* of T. The *centroid* of T is the set of all centroid vertices of T and we denote it by $C_d(T)$.

Proposition 1.2.3 ([6], Theorem 2.3). *The centroid of a tree consists of either a single vertex or two adjacent vertices.*

Since the centroid is defined for trees only, many people tried to generalise the definition of the centroid to graphs in different ways. As a consequence, the median of a graph was observed as a central part of a graph by Zelinka [51] in 1968. The median of a graph was first introduced by Ore [28], in 1962.

For $v \in V(G)$, the *distance* $D_G(v)$ of v is defined as $D_G(v) = \sum\limits_{u \in V(G)} d(v,u)$.

A vertex of minimum distance is called a *median vertex* of G and the set of all median vertices is called the *median* of G. In [51], Zelinka proved the following facts regarding median.

Proposition 1.2.4 ([51],Theorem 2 and 3). *The median of a tree consists of either a single vertex or two adjacent vertices and it coincides with the centroid.*

A result similar to Proposition 1.2.2 for median is proved in [43].

Proposition 1.2.5 ([43], Theorem 3). *The median of a graph G is contained in a block of G.*

In 1975, Slater [34] defined the *security center* of a graph, which he felt, a better generalisation of the centroid than the median. For $u, v \in V(G)$, let $V_{uv} = \{x \in V(G) : d(x,u) < d(x,v)\}$ and let $g(u,v) = |V_{uv}| - |V_{vu}|$. The *security number* of $u \in V(G)$ is denoted by $s(u)$ and defined as $s(u) = \min\{g(u,v) : v \in V(G) - u\}$. The *security center* $\mathbb{S}(G)$ of G is the set of vertices x for which $s(x)$ is maximum. Slater proved the following result which is a motivation towards considering the security center as a central part of a graph.

Proposition 1.2.6 ([34], Theorem 1, Corollary 1a). *The security center of a tree coincides with its centroid and hence it consists of either one vertex or two adjacent vertices.*

Smart and Slater in 1999 proved the following result regarding the position of the security center of a graph.

Proposition 1.2.7 ([36], Theorem 6). *For any graph G, the median and the security center lie in the same block of G and hence $\mathbb{S}(G)$ is contained in a block of G.*

Though the median and the security center lie in the same block of G, by an example the authors have shown in [36] that $\mathbb{S}(\mathbb{G})$ and $M(G)$ may not be same for every graph.

Many other central parts of trees are defined in different ways by several researchers. For example, In 1978, Mitchel defined a central part of a tree known as the *telephone center* ([26]) and shown that it coincides with its centroid. Let T be a tree. Suppose the vertices of T represents telephone lines and the path between two vertices u and v represents a telephone call between them. Assuming that at a given time, a vertex can be involved in only one call, define the *switchboard number* $sb(v)$ of v as the maximum number of calls which can pass through v at a given time. The *telephone center* of T is the set of vertices having maximum switchboard number. The following result regarding the telephone center is due to Mitchell.

Proposition 1.2.8 ([26], Corollary 3). *The telephone center of a tree consists of either a single vertex or two adjacent vertices and it coincides with the centroid.*

A lot of other interesting central parts for trees can be found in the survey paper [31], many of which coincide with the centroid. In 2005, Sźekely and Wang [38] defined a new central part of a tree different from both the center and the centroid.

For a vertex v of a tree T, let $f_T(v)$ be the number of subtrees of T containing v. The *subtree core* of T is the set of vertices of T maximizing $f_T(v)$. The following result is a motivation towards considering the subtree core as a central part of a tree.

Proposition 1.2.9 ([38], Theorem 9.1)**.** *The subtree core of a tree consists of either a single vertex or two adjacent vertices.*

To prove the Proposition 1.2.9, the authors have shown that f_T is concave in the following sense.

Proposition 1.2.10 ([38])**.** *If u, v and w are three vertices of a tree T with $\{u, v\}, \{v, w\} \in E(T)$, then $2f_T(v) - f_T(u) - f_T(w) > 0$.*

All the above central parts for trees or graphs are defined combinatorially. There is a central part for trees raised from the Fiedler theory [13, 27] which is defined algebraically. For a graph G with $V(G) = \{v_1, v_2, \ldots, v_n\}$, the *degree matrix* $D(G) = (d_{ij})$ is the $n \times n$ diagonal matrix with d_{ii} is equal to the degree of the vertex v_i, for $i = 1, 2, \ldots, n$. The *adjacency matrix* $A(G) = (a_{ij})$ is the $n \times n$ matrix where $a_{ij} = 1$ if v_i and v_j are adjacent and 0 otherwise. The *Laplacian matrix* $L(G)$ of G is defined as $L(G) = D(G) - A(G)$. It is known that $L(G)$ is real, symmetric and positive semi-definite. The smallest eigenvalue of $L(G)$ is 0 with all one vector as a corresponding eigenvector. The second smallest eigenvalue of $L(G)$ is called the *algebraic connectivity* of G as it is positive if and only if G is connected (see [14]). We denote the second smallest eigenvalue of $L(G)$ by $\mu(G)$. An eigenvector corresponding to $\mu(G)$ is called a *Fiedler vector* of G.

Let Y be a Fidler vector of G. By $Y(v)$ we mean the co-ordinate of Y corresponding to the vertex v of G. A vertex v is called a *characteristic vertex* of G with respect to (w.r.t.) Y if it satisfies one of the following two conditions.

(*i*) $Y(v) = 0$ and there exists a vertex u adjacent to v such that $Y(u) \neq 0$.

(*ii*) there exists a vertex u adjacent to v such that $Y(v)Y(u) < 0$.

The set of all characteristic vertices of G w.r.t. Y is called the *characteristic set* of G w.r.t. Y. We denote the characteristic set of G w.r.t. Y by $\chi(G, Y)$. It is observed that the the characteristic set behaves like a central part in trees. One of the important reason to consider it as a central part of a tree is the following proposition.

Proposition 1.2.11 ([13], Theorem 3,14 and [27],Theorem 2)**.** *Let Y be a Fiedler vector of a tree T. Then $\chi(T, Y)$ is either a single vertex or two adjacent vertices. Furthermore, $\chi(T, Y)$ is fixed for any Fiedler vector Y.*

Note that for a characteristic vertex v, if condition (*ii*) holds then u is also a characteristic vertex of G w.r.t. Y. In this case, the edge $\{u, v\}$ is known as a *characteristic edge* of G corresponding to Y. Thus by a characteristic edge of G w.r.t. Y, we mean two adjacent characteristic vertices of G w.r.t. Y. The concept of characteristic set in terms of characteristic vertices and characteristic edges was first introduced and studied by Bapat and Pati in [4].

We now discuss some important results related to the study of the position of the characteristic set in a tree. Let v be a vertex of G and $C_1, C_2, \ldots, C_k$ be the connected components of $G - v$. Note that $k \geqslant 2$ if and only if v is a cut vertex of G. For each such component, let $\hat{L}(C_i), i = 1, 2, \ldots, k$ be the principal submatrix of $L(G)$ corresponding to the vertices of C_i. Then $\hat{L}(C_i)$ is invertible and $\hat{L}(C_i)^{-1}$ is a positive matrix which is called the *bottleneck matrix* for C_i. By Perron-Frobenius theorem, $\hat{L}(C_i)^{-1}$ has a simple dominant eigenvalue, called the *Perron value* of C_i at

v. The component C_j is called a *Perron component* at v if its Perron value is maximal among the components $C_1, C_2, \ldots, C_k$, at v. The next result describes the entries of bottleneck matrices for trees which is very useful for our study.

Lemma 1.2.12 ([21], Proposition 1)**.** *Let T be a tree and let $v \in V(T)$. Let T_1 be a component of $T - v$ and L_1 be the submatrix of $L(T)$ corresponding to T_1. Then $L_1^{-1} = (m_{ij})$, where m_{ij} is the number of edges in common between the paths P_{iv} and P_{jv}, where P_{iv} denotes the path joining the vertices i and v.*

A connection between Perron components and characteristic set of a tree is described in next three results.

Proposition 1.2.13 ([21], Corollary 1.1)**.** *Let T be a tree on n vertices. Then the edge $\{i, j\}$ is the characteristic edge of T if and only if the component T_i at vertex j containing the vertex i is the unique Perron component at j while the component T_j at vertex i containing the vertex j is the unique Perron component at i.*

Proposition 1.2.14 ([21], Corollary 2.1)**.** *Let T be a tree on n vertices. Then the vertex v is the characteristic vertex of T if and only if there are two or more Perron components of T at v.*

Proposition 1.2.15 ([21], Proposition 2)**.** *Let T be a tree and suppose that v is not a characteristic vertex of T. Then the unique Perron component at v contains the characteristic set of T.*

Let $P_n : 12 \cdots n$ be the path on n vertices. As an application of Lemma 1.2.12, Proposition 1.2.13 and Proposition 1.2.14, we have the following remarks.

Remark 1.2.1. *For any Fiedler vector Y of P_n,*

$$\chi(P_n, Y) = \begin{cases} \{\frac{n}{2}, \frac{n}{2}+1\} & \text{if } n \text{ is even,} \\ \{\frac{n+1}{2}\} & \text{if } n \text{ is odd.} \end{cases}$$

Remark 1.2.2. *For any Fiedler vector Y of $K_{1,n-1}$, $\chi(K_{1,n-1}, Y) = \{v\}$ where v is the vertex of degree $n-1$ in $K_{1,n-1}$.*

The centrality nature of the characteristic set of a tree and its relation with other central parts of trees have been studied by many people. One can see some of the related studies in [1, 8, 29, 55].

1.2.1 Two new central parts

By Proposition 1.2.11, it is clear that the characteristic set of a tree is independent of the choice of the Fiedler vector but this is not true for general graphs. We have the following example.

Example 1.2.1. *In the cycle C_4, $\mu(C_4) = 2$ and $Y_1 = (1, 0, -1, 0)$ and $Y_2 = (0, 1, 0, -1)$ are two Fiedler vectors. If C_4 is $v_0v_1v_2v_3v_0$, then we get $\chi(C_4, Y_1) = \{v_1, v_3\}$ and $\chi(C_4, Y_2) = \{v_0, v_2\}$.*

The above example shows that, the characteristic set of a graph can be different for different Fiedler vectors. So, claiming it a central part in graphs is ill-suited. This motivates us to give a more general definition of the characteristic set to consider it as a central part of a graph.

Definition 1.2.16. *Let G be a connected graph and $L(G)$ be the Laplacian matrix of*

G. Then the **characteristic center** *$\chi(G)$ of G is given by*

$$\chi(G) = \{v \in V(G) : v \in \chi(G, Y) \ \textit{for some Fiedler vector } Y\}.$$

The term characteristic center (in place of characteristic set) of a tree is first used by Zimmermann in [55]. Clearly, $\chi(G)$ is independent of the choice of the Fiedler vector and for a tree T, $\chi(T) = \chi(T, Y)$ for any Fiedler vector Y. So, we note the following remark on the characteristic center of a tree.

Remark 1.2.3. *The characteristic center of a tree consists of either one vertex or two adjacent vertices.*

For the remaining part of the thesis, we use the term *characteristic center* of a tree instead of the *characteristic set* of a tree.

The subtree core is exclusively defined for trees. We give a very natural extension of the subtree core of a tree to general graphs. As trees have subtrees, graphs have connected subgraphs. So we define the subgraph core of a graph as follow.

Definition 1.2.17. *Let G be a graph and $v \in V(G)$. The subgraph number $f_G(v)$ of v is the number of connected subgraphs of G containing v. The set of vertices of G which have maximum subgraph number is called the* **subgraph core** *of G and we denote it by $S_c(G)$.*

Note that for a tree T, the subgraph core of T is same as the subtree core of T. So, we continue using the term subtree core for trees.

In section 1.4, we give an example of a tree in which the center, median, subtree core and the characteristic center are distinct. In Chapter 2, we study more about the characteristic center and the subgraph core, with a focus on their behaviour resembling with other central parts.

1.3 Indices related to some central parts

There are many topological indices defined for a graph. We observed that some of these indices are associated with some central parts of graphs. The Wiener index and the total eccentricity index are the two among them associated with the median and the center of a graph respectively. We introduce the *subgraph index* associated with the subgraph core of a graph.

The Wiener index is the oldest known and extensively studied graphical index. The Wiener index of a graph was first introduced by the Chemist H. Wiener in 1947 [45]. The *Wiener index* $W(G)$ of G is defined as the sum of distances between all unordered pairs of its vertices. $i.e.$

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

The Wiener index of a graph can also be defined through the distances of its vertices as follow.

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

This indicates that the distance of a vertex of G is a local version of the Wiener index of G. Since both $M(G)$ and $W(G)$ depend upon the distances of the vertices, the Wiener index of a graph can be observed as an index associated with its median.

The *total eccentricity index* of G is defined as the sum of eccentricities of all its vertices and we denote it by $\varepsilon(G)$. Thus in a graph G, the eccentricity of a vertex is a local version of the total eccentricity index. As the center of a graph is the set of vertices having minimum eccentricity, we see the total eccentricity index as an index associated with the center of a graph. The quantity closely related to the total eccentricity index is the average eccentricity of a graph. The *average eccentricity* of G, denoted by $avec(G)$, is defined as $avec(G) = \frac{\varepsilon(G)}{n}$, where n is the order of G. The average eccentricity is first defined by Buckley and Harary in 1990 (see [6], Exercise 9.1, problem 4) by the name *eccentric mean.*

In 2005, Székely and Wang ([38], [39]) started studying the number of subtrees of trees. They found the trees which maximizes or minimizes the number of subtrees over binary trees on n vertices. They observed that the number of subtrees of trees have some kind of reverse correlation with the Wiener index of trees. In many classes of trees, the tree which maximizes (minimizes) the number of subtrees are the trees which minimizes (maximizes) the Wiener index. With this a number of extremal problems regarding maximum or minimum number of subtrees in different class of trees arose and answered by many people. Some of them can be seen in [20, 23, 33, 53] and [54].

Motivated from the extremal problems on subtrees of trees, we chose to work on extremal problems of number of connected subgraphs of graphs. We define the **subgraph index** of G as the number of connected subgraphs of G and denote it by $F(G)$. From the definition of $F(G)$ and $f_G(v)$, it can be observed that in a graph G, the subgraph number of a vertex is a local version of the subgraph index. As both $S_c(G)$ and $F(G)$ are dependant on the number of connected subgraphs of G, we see the subgraph index as an index associated with the subgraph core.

The Wiener index, the total eccentricity index and the subgraph index are the three graphical indices of our interest. It can be observed that the Wiener index and the total eccentricity index are correlated in the sense that, in certain classes of graphs, the graph maximizing (minimizing) the Wiener index is same as the graph maximizing (minimizing) the total eccentricity index. The subgraph index of a graph is inversely correlated with both the Wiener index and the total eccentricity index in the same sense.

1.4 Motivation for the work

Motivated from the median and the security center of a graph as a generalisation of the centroid of a tree, we found it interesting to study the centrality behaviour of the subgraph core and the characteristic center in general graphs.

Let τ_n be the set of all trees on n vertices. Consider the path $P_n : 12\cdots n$ and the star $K_{1,n-1}$ in which v is the vertex of degree $n-1$. We have discussed the characteristic center of P_n and $K_{1,n-1}$ in Remark 1.2.1 and Remark 1.2.2. It can be easily observed that, the other central parts of P_n or $K_{1,n-1}$ coincide with the characteristic center. So we have,

$$C(P_n) = C_d(P_n) = S_c(P_n) = \chi(P_n) = \begin{cases} \{\frac{n}{2}, \frac{n}{2}+1\} & \text{if n is even,} \\ \{\frac{n+1}{2}\} & \text{if n is odd} \end{cases} \tag{1.4.1}$$

and

$$C(K_{1,n-1}) = C_d(K_{1,n-1}) = S_c(K_{1,n-1}) = \chi(K_{1,n-1}) = \{v\}. \tag{1.4.2}$$

But this is not true for every tree. We have the following examples in which the four central parts are mutually disjoint.

Example 1.4.1. *In the tree T in Figure 1.3, the center $C(T) = \{6\}$ as $e(6) = 5$ and eccentricity of any other vertex is more than 5. The centroid $C_d(T) = \{9\}$ as $\omega(9) = 8$ and weight of any other vertex is more than 8. The subtree core $S_c(T) = \{10\}$*

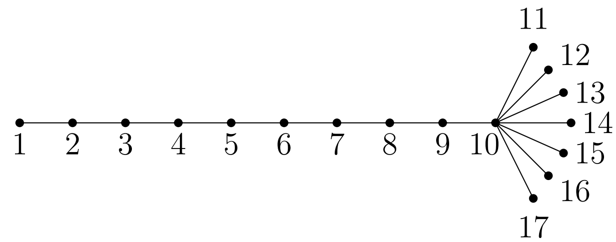


Figure 1.3: A tree T with disjoint central parts

as $f_T(10) = 10 \times 2^7$ *and the the number of subtrees containing any other vertex is less than* 10×2^7*. Also* $\mu(T) = .0483$ *and* $Y = (-0.4116, -0.3917, -0.3528, -0.2970, -0.2267, -0.1455, -0.0573, 0.0337, 0.1231, 0.2065, 0.2170, 0.2170, 0.2170, 0.2170, 0.2170, 0.2170, 0.2170)^T$ *is a Fiedler vector. So* $\chi(T) = \{7, 8\}$*, which is disjoint from each of the center, centroid and subtree core.*

Since the center, centroid, subtree core and the characteristic center coincide in both paths and stars, it follows that the minimum distance between any two of these central parts over τ_n is zero. It is natural to think about the maximum possible distances between any two of them, over τ_n. Next we introduce a class of trees which plays an important role in the study of maximizing the distances between different central parts of trees on n vertices.

For positive integers n and g with $g < n$, consider the tree obtained from the path P_{n-g} and the star $K_{1,g}$ by identifying one pendant vertex of P_{n-g} with the center of $K_{1,g}$. We denote this tree by $P_{n-g,g}$ and call it a *path-star tree*. Note that for a fixed n, we get different path-star trees by varying g. Also for $g = 1$, $P_{n-g,g} \cong P_n$ and for $g = n-1, n-2$, $P_{n-g,g} \cong K_{1,n-1}$. We keep the labelling of the vertices of $P_{n-g,g}$ fixed as in Figure 1.4.

In last two decades, the problems of maximizing the pairwise distances between different central parts of trees on n vertices have been studied by many researchers . We recall these results from the literature.

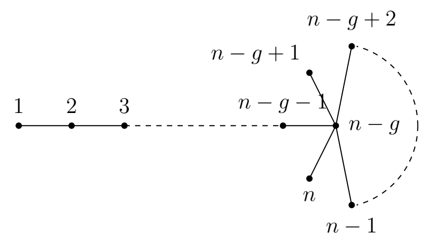


Figure 1.4: The path-star tree $P_{n-g,g}$

Proposition 1.4.1 ([29] and [37]). *For $n \geqslant 5$ and $T \in \tau_n$, $d_T(C, C_d) \leqslant \lfloor \frac{n-3}{4} \rfloor$ and the bound is attained by $P_{n-\lfloor \frac{n}{2} \rfloor, \lfloor \frac{n}{2} \rfloor}$.*

Proposition 1.4.2 ([12] and [37]). *Let $n \geqslant 5$ and let g_0 be the smallest positive integer satisfying $2^{g_0} + g_0 > n - 1$. For $T \in \tau_n$, we have*

(i) $d_T(C, S_c) \leqslant \lfloor \frac{n-g_0}{2} \rfloor - 1$ and the bound is attained by P_{n-g_0,g_0}.

(ii) $d_T(C_d, S_c) \leqslant \lfloor \frac{n-1}{2} \rfloor - g_0$ and the bound is attained by P_{n-g_0,g_0}.

Proposition 1.4.3 ([1] and [29]). *For $n \geqslant 5$ and $T \in \tau_n$, we have*

(i) $d_T(C_d, \chi) \leqslant d_{P_{n-\lfloor \frac{n}{2} \rfloor, \lfloor \frac{n}{2} \rfloor}}(C_d, \chi)$.

(ii) $d_T(C, \chi) \leqslant d_{P_{n-g,g}}(C, \chi)$, for some $2 \leqslant g \leqslant n - 3$.

Note that all the above maximum distances are attained in a path-star tree. The maximum distance between the characteristic center and the subtree core over τ_n is not studied yet. This motivated us to find the trees which maximizes the distance between the characteristic center and the subtree core over τ_n. This further motivated us to extend the study to some other classes of trees. We got to know about an unsolved problem on distances between different central parts in binary trees, which we discuss now. To introduce the problem, we need to describe the structure of a specific binary tree.

Let $n \geqslant 4$ be an even integer and let $l \geqslant 3$ be an odd integer such that $l < n$. Let $T_{rg}^{n,l}$ be the tree on n vertices which is obtained by identifying the root of the rgood tree T_{rg}^{l} with a vertex of maximum eccentricity of a binary caterpillar on $n-l+1$ vertices (see figure 1.5). The tree $T_{rg}^{n,l}$ is called a *crg tree*. The binary caterpillar on $n \geqslant 6$ vertices can be considered as one of $T_{rg}^{n,1}$, $T_{rg}^{n,3}$ or $T_{rg}^{n,5}$. We denote by Ω_n the class of all crg trees on n vertices.

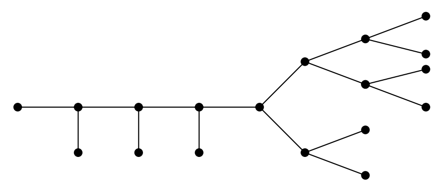


Figure 1.5: The crg tree $T_{rg}^{18,11}$

We observe that, due to symmetry in vertices, the center, centroid, subtree core and the characteristic center coincide in binary caterpillars. This shows that among all binary trees on n vertices the minimum distance between any two of these central parts is zero. Regarding the maximum distance between two central parts, Smith et al. conjectured the following in [37] (see Conjecture 3.10).

Among all binary trees on n vertices, the pairwise distance between any two of center, centroid and subtree core is maximized by some trees of the family Ω_n.

The above proposed conjecture for binary trees motivated us to study the pairwise distances between different central parts in binary trees.

In [38], Sźekely and wang have proved some extremization results on the number of subtrees of trees. Since then a lot has been studied regarding characterization of trees maximizing or minimizing the the number of subtrees in different classes of trees (see

[9, 20, 23, 33, 39, 47, 48, 52, 53, 54]). From this we get the motivation to characterize the graphs maximizing or minimizing the number of connected subgraphs in various classes of graphs. In this direction, we continue our study for the Wiener index and the total eccentricity index also.

Chapter 2

Central parts of trees and graphs

This chapter is divided into three sections. In Section 2.1 we discuss the centrality nature of the characteristic center and the subgraph core of a graph. In Section 2.2 we study the distances between different central parts of trees for some classes of trees. Finally we conclude the chapter with some open problems related to different central parts of graphs.

2.1 The characteristic center and the subgraph core

In Chapter 1, we defined the characteristic center and the subgraph core of a graph as a generalization of the characteristic set and the subtree core of a tree, respectively. Here we discuss their centrality nature in graphs. The center, median and the security center are the three central parts defined for any connected graphs. All these three have some similar features. We show that the new central parts we defined also have these features, which suggest that they behave like central parts in graphs.

Like center, median and security center, the subgraph core and the characteristic center of a tree contain either a single vertex or two adjacent vertices. For the path

$P_n : 12 \cdots n$ and the star $K_{1,n-1}$, we have

$$C(P_n) = M(P_n) = \mathbb{S}(P_n) = \begin{cases} \{\frac{n}{2}, \frac{n}{2}+1\} & \text{if n is even,} \\ \\ \{\frac{n+1}{2}\} & \text{if n is odd} \end{cases} \tag{2.1.1}$$

and

$$C(K_{1,n-1}) = M(K_{1,n-1}) = \mathbb{S}(K_{n-1}) = \{v\} \tag{2.1.2}$$

where $v \in V(K_{1,n-1})$ is the vertex of degree $n-1$.

In the complete graph K_n, $e(v) = 1$ and $D(v) = n-1$ for any $v \in V(K_n)$. Also for $u, v \in V(K_n)$, $V_{vu} = \{v\}$ and $V_{uv} = \{u\}$ which gives $s(v) = 0$ for all $v \in V(K_n)$. Hence we get

$$C(K_n) = M(K_n) = \mathbb{S}(K_n) = V(K_n). \tag{2.1.3}$$

Similarly in C_n, $e(v) = \lfloor \frac{n}{2} \rfloor$ and $D(v) = \lfloor \frac{n^2}{4} \rfloor$ for any $v \in V(C_n)$. Also For $u, v \in V(C_n)$, there are two paths from u to v, one in clockwise direction and the other in anti clockwise direction. In each of these paths the number of vertices closure to u than v is same as the number of vertices closure to v than u. So $|V_{vu}| = |V_{uv}|$, implying $s(v) = 0$ for any $v \in V(C_n)$. Hence we get,

$$C(C_n) = M(C_n) = \mathbb{S}(C_n) = V(C_n). \tag{2.1.4}$$

In Chapter 1, it is also mentioned that the center, median and the security center of a graph is contained in a block. To explain the centrality behaviour of the two newly defined central parts of graphs, we try to establish the above centrality features for them.

2.1.1 The characteristic center

From Remark 1.2.3, the characteristic center of a tree consists of either a single vertex or two adjacent vertices. Also from Remark 1.2.1 and Remark 1.2.2, it follows that

$$\chi(P_n) = \begin{cases} \{\frac{n}{2}, \frac{n}{2}+1\} & \text{if } n \text{ is even,} \\ \{\frac{n+1}{2}\} & \text{if } n \text{ is odd.} \end{cases}$$

and

$$\chi(K_{1,n-1}) = \{v\}$$

where v is the vertex of degree $n-1$ in $K_{1,n-1}$.

Now we obtain the characteristic center of K_n and C_n.

Theorem 2.1.1. *For $n \geqslant 2$, $\chi(K_n) = V(K_n)$.*

Proof. Let $V(K_n) = \{v_1, v_2, \ldots, v_n\}$. The Laplacian eigenvalues of K_n are 0 with multiplicity 1 and n with multiplicity $n-1$. So $\mu(K_n) = n$. It is easy to check that $Y = (1, -1, 0, 0, \ldots, 0)$ is a Fiedler vector of K_n. Since $Y(v_1)Y(v_2) = -1$, so $v_1, v_2 \in \chi(K_n)$. Also for $i \geqslant 3$, $Y(v_i) = 0$ and v_i adjacent to v_1 with $Y(v_1) \neq 0$. This gives $v_i \in \chi(G)$ for $i = 3, 4, \ldots n$ and hence, $\chi(G) = V(K_n)$. □

Theorem 2.1.2. *For $n \geqslant 3$, $\chi(C_n) = V(C_n)$.*

Proof. Let $C_n : v_0 v_1 \cdots v_{n-1} v_0$ be the cycle on n vertices. The Laplacian eigenvalues of C_n are $2 - 2\cos(\frac{2\pi j}{n}), j = 1, 2, \ldots, n$ (see [5], Lemma 4.9). Since cosine function is decreasing in $[0, \pi]$ and $\cos(2\pi - \theta) = \cos\theta$, it follows that the algebraic connectivity of C_n is $2(1 - \cos(\frac{2\pi}{n}))$ with multiplicity 2. Consider the vectors $X = \Big(1, \cos(\frac{2\pi}{n}), \cos(\frac{4\pi}{n}), \ldots, \cos(\frac{2(n-1)\pi}{n})\Big)$ and $Y = \Big(0, \sin(\frac{2\pi}{n}), \sin(\frac{4\pi}{n}), \ldots, \sin(\frac{2(n-1)\pi}{n})\Big)$. It is easy to check that X and Y are two linearly independent Fiedler vectors of C_n. As

$n \geqslant 3$, $\sin(\frac{2\pi}{n}) \neq 0$, so Y is a Fiedler vector with $Y(v_0) = 0$ and $Y(v_1) \neq 0$ which implies v_0 is a characteristic vertex of C_n with respect to Y. Since there is no $\theta \in [0, 2\pi]$ such that $\sin(\theta) = \cos(\theta) = 0$, hence $X(v_i)$ and $Y(v_i)$ can never be simultaneously zero for any $i = 1, 2, \ldots, n-1$. So for $j = 1, 2, \ldots, n-1$, $Z_j = \sin(\frac{2\pi j}{n})X - \cos(\frac{2\pi j}{n})Y = \Big(\sin(\frac{2\pi j}{n}), \sin(\frac{2\pi(j-1)}{n}), \sin(\frac{2\pi(j-2)}{n}), \ldots, \sin(\frac{2\pi(j-n+1)}{n})\Big)$ is also a Fiedler vector of C_n. Note that for $j = 1, 2, \ldots, n-1$, $Z_j(v_j) = 0$ and $Z_j(v_{j-1}) = \sin(\frac{2\pi}{n}) \neq 0$. This implies that, v_j is a characteristic vertex of C_n w.r.t. Z_j for each $j = 1, 2, \ldots, n-1$. Hence $\chi(C_n) = \{v_0, v_1, \ldots, v_{n-1}\} = V(C_n)$. □

An important feature of any central part of a graph G is that it lies in a block of G. To support the centrality nature of the characteristic center, next we show that $\chi(G)$ lies in a block of G. Let Y be a Fiedler vector of G. We call a vertex v has a positive valuation, negative valuation or zero valuation depending upon whether $Y(v)$ is positive, negative or zero, respectively.

Proposition 2.1.3 ([13], Theorem 3,12). *Let G be a connected graph and Y be a Fiedler vector of G. Then exactly one of the following cases holds.*

Case A: *There is a single block B_0 in G which contains vertices with both positive and negative valuations. Each other block contains either only positively valuated vertices, only negatively valuated vertices or only zero valuated vertices. Every path P starting from B_0, which contains at most two cut vertices in each block and exactly one vertex k in B_0 has the property that the valuations of the cut vertices of G lying in P, form either an increasing or a decreasing or a zero sequence along this path according to whether $Y(k) > 0, Y(k) < 0$ or $Y(k) = 0$. In the last case all the vertices on P have valuation zero.*

Case B: *No block of G contains both positively and negatively valuated vertices. There* *exists a unique vertex z of valuation zero which is adjacent to a vertex with non-zero valuation. This vertex z is a cut vertex. Each block contains (with the exception of z) either the vertices with positive valuations only, vertices with negative valuations only or vertices with zero valuations only. Every path P starting from z which contains at most two cut vertices in each block has the property that the valuations at its cut vertices either increases and then all valuations of vertices on P are positive(with the exception of z), or decreases and then all valuations of the vertices on P are negative (with the exception of z) or all valuations of the vertices on P are zero. Every path containing both positively and negatively valuated vertices passes through z.*

Kirkland and Fallat proved the following result which tells about the position of characteristic center in a graph .

Lemma 2.1.4 ([22], Corollary 2.1)**.** *Let G be a graph. Then either Case A holds for every Fiedler vector, and each such Fiedler vector identifies the same block as being the one with both positively and negatively valuated vertices, or Case B holds for every Fiedler vector, and each such vector identifies the same vertex z which has zero valuation and is adjacent to one with nonzero valuation.*

The next result follows from Lemma 2.1.4, which affirms the centrality nature of the characteristic center.

Theorem 2.1.5. *The characteristic center of a graph G is contained in a block of G.*

The above deliberations show that the features of the characteristic center of a graph resembles with center, median and security center, which indicates that the characteristic center behaves like a central part of a graph. The following example shows that the center, characteristic center, median and security center can be different in a graph.

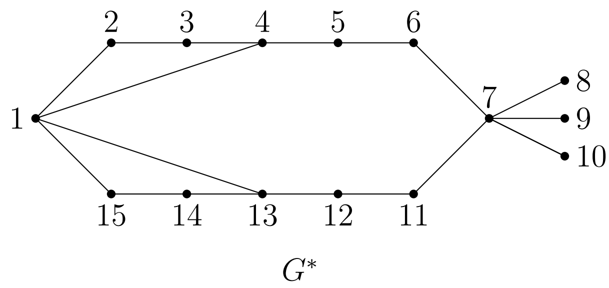


Figure 2.1: A graph with different center, characteristic center, median and security center

Example 2.1.1. *In Figure 2.1, the center* $C(G^*) = \{4, 5, 12, 13\}$*, the median* $M(G^*) = \{4, 13\}$*, and the security center* $\mathbb{S}(G^*) = \{1, 4, 5, 6, 7, 11, 12, 13\}$ *(see [34], Section 1). It can be checked using Matlab that* $\mu(G^*) = 0.2$ *and* $Y = (-0.2485, -0.2837, -0.2623, -0.1883, -0.0166, 0.1584, 0.3018, 0.3772, 0.3772, 0.3772, 0.1584, -0.0166, -0.1883, -0.2623, -0.2837)^T$ *is the unique Fiedler vector up to a scalar multiplication. So it follows that* $\chi(G^*) = \{5, 6, 11, 12\}$.

2.1.2 The subgraph core

The subgraph core of a graph is a natural extension of the subtree core of trees. So by Proposition 1.2.9, the subgraph core of a tree consists of either a single vertex or two adjacent vertices. Also, we have

$$S_c(P_n) = \begin{cases} \{\frac{n}{2}, \frac{n}{2}+1\} & \text{if } n \text{ is even,} \\ \{\frac{n+1}{2}\} & \text{if } n \text{ is odd} \end{cases}$$

and

$$S_c(K_{1,n-1}) = \{v\}$$

where v is the vertex of degree $n-1$ in $K_{1,n-1}$.

Now we obtain the subgraph core of K_n and C_n.

Theorem 2.1.6. *For any positive integer n, $S_c(K_n) = V(K_n)$.*

Proof. For any vertex v of K_n, we have $F(K_n) = F(K_{n-1}) + f_{K_n}(v)$. Here $F(K_{n-1})$ counts the number of connected subgraphs of K_n not containing v and $f_{K_n}(v)$ counts the number of connected subgraphs of K_n containing v. Thus, we get $f_{K_n}(v) = F(K_n) - F(K_{n-1})$ for any $v \in V(K_n)$. This implies $S_c(K_n) = V(K_n)$.

□

Theorem 2.1.7. *For $n \geqslant 3$, $S_c(C_n) = V(C_n)$.*

Proof. Let $v \in V(C_n)$. Then the single vertex v and the cycle C_n are two connected subgraphs of C_n containing v. All other connected subgraphs of C_n containing v are paths with at least two vertices. The number of paths in C_n containing v as a pendant vertex is $2(n-1)$ and the number of paths in C_n containing v as a non-pendant vertex is $\binom{n-1}{2}$. Thus, we have $f_{C_n}(v) = 2n + \binom{n-1}{2}$ for all $v \in V(C_n)$ and hence $S_c(C_n) = V(C_n)$. □

Thus the subgraph core of a graph fulfils many features of a central part. By Example 1.4.1 it follows that the subgraph core of a graph can be different from the center, median and the characteristic center. One of the most important feature of a central part of a graph is that, it should be contained in a block. We strongly feel that the subgraph core fulfils this feature, but we are not able to prove it. So we propose the following conjecture.

Conjecture 2.1.8. *The subgraph core of a graph G is contained in a block of G.*

This influences us to consider the subgraph core as a central part of a graph. By examples 1.4.1 and 2.1.1, it is clear that the center, median, security center, characteristic center and the subgraph core may be different in a graph. Thus we have five distinct central parts in graphs among which four are combinatorially defined and one is algebraically defined.

2.2 Distance between different central parts of trees

In this section, we study the distance between the characteristic center and the subtree core among all trees on n vertices. We also study the asymptotic nature of the distances between different central parts of trees. Finally we discuss the distance between different central parts of trees with fixed diameter.

2.2.1 Some results from the literature

The following two lemmas related to the subtree core of trees are important for our study.

Lemma 2.2.1 ([12], Lemma 2.2)**.** *Let T be a tree, $v \in S_c(T)$ and y be a pendant vertex of T not adjacent to v. If $\tilde{T}$ is the tree obtained from T by detaching y from T and adding it as a pendant vertex adjacent to v, then $S_c(\tilde{T}) = \{v\}$.*

Lemma 2.2.2 ([12], Lemma 3.1)**.** *Let T be a tree, $v \in S_c(T)$ and B be a branch at v. Let u be the vertex in B adjacent to v and x be a pendant vertex of T in B. Suppose that B is not a path. Let y be the vertex closest to x with $\deg(y) \geqslant 3$ and $[y, y_1, y_2, \ldots, y_m = x]$ be the path connecting y and x. Let $z \neq y$ be a vertex of B such that the path from v to z contains y but not y_1. Let $\tilde{T}$ be the tree obtained from T by detaching the path $[y_1, y_2, \ldots, y_m]$ from y and attaching it to z. Then $f_{\tilde{T}}(v) > f_{\tilde{T}}(u)$.*

The path-star trees play an important role in the study of distance between the characteristic center and the subtree core of a tree. The following lemma tells about the subtree core of path-star trees.

Lemma 2.2.3 ([12], Theorem 2.4). *The subtree core of the path-star tree $P_{n-g,g}$ is given by*

$$S_c(P_{n-g,g}) = \begin{cases} \begin{cases} \{\frac{n-g+2^g}{2}\} & \text{if } n-g \text{ is even,} \\ \{\frac{n-g-1+2^g}{2}, \frac{n-g+1+2^g}{2}\} & \text{if } n-g \text{ is odd,} \end{cases} & \text{if } 2^g+1 \leqslant n-g, \\ \{n-g\} & \text{if } 2^g+1 > n-g. \end{cases}$$

The next two results are related to the study of the position and the movement of characteristic center in path-star trees.

Lemma 2.2.4 ([29], Lemma 2.2). *The characteristic center of $P_{n-2,2}$ is given by*

$$\chi(P_{n-2,2}) = \begin{cases} \{\frac{n}{2}, \frac{n}{2}+1\} & \text{if } n \text{ is even,} \\ \{\frac{n-1}{2}, \frac{n+1}{2}\} & \text{if } n \text{ is odd.} \end{cases}$$

Lemma 2.2.5 ([29], Proposition 3.1, 3.2, 3.3 and 3.4). *The following hold for the path-star tree $P_{n-g,g}$.*

(i) If $\chi(P_{n-g,g}) = \{i, i+1\}$ where $g \geqslant 3$ and $2 \leqslant i \leqslant n-g-1$, then $\chi(P_{n-g+1,g-1}) = \{i, i+1\}$ or $\{i+1\}$ or $\{i+1, i+2\}$.

(ii) If $\chi(P_{n-g,g}) = \{i\}$, where $g \geqslant 3$, then $\chi(P_{n-g+1,g-1}) = \{i, i+1\}$.

(iii) If $\chi(P_{n-g,g}) = \{i, i+1\}$ where $g \leqslant n-4$, then $\chi(P_{n-g-1,g+1}) = \{i-1, i\}$ or $\{i\}$ or $\{i, i+1\}$.

(iv) If $\chi(P_{n-g,g}) = \{i\}$ where $g \leqslant n-4$, then $\chi(P_{n-g-1,g+1}) = \{i-1, i\}$.

2.2.2 The characteristic center and the subtree core

The center, centroid, subtree core and the characteristic center coincide for both path and star. It shows that, among all trees on n vertices the minimum distance between any two of the four central parts is zero. Except for the pair {characteristic center, subtree core} the problems of maximizing the distances between all other five pairs of central parts are studied (see Proposition 1.4.1, 1.4.2 and 1.4.3) . We now discuss the same for the pair {characteristic center, subtree core}.

Lemma 2.2.6. *For the path-star tree $P_{n-2,2}$, $d_{P_{n-2,2}}(S_c, \chi) = 0$.*

Proof. By Lemma 2.2.3, if $n < 7$ then $S_c(P_{n-2,2}) = \{n-2\}$ and if $n \geqslant 7$,

$$S_c(P_{n-2,2}) = \begin{cases} \{\frac{n}{2}+1\} & \textit{if } n \textit{ is even,} \\ \{\frac{n+1}{2}, \frac{n+3}{2}\} & \textit{if } n \textit{ is odd.} \end{cases}$$

Hence by Lemma 2.2.4, $d_{P_{n-2,2}}(S_c, \chi) = 0$. □

Theorem 2.2.7. *Among all trees on $n \geqslant 5$ vertices, the distance between the subtree core and the characteristic center is maximized by some path-star tree.*

Proof. Let T be a tree on n vertices. Our aim is to construct a path-star tree $P_{n-g,g}$ such that $d_{P_{n-g,g}}(S_c, \chi) \geqslant d_T(S_c, \chi)$. By Lemma 2.2.6, $d_{P_{n-2,2}}(S_c, \chi) = 0$, so we assume that $d_T(S_c, \chi) \geqslant 1$.

As the subtree core of a tree consists of either one vertex or two adjacent vertices and the characteristic center of a tree consists of a vertex or an edge (two adjacent vertices), so we need to consider four cases. Here, we prove the case when subtree core consists of two adjacent vertices and the characteristic center consists of an edge. The proofs of the other three cases are similar.

Let $\chi(T) = \{u_1, v_1\}$ and $S_c(T) = \{u_2, v_2\}$. Also suppose that $d_T(S_c, \chi) = d(v_1, u_2)$. Let $C_1, C_2, \ldots, C_k$ be the components of $T - v_2$ where C_1 is the component containing u_2. If $|V(C_i)| = 1$ for $2 \leqslant i \leqslant k$, then rename the tree T as $\tilde{T}$. Otherwise, let $C = \bigcup_{i=2}^{k} C_i$ and $|V(C)| = s$. Construct a new tree $\tilde{T}$ from T by removing C and adding s pendant vertices at v_2. By Lemma 2.2.1, $S_c(\tilde{T}) = \{v_2\}$. We will now check the effect of this perturbation on the distance between characteristic center and subtree core in $\tilde{T}$. For that we will obtain $\tilde{T}$ from T little differently. In T at v_1, let T_1 be the component containing u_1 and T_2 be the component containing u_2. By Theorem 1.2.13, T_1 is the only Perron component at v_1 in T. In T at v_1, replace the component T_2 by another component $\tilde{T_2}$, where $\tilde{T_2}$ is obtained from T_2 by removing C and adding s pendant vertices at v_2. The new tree is $\tilde{T}$ and by Lemma 1.2.12, $\hat{L}(\tilde{T_2})^{-1} \ll \hat{L}(T_2)^{-1}$. So, $\rho(\hat{L}(\tilde{T_2})^{-1}) < \rho(\hat{L}(T_2)^{-1})$ and hence in $\tilde{T}$ at v_1, T_1 is the only Perron component. By Theorem 1.2.15, the characteristic center of $\tilde{T}$ is either $\{u_1, v_1\}$ or moves away from u_2. So $d_{\tilde{T}}(S_c, \chi) \geqslant d_T(S_c, \chi)$.

If $\tilde{T}$ is a path-star tree, then the result follows. Suppose $\tilde{T}$ is not a path-star tree. In $\tilde{T}$, let v_3 be the characteristic vertex nearest to the subtree core v_2. Let $A_1, A_2, \ldots, A_p$ be the connected components of $\tilde{T} - v_3$ with A_1 as the component containing the subtree core. If $p = 2$ and A_2 is a path then rename the tree $\tilde{T}$ as $\hat{T}$. Otherwise, let $\tilde{C} = \bigcup_{i=2}^{p} A_i$. Construct a new tree $\hat{T}$ from $\tilde{T}$ by replacing $\tilde{C}$ with a path P on $|\tilde{C}|$ vertices. Then by Lemma 1.2.12, $\hat{L}(\tilde{C})^{-1} \ll \hat{L}(P)^{-1}$. So, $\rho(\hat{L}(\tilde{C})^{-1}) < \rho(\hat{L}(P)^{-1})$ and hence in $\hat{T}$ at v_3, the component not containing v_2 is the only Perron component. By Theorem 1.2.15, the characteristic center of $\hat{T}$ is either $\{u_3, v_3\}$ or moves away from v_2. The tree $\hat{T}$ can also be obtained from $\tilde{T}$ by following the perturbation mentioned in Lemma 2.2.2. Hence by Lemma 2.2.2, $S_c(\hat{T}) = \{v_2\}$. So $d_{\hat{T}}(S_c, \chi) \geqslant d_{\tilde{T}}(S_c, \chi)$.

If $\hat{T}$ is a path-star tree, then the result follows. Otherwise, $\hat{T}$ has three parts. The first part is the path from vertex 1 to u_3, second is a tree T' containing v_3 and u_2 and the third part is the star $K_{1,s}$ centred at v_2. Clearly T' is not a path. Let Q be the $v_3 - u_2$ path in T' and let there are l vertices of T' which are not in Q. Delete all the vertices from T' which are not in the path Q and add a path on l vertices at 1, to form a new tree $\bar{T}$. Note that $\bar{T} \cong P_{n-s,s}$. At v_3 in $\bar{T}$, there are two components and the component containing u_3 is the Perron component. By Theorem 1.2.15, the characteristic center of $\bar{T}$ is either $\{u_3, v_3\}$ or moves away from v_2. The tree $\bar{T}$ can also be obtained from $\hat{T}$ by following the perturbation mentioned in Lemma 2.2.2. Hence by Lemma 2.2.2, $S_c(\hat{T}) = \{v_2\}$. So $d_{\bar{T}}(S_c, \chi) \geqslant d_{\hat{T}}(S_c, \chi)$. This proves the result. □

For $1 \leqslant i \leqslant n-g$, the number of subtrees containing the vertex i in the path-star tree $P_{n-g,g}$ is given by

$$f_{P_{n-g,g}}(i) = i(n-g-i) + i(2^g). \tag{2.2.1}$$

Here the first term counts the number of subtrees of $P_{n-g,g}$ containing the vertex i but not $n-g$, while the second term counts the number of subtrees of $P_{n-g,g}$ containing both i and $n-g$. The following lemma describes the movement of the subtree core while changing a path-star tree on n vertices by decreasing the size of its star part.

Lemma 2.2.8. *Let g_0 be the smallest positive integer such that $2^{g_0}+1 > n-g_0$. Then for $1 \leqslant k \leqslant g_0 - 2$, a vertex $n - g_0 - \alpha \in S_c(P_{n-g_0+k,g_0-k})$ for some $\alpha \geqslant 0$.*

Proof. Since $2^{g_0} + 1 > n - g_0$, by Lemma 2.2.3, $S_c(P_{n-g_0,g_0}) = n - g_0$. For $1 \leqslant k \leqslant g_0 - 2$, by (2.2.1), we have

$$f_{P_{n-g_0+k,g_0-k}}(n-g_0) = (n-g_0)(k + 2^{g_0-k})$$

and

$$f_{P_{n-g_0+k,g_0-k}}(n-g_0+1) = (n-g_0+1)(k-1+2^{g_0-k}).$$

Then

$$\begin{aligned}
&f_{P_{n-g_0+k,g_0-k}}(n-g_0) - f_{P_{n-g_0+k,g_0-k}}(n-g_0+1)\\
&= n-g_0-(k-1+2^{g_0-k})\\
&= [n-(g_0-1)-(2^{g_0-1}+1)] + 2^{g_0-1} - 2^{g_0-k} - k + 1\\
&\geqslant 2^{g_0-k}(2^{k-1}-1) - k + 1\\
&\geqslant 0.
\end{aligned}$$

By Proposition 1.2.10, the function f_T is strictly concave, hence the result follows. □

Theorem 2.2.9. *Let g_0 be the smallest positive integer such that $2^{g_0}+1 > n-g_0$. Then among all trees on $n \geqslant 5$ vertices, the path-star tree P_{n-g_0,g_0} maximizes the distance between the subtree core and the characteristic center.*

Proof. By Theorem 2.2.7, we need to consider path-star trees only. Consider the path-star tree P_{n-g_0,g_0}. Let $d_{P_{n-g_0,g_0}}(\chi, S_c) = r$. We show that for $g \neq g_0$, $d_{P_{n-g,g}}(\chi, S_c) \leqslant r$. By Lemma 2.2.3, $S_c(P_{n-g_0,g_0}) = \{n-g_0\}$. So $\chi(P_{n-g_0,g_0}) = \{n-g_0-r\}$ or $\{n-g_0-r-1, n-g_0-r\}$.

First suppose that $g = g_0+1$. Then by Lemma 2.2.3, $S_c(P_{n-g,g}) = S_c(P_{n-g_0-1,g_0+1}) = \{n-g_0-1\}$. By Lemma 2.2.5, if $\chi(P_{n-g_0,g_0}) = \{n-g_0-r\}$, then $\chi(P_{n-g_0-1,g_0+1}) = \{n-g_0-r-1, n-g_0-r\}$ and if $\chi(P_{n-g_0,g_0}) = \{n-g_0-r-1, n-g_0-r\}$, then $\chi(P_{n-g_0-1,g_0+1}) = \{n-g_0-r-2, n-g_0-r-1\}$ or $\{n-g_0-r-1\}$ or $\{n-g_0-r-1, n-g_0-r\}$. It is easy to check that $d_{P_{n-g_0-1,g_0+1}}(\chi, S_c) \leqslant r$. Same argument holds for any $g > g_0$.

Let $1 \leqslant k \leqslant g_0-2$. Now suppose that $g = g_0-k$. Then by Lemma 2.2.8, the subtree core of P_{n-g_0+k,g_0-k} moves at least k steps and by Lemma 2.2.5 the characteristic center moves at most k steps towards center. So $d_{P_{n-g_0+k,g_0-k}}(\chi, S_c) \leqslant r$ and hence the result follows. $\square$

2.2.3 Asymptotic distance between two central parts

We define $\delta_n(\chi, S_c) = \max\{d_T(\chi, S_c)$:T is a tree on n vertices$\}$. Analogously we define $\delta_n(C, S_c)$, $\delta_n(C, C_d)$, $\delta_n(C_d, S_c)$, $\delta_n(C, \chi)$ and $\delta_n(C_d, \chi)$. In [1], the authors have established the limits $\lim\limits_{n\to\infty} \frac{\delta_n(C,\chi)}{n}$ and $\lim\limits_{n\to\infty} \frac{\delta_n(C_d,\chi)}{n}$. We will now do the same for the remaining four. We need the following lemma to prove our results.

Lemma 2.2.10 ([29], Theorem 3.3 and [12], Proposition 4.1)**.** *In any path-star tree the following hold.*

(i) The characteristic center lies in the path joining the center and the centroid.

(ii) The centroid lies in the path joining the center and the subtree core.

Theorem 2.2.11. *For the asymptotic distances between different central parts of trees, we have the following:*

(i) $\lim\limits_{n\to\infty} \frac{\delta_n(C,C_d)}{n} = \frac{1}{4}$.

(ii) $\lim\limits_{n\to\infty} \frac{\delta_n(C,S_c)}{n} = \frac{1}{2}$.

(iii) $\lim\limits_{n\to\infty} \frac{\delta_n(C_d,S_c)}{n} = \frac{1}{2}$.

(iv) $\lim\limits_{n\to\infty} \frac{\delta_n(\chi,S_c)}{n} = \frac{1}{2}$.

Proof. (i) Follows from Proposition 1.4.1.

(ii) For $n \geqslant 5$, let g_0 be the smallest positive integer such that $2^{g_0} + g_0 > n - 1$. So $2^{g_0-1} + g_0 - 1 \leqslant n - 1$. This implies $2^{g_0-1} < n$. Taking logarithm with base 2 on both side, we have $g_0 < 1 + \log_2 n$. As $n \geqslant 5$, so $0 < g_0 < 1 + \log_2 n$. Since $\lim\limits_{n\to\infty} \frac{\log_2 n}{n} = 0$, so $\lim\limits_{n\to\infty} \frac{g_0}{n} = 0$. By Proposition 1.4.2($i$), $\delta_n(C, S_c) = \lfloor \frac{n-g_0}{2} \rfloor - 1$. This implies that

$$\lim_{n\to\infty} \frac{\delta_n(C, S_c)}{n} = \lim_{n\to\infty} \frac{\lfloor \frac{n-g_0}{2} \rfloor - 1}{n} = \frac{1}{2}.$$

(iii) Since $\lim\limits_{n\to\infty} \frac{g_0}{n} = 0$, the result follows from Proposition 1.4.2(ii).

(iv) By Theorem 2.2.9, we have $\delta_n(\chi, S_c) = d_{P_{n-g_0,g_0}}(\chi, S_c)$. Also by Proposition 1.4.2(i), $\delta_n(C, S_c) = d_{P_{n-g_0,g_0}}(C, S_c)$ and by Proposition 1.4.2(ii), $\delta_n(C_d, S_c) = d_{P_{n-g_0,g_0}}(C_d, S_c)$. Now from Lemma 2.2.10, it follows that

$$\delta_n(C_d, S_c) \leqslant \delta_n(\chi, S_c) \leqslant \delta_n(C, S_c)$$

$$\Rightarrow \lim_{n\to\infty} \frac{\delta_n(C_d, S_c)}{n} \leqslant \lim_{n\to\infty} \frac{\delta_n(\chi, S_c)}{n} \leqslant \lim_{n\to\infty} \frac{\delta_n(C, S_c)}{n}.$$

As $\lim\limits_{n\to\infty} \frac{\delta_n(C,S_c)}{n} = \frac{1}{2} = \lim\limits_{n\to\infty} \frac{\delta_n(C_d,S_c)}{n}$, it follows that $\lim\limits_{n\to\infty} \frac{\delta_n(\chi,S_c)}{n} = \frac{1}{2}$.

□

2.2.4 Trees with fixed diameter

In this section, we try to obtain the trees which extremize the distances between two central parts among all trees on n vertices with diameter d. It is clear that K_2 is the unique tree with diameter 1 and any tree of diameter 2 is a star on $n \geqslant 3$ vertices. Also given $n \geqslant 2$, the path is the only tree with diameter $n - 1$. So we assume that $n \geqslant 3$ and $3 \leqslant d \leqslant n - 2$.

For a tree T and the edge $e = \{u, v\} \in E(T)$, we denote the component of $T - e$ containing u by $T_e(u)$. The following result helps us to find the location of the subtree core in a tree.

Proposition 2.2.12 ([37], Proposition 1.7)**.** *Let T be a tree. A vertex $u \in S_c(T)$ if and only if for each neighbour v of u, $f_{T_e(u)}(u) \geqslant f_{T_e(v)}(v)$ where $e = \{u, v\}$. Furthermore, if $u \in S_c(T)$ and equality holds then $v \in S_c(T)$.*

We denote the set of all trees on n vertices with diameter d by Γ_n^d. Take the path $P_{d+1} : v_1 v_2 \cdots v_{d+1}$ and construct a new tree by adding $n - d - 1$ pendant vertices at the vertex $v_{\lfloor \frac{d+2}{2} \rfloor}$ of P_{d+1}. We denote the new tree by T_n^d. Clearly $T_n^d \in \Gamma_n^d$.

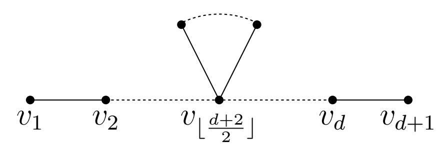


Figure 2.2: The tree T_n^d

Theorem 2.2.13. *Among all trees on n vertices with diameter d, the minimum distance between any two of the central parts center, centroid, subtree core and characteristic center is* 0.

Proof. Since $T_n^d \in \Gamma_n^d$, it is sufficient to show that the distance between different central parts in T_n^d is zero. We consider two cases depending on d is even or odd.

Case I: d is even

It is easy to check that $C(T_n^d) = C_d(T_n^d) = \{v_{\frac{d+2}{2}}\}$. Also at $v_{\frac{d+2}{2}}$ in T_n^d, there are two Perron components (since $d > 2$), so by Proposition 1.2.14 $\chi(T_n^d) = \{v_{\frac{d+2}{2}}\}$.

Since $n \geqslant 3$, so the subtree core $S_c(T_n^d)$ does not contain any pendent vertex (see [12], Remark 1.5). Consider the edge $e = \{v_{\frac{d}{2}}, v_{\frac{d+2}{2}}\}$. Let C_1 and C_2 be the components of $T-e$ containing $v_{\frac{d}{2}}$ and $v_{\frac{d+2}{2}}$, respectively. Since a copy of C_1 is properly contained in C_2, $f_{C_2}(v_{\frac{d+2}{2}}) > f_{C_1}(v_{\frac{d}{2}})$. By symmetry and Proposition 2.2.12, we have $S_c(T_n^d) = \{v_{\frac{d+2}{2}}\}$ and hence the result follows.

Case II: d is odd

Since $n > d+1$, we have $C(T_n^d) = \{v_{\frac{d+1}{2}}, v_{\frac{d+3}{2}}\}$ and $C_d(T_n^d) = \{v_{\frac{d+1}{2}}\}$. At $v_{\frac{d+1}{2}}$, the component containing $v_{\frac{d+3}{2}}$ is the only Perron component and at $v_{\frac{d+3}{2}}$ the component containing $v_{\frac{d+1}{2}}$ is the only Perron component, so by Proposition 1.2.13, $\chi(T_n^d) = \{v_{\frac{d+1}{2}}, v_{\frac{d+3}{2}}\}$. Also using similar technique as in Case I, it can be checked that $S_c(T_n^d) = \{v_{\frac{d+1}{2}}\}$. Hence the result follows. $\square$

Now we try to obtain the trees , which maximize the distance between two central parts over Γ_n^d. Smith et al. have studied the same for the pairs {center, centroid} and {center, subtree core} (see [37], Proposition 4.1 and Proposition 4.2). We will discuss the maximum distances over Γ_n^d for the pairs {center, characteristic center} and {centroid, characteristic center}.

Theorem 2.2.14. *The path-star tree $P_{d,n-d}$ maximizes the distance between the center and the characteristic center over Γ_n^d.*

Proof. Let $T \in \Gamma_n^d$. We will prove that $d_{P_{d,n-d}}(C,\chi) \geqslant d_T(C,\chi)$. Without loss of generality we can take $d_T(C,\chi) \geqslant 1$. The center of T lies in all the longest paths of T. We consider two cases depending on the position of characteristic center of T.

Case I: Characteristic center of T lies in a longest path

Let P be a longest path of T containing both $C(T)$ and $\chi(T)$. Then the diameter of the path P is d. Let v be the vertex in the characteristic center which is farthest from $C(T)$. Let $C_1, C_2, \ldots, C_l$ be the components of $T-v$ where C_1 is the component containing the center of T. If $|C_j| = 1$ for $j = 2, 3, \ldots l$, then rename the tree T as $\tilde{T}$. Otherwise, let $C = \bigcup_{j=2}^{l} C_j$ and $|V(C)| = s$.

For $2 \leqslant i \leqslant l$, let $x_i \in V(C_i)$ be the vertex adjacent to v in T and $\beta_i = \max\{d(x_i, z) : z \in V(C_i)\}$. Construct a new tree $\tilde{T}$ from T by replacing C with a path-star tree $P_{g,s-g}$ at v, where $g = \max\{\beta_2, \beta_3, \ldots, \beta_l\}$. Then $\tilde{T} \in \Gamma_n^d$. Suppose $\tilde{M}$ is the bottleneck matrix of $P_{g,s-g}$ at v in $\tilde{T}$. Then by Lemma 1.2.12, $\tilde{M} \gg \hat{L}(C)^{-1}$ and the characteristic center of $\tilde{T}$ is either same as characteristic center of T or it moves away from its center towards the path-star part. So, $d_{\tilde{T}}(C, \chi) \geqslant d_T(C, \chi)$.

If $\tilde{T}$ is a path-star tree then the result follows. Otherwise at v, one of the components in $\tilde{T}$ is a path-star tree. In the other component at v, choose a longest path P_1 which contains the center of $\tilde{T}$. Delete the vertices which are not on P_1, and add the same number of vertices (as pendants) to the star part (of the other component) to get a new tree $\hat{T}$. Clearly $\hat{T}$ is the path-star tree $P_{d,n-d}$. Then $C(\tilde{T}) = C(\hat{T})$ and the characteristic center of $\hat{T}$ is either same as characteristic center of $\tilde{T}$ or it moves away from its center towards the path-star part. So, $d_{\hat{T}}(C, \chi) \geqslant d_{\tilde{T}}(C, \chi) \geqslant d_T(C, \chi)$. Hence the result follows.

Case II: Characteristic center of T does not lie in any of the longest path

Let P be a longest path of T containing both $C(T)$ and $\chi(T)$. Then the diameter of the path P is less than d. Let v be the vertex in the characteristic center which is farthest from $C(T)$ and let u be the pendant vertex of P farthest from v. Let $d_T(u, v) = \alpha$. Let $C_1, C_2, \ldots, C_l$ be the components of $T - v$ where C_1 is the component containing $C(T)$. For $2 \leqslant i \leqslant l$, let $x_i \in V(C_i)$ be the vertex adjacent to v in T and $\beta_i = \max\{d(x_i, z) : z \in V(C_i)\}$. Since $diam(P) < d$ and $d(u, v) = \alpha$, so $\max\{\beta_2, \beta_3, \ldots, \beta_l\} \leqslant d - \alpha - 2$. Let $C \equiv \bigcup_{j=2}^{l} C_j$ and $|V(C)| = s$. As $\alpha > \frac{d}{2}$ and v is in the characteristic center, so $s \geqslant d - \alpha$. Construct a new tree $\tilde{T}$ from T by replacing C with a path-star tree $P_{d-\alpha-1, s-(d-\alpha-1)}$ at v. Then $\tilde{T} \in \Gamma_n^d$. Suppose $\tilde{M}$ is the bottleneck matrix of $P_{d-\alpha-1, s-(d-\alpha-1)}$ at v in $\tilde{T}$. Then by Lemma 1.2.12 $\tilde{M} \gg \hat{L}(C)^{-1}$ and the characteristic center of $\tilde{T}$ is either same as the characteristic center of T or it moves away from its center towards the path-star part. So, $d_{\tilde{T}}(C,\chi) \geqslant d_T(C,\chi)$.

Now the center and characteristic center of $\tilde{T}$ lie in a longest path of it and the result follows from Case I. $\square$

For positive integers l, m, d with $n = l + m + d$, let $T(l,m,d)$ be the tree of order n obtained by taking the path $P_d : v_1 v_2 \cdots v_d$ and adding l pendant vertices adjacent to v_1 and m pendant vertices adjacent to v_d. Note that $T(l,m,d) \in \Gamma_n^{d+1}$.

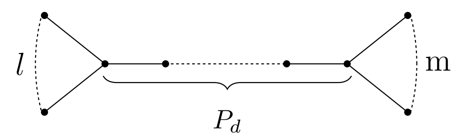


Figure 2.3: The tree $T(l,m,d)$

Theorem 2.2.15. *Let $d \leqslant \lceil \frac{n}{2} \rceil$. Then over Γ_n^d, the distance between the centroid and the characteristic center is maximized by the tree $T(n - \lfloor \frac{n}{2} \rfloor - d + 1, \lfloor \frac{n}{2} \rfloor, d - 1)$.*

Proof. Let $T \in \Gamma_n^d$. Without loss of generality we can take $d_T(C_d,\chi) \geqslant 1$. Let $u \in \chi(T)$ and $v \in C_d(T)$ such that $d_T(C_d,\chi) = d_T(u,v)$. Let $C_1, C_2, \ldots, C_l$ be the components of $T - v$ where C_1 is the component containing $\chi(T)$. If $|V(C_i)| = 1$ for $i = 2, 3, \ldots l$ then name the tree T as $\tilde{T}$. Otherwise, let $C = \bigcup_{j=2}^{l} C_j$ and $|V(C)| = s$. Construct $\tilde{T}$ from T by removing C and adding s pendant vertices at v. Observe that $C_d(\tilde{T}) = \{v\}$ and $diam(\tilde{T}) \leqslant d$. Let M be the bottleneck matrix of the component of $T - u$ containing v and let $\tilde{M}$ be the bottleneck matrix of the component of $\tilde{T} - u$ containing v. Then by Lemma 1.2.12 $M \gg \tilde{M}$ and by Proposition 1.2.15 the characteristic center of $\tilde{T}$ is either same as the characteristic center of T or it moves away from v. So, $d_{\tilde{T}}(C_d,\chi) \geqslant d_T(C_d,\chi)$.

Let $w \in \chi(\tilde{T})$ such that w is nearest to v. Let $D_1, D_2, \ldots, D_p$ be the components of $\tilde{T} - w$ where D_1 is the component containing the vertex v. For $i = 2, 3, \ldots, p$, let $x_i \in V(D_i)$ be the vertex adjacent to w in $\tilde{T}$and $\beta_i = \max\{d(x_i,z) : z \in V(D_i)\}$.

Let $D = \bigcup_{j=2}^{p} D_j$ and $|V(D)| = q$. Construct a new tree $\hat{T}$ from $\tilde{T}$ by replacing D at w with a path-star tree $P_{g,q-g}$ at w, where $g = \max\{\beta_2, \beta_3, \ldots, \beta_p\}$. Observe that $C_d(\hat{T}) = C_d(\tilde{T})$ and the characteristic center of $\hat{T}$ is either same as characteristic center of $\tilde{T}$ or it moves away from v. So, $d_{\hat{T}}(C_d, \chi) \geqslant d_{\tilde{T}}(C_d, \chi)$. Also $diam(\hat{T}) = diam(\tilde{T}) \leqslant d$.

Let w_1 be the center of the star part of $P_{g,q-g}$. In $\hat{T}$, let v' and w_1' be the non-pendant vertices adjacent to v and w_1, respectively. Consider the maximal subtree of $\hat{T}$ not containing v and w_1. Delete all the vertices of this subtree which are not in the $w_1' - v'$ path and add them as pendant vertices at w_1 to form a new tree $\hat{T}_1$ from $\hat{T}$. Clearly $d_{\hat{T}_1}(C_d, \chi) \geqslant d_{\hat{T}}(C_d, \chi)$ and $diam(\hat{T}_1) = diam(\hat{T}) \leqslant d$.

Since $C_d(\hat{T}_1) = \{v\}$, so at least $\lfloor \frac{n}{2} \rfloor$ pendant vertices are adjacent to v. If the number of pendant vertices adjacent to v is α then remove $\alpha - \lfloor \frac{n}{2} \rfloor$ pendant vertices from v and add them as pendant vertices at w_1 to form a new tree $\hat{T}_2$ from $\hat{T}_1$. Then $C_d(\hat{T}_2) = C_d(\hat{T}_1) = \{v\}$ and either $\chi(\hat{T}_2) = \chi(\hat{T}_1)$ or $\chi(\hat{T}_2)$ moves towards w_1. So $d_{\hat{T}_2}(C_d, \chi) \geqslant d_{\hat{T}_1}(C_d, \chi)$ and $diam(\hat{T}_2) = diam(\hat{T}_1) \leqslant d$.

If $diam(\hat{T}_2) = d$, then we are done. Otherwise let $u' \in \chi(\hat{T}_2)$ such that u' is closer to v and $d_{\hat{T}_2}(u', v) = \beta$. Let E_1 be the component of $\hat{T}_2$ at u' containing w_1. Then $diam(E_1) < d - \beta - 2 = \gamma_1$(say) and order of E_1 is $n - (\lfloor \frac{n}{2} \rfloor + \beta + 1) = \gamma_2$(say). Construct a new tree $\hat{T}_3$ from $\hat{T}_2$ by replacing E_1 at u' with a path-star tree $P_{\gamma_1, \gamma_2 - \gamma_1}$. The new tree $\hat{T}_3$ is the tree $T(n - \lfloor \frac{n}{2} \rfloor - d + 1, \lfloor \frac{n}{2} \rfloor, d - 1)$ and $d_{\hat{T}_3}(C_d, \chi) \geqslant d_{\hat{T}_2}(C_d, \chi)$. Hence the result follows. $\square$

2.3 Some open problems

The center, centroid and subtree core of a path-star tree is explicitly known. But it is still open to give an expression for the characteristic center of a path-star tree. In this regard we conjecture the following.

Conjecture 2.3.1. *For $2 \leqslant g \leqslant n-3$, $\chi(P_{n-g,g})$ consists of two adjacent vertices.*

Among all trees on n vertices, the trees which attain the maximum distance between two central parts are known. Also an strict upper bound on the distance for the pairs {center, centroid} [29], {center, subtree core} and {centroid, subtree core}[12] are established. Since the exact location of the characteristic center of a path-star tree is not known, we are not able to give an upper bound on the distances for the pairs consisting of the characteristic center. If the position of the characteristic center of path-star trees are known, then an upper bound on such distances can be given.

Over Γ_n^d, the following problems are open.

- Obtain a tree which maximizes the distance between centroid and characteristic center when $d > \lceil \frac{n}{2} \rceil$.
- Obtain a tree which maximizes the distance between subtree core and the characteristic center.
- Obtain a tree which maximizes the distance between centroid and subtree core.

We name the subgraphs induced by the center, median, security center, characteristic center and the subgraph core of a graph by the *center subgraph, median subgraph, security subgraph, characteristic subgraph* and the *core subgraph*, respectively. In [7], the authors have shown that for any graph G (may be disconnected) , there exists a super graph H containing G such that the center subgraph of H is isomorphic to G. In [35], it is shown that, for any graph G (may be disconnected), there exists a super graph H containing G such that the median subgraph of H is isomorphic to G. In this construction the size of H is much larger than the size of G. For G

with no isolated vertices, a simple construction of H on $2|V(G)|$ vertices, is given in [36] whose median subgraph is isomorphic to G. The same construction works for the security subgraph also. i.e. The security subgraph of the same super graph H is isomorphic to G (without isolated vertices). These results motivate us to raise the following questions.

1. Given a graph G, does there exist a super graph H containing G, such that the characteristic subgraph of H is isomorphic to G ?

2. Given a graph G, does there exist a super graph H containing G, such that the core subgraph of H is isomorphic to G ?

Further study on the characteristic center and the subgraph core may be needed to answer these questions.

Chapter 3

Distances between central parts in binary trees

In this chapter, we prove the conjecture posed by Smith et al. in [37] which says that among all binary trees on n vertices the distances between any two of center, centroid and the subtree core is maximized by some crg tree. Further, we obtain the crg trees which achieve these distances.

3.1 Binary and rooted binary trees

For $n \geqslant 3$, let h be the height of the rgood binary tree T_{rg}^n. Then $2^h+1 \leqslant n \leqslant 2^{h+1}-1$ and there exists a positive integer α such that $n = 2^h+\alpha$, which gives $h = \log_2(n-\alpha)$. There are two branches at the root of an rgood binary tree. The branch having maximum weight between the two, is termed as the *heavier branch*. If both the branches have same weight then we say the rgood binary tree is complete. In this case any branch can be considered as heavier.

Let T be a rooted binary tree. If the pendant vertices of T are in at least three different levels, then form a new rooted binary tree T' from T by moving a pair of pendant vertices with same parent from the highest level to the lowest level. Then $ht(T') \leqslant ht(T)$. This leads us to the next result which is straightforward and tells about the rooted binary trees with minimum height.

Lemma 3.1.1. *Among all rooted binary trees on n vertices, $ht(T^n_{rg}) \leqslant ht(T)$ and equality holds, when T is a rooted binary tree in which the heights of any two pendant vertices differ by at most one.*

The following result determines the binary tree on n vertices with maximum diameter.

Lemma 3.1.2. *Among all binary trees on n vertices, the binary caterpillar has the maximum diameter.*

Proof. Let T be a binary tree on n vertices with diameter d. Let $P : u_0u_1 \dots u_d$ be a path of diameter d in T. Suppose T is not caterpillar. Then there exist two pendant vertices $v_1, v_2 \in V(T) - V(P)$ adjacent to v such that v is not on the path P. Delete the vertices v_1, v_2 and add them as pendant vertices at u_0 to get a new tree T'. Then $diam(T') > diam(T)$. Repeat the process till a binary caterpillar is achieved. $\square$

The weight of a branch B at v is the number of edges in B and we denote it as $\omega_v(B)$.

Lemma 3.1.3. *Let $e = \{u, v\} \in E(T)$. Then $|V(T_e(u))| > |V(T_e(v))|$ if and only if $C_d(T) \subseteq V(T_e(u))$.*

Proof. Let $|V(T_e(u))| = k$ and $|V(T_e(v))| = k'$. First suppose $|V(T_e(u))| > |V(T_e(v))|$. Since $k > k'$, it follows that $\omega(v) = k$ and for any $w' \in V(T_e(v)), w' \neq v, \omega(w') > \omega(v)$. So the only possible vertex of $T_e(v)$ which may belong to $C_d(T)$ is v. Let B be the branch at u containing v. If $\omega(u) = \omega_u(B)$, then $\omega(u) = k' < k = \omega(v)$. If

$\omega(u) \neq \omega_u(B)$, then $\omega(u)$ is the weight of a branch of $T_e(u)$ at u and so $\omega(u) \leqslant k-1 < k = \omega(v)$. Hence, $\min\{\omega(z) : z \in V(T)\} \leqslant \omega(u) < \omega(v)$. This implies $C_d(T) \subseteq V(T_e(u))$.

Now suppose $C_d(T) \subseteq V(T_e(u))$. Let $w \in C_d(T)$, then $\omega(w) \geqslant k'$ as the branch at w containing v has weight at least k'. Since $v \notin C_d(T)$, so $\omega(v) > \omega(w) \geqslant k'$. This implies $\omega(v)$ is the weight of the branch at v containing u, i.e. $\omega(v) = k$ and hence $k > k'$. $\square$

Corollary 3.1.4. *Let v be the root of the rgood part of $T_{rg}^{n,l}$ and let v' be the vertex in a heavier branch of the rgood part at v such that $\{v, v'\} \in E(T_{rg}^{n,l})$. If $l \geqslant \frac{n}{2} + 1$ then $C_d(T_{rg}^{n,l}) \subseteq \{v, v'\}$. Moreover, if the rgood part is complete then $C_d(T_{rg}^{n,l}) = \{v\}$.*

Proof. Let T be a crg tree with $l \geqslant \frac{n}{2} + 1$ and let T' be the rgood part of T. Since $l \geqslant \frac{n}{2} + 1$, so by Lemma 3.1.3, $C_d(T) \subseteq V(T')$.

First suppose that T' is not complete. Let $e = \{w, v\} \in E(T')$ where w is not on the heavier branch of T'. Then a copy of $T'_e(w)$ is properly contained in $T'_e(v)$ and so $|V(T_e(v))| > |V(T_e(w))|$. Since $C_d(T) \subseteq V(T')$, so by Lemma 3.1.3, $C_d(T)$ is contained in the heavier branch of T'. Suppose $e_1 = \{u, v'\} \in E(T')$ where $ht(u) = 2$ in T'. Then a copy of $T'_{e_1}(u)$ is properly contained in $T'_{e_1}(v')$ and so $|V(T_{e_1}(v'))| > |V(T_{e_1}(u))|$. Hence by Lemma 3.1.3, $C_d(T) \subseteq \{v, v'\}$.

If T' is complete, then T' has two heavier branches at v. Since centroid of T contains either a single vertex or two adjacent vertices, so $C_d(T) = \{v\}$. $\square$

For $l \geqslant \frac{n}{2} + 1$, in Corollary 3.1.4, we proved that $C_d(T_{rg}^{n,l}) = \{v\}$ or $\{v'\}$ or $\{v, v'\}$. We also showed that $C_d(T_{rg}^{n,l}) = \{v\}$ if the rgood part is complete. For many values of n and l, the other two cases will also happen. For example, it can be checked that $C_d(T_{rg}^{12,11}) = \{v'\}$ and $C_d(T_{rg}^{14,13}) = \{v, v'\}$.

Corollary 3.1.5. *Let v be the root of the rgood part of $T_{rg}^{n,l}$ and let v' be the vertex in a heavier branch of the rgood part at v such that $\{v, v'\} \in E(T_{rg}^{n,l})$. If $n = 4k$ and $l \geqslant 2k+1$ then $C_d(T_{rg}^{n,l}) = \{v\}$ or $\{v'\}$.*

Proof. Let T be a crg tree with $n = 4k$ and $l \geqslant 2k+1$. By Corollary 3.1.4, $C_d(T) = \{v\}$ or $\{v'\}$ or $\{v, v'\}$. Let $e = \{v, v'\} \in E(T)$. If $C_d(T) = \{v, v'\}$ then $|V(T_e(v))| = |V(T_e(v'))| = 2k$. But both $T_e(v)$ and $T_e(v')$ are binary rooted trees with roots v and v', respectively and hence both must have odd number of vertices. Thus a contradiction arises, so $C_d(T) = \{v\}$ or $\{v'\}$. □

We will now prove a result similar to Lemma 3.1.3 related to subtree core of trees.

Lemma 3.1.6. *Let $e = \{u, v\} \in E(T)$. Then $S_c(T) \subseteq V(T_e(u))$ if and only if $f_{T_e(u)}(u) > f_{T_e(v)}(v)$.*

Proof. We have

$$f_T(u) = f_{T_e(u)}(u) + f_{T_e(u)}(u) f_{T_e(v)}(v)$$

and

$$f_T(v) = f_{T_e(v)}(v) + f_{T_e(u)}(u) f_{T_e(v)}(v).$$

So,

$$f_T(u) - f_T(v) = f_{T_e(u)}(u) - f_{T_e(v)}(v).$$

Now the result follows from Proposition 1.2.10. □

Next, we discuss about the position of the center, centroid and subtree core for rgood and crg trees.

Lemma 3.1.7. *Let v be the root of T_{rg}^n and let v' be the vertex in a heavier branch of T_{rg}^n such that $e = \{v, v'\} \in E(T_{rg}^n)$. Then center, centroid and subtree core of T_{rg}^n are* *contained in the set* $\{v, v'\}$. *Moreover, if* T^n_{rg} *is complete then* $C(T^n_{rg}) = C_d(T^n_{rg}) = S_c(T^n_{rg}) = \{v\}$.

Proof. Let P be a longest path of T^n_{rg}. Then it must go through v and $C(P) = \{v\}$ or $\{v, v'\}$ depending on the length of P is even or odd, respectively. So, $C(T^n_{rg}) = \{v\}$ or $\{v, v'\}$.

Let $w' \neq v'$ and $e' = \{v, w'\} \in E(T^n_{rg})$. Since v' is in a heavier branch, so $|V(T_{e'}(v))| > |V(T_{e'}(w'))|$. By Lemma 3.1.3, $C_d(T^n_{rg}) \subseteq V(T_{e'}(v))$. If $n > 3$ then $\deg(v') = 3$. Let $e_1 = \{v', v_1\}, e_2 = \{v', v_2\} \in E(T^n_{rg})$. For $i = 1, 2$, $T_{e_i}(v')$ contains a copy of $T_{e_i}(v_i)$. By Lemma 3.1.3, $C_d(T^n_{rg}) \subseteq V(T_{e_i}(v'))$. Hence $C_d(T^n_{rg}) \subseteq \{v, v'\}$.

Since v' is in a heavier branch, so the tree $T_{e'}(v)$ contains a copy of the rooted binary tree $T_{e'}(w')$ with root w'. So $f_{T_{e'}(v)}(v) > f_{T_{e'}(w')}(w')$ and hence by Lemma 3.1.6, $S_c(T^n_{rg}) \subseteq V(T_{e'}(v))$. Also for $i = 1, 2$, the rooted binary tree $T_{e_i}(v')$ with root v' contains a copy of the rooted binary tree $T_{e_i}(v_i)$ with root v_i. So by Lemma 3.1.6, $S_c(T^n_{rg}) \subseteq V(T_{e_i}(v'))$ for $i = 1, 2$. Hence $S_c(T^n_{rg}) \subseteq \{v, v'\}$.

If T^n_{rg} is complete, then T^n_{rg} has two heavier branches at v and in this case we have $C(T^n_{rg}) = C_d(T^n_{rg}) = S_c(T^n_{rg}) = \{v\}$. $\square$

We label the vertices of a longest path of the caterpillar part of $T^{n,l}_{rg}$ by $1, 2, \ldots, \frac{n-l+3}{2} = v$, where v is the root of the rgood part of it. We continue this labelling for a longest path in a heavier branch of the rgood part starting from v as $\frac{n-l+3}{2}, \frac{n-l+5}{2}, \ldots, \frac{n-l+3}{2}+h$ where h is the height of the rgood part of $T^{n,l}_{rg}$.

Corollary 3.1.8. *Let* v *be the root of the rgood part of* $T^{n,l}_{rg}$ *and let* v' *be the vertex in a heavier branch at* v *with* $\{v, v'\} \in E(T^{n,l}_{rg})$. *Then center, centroid and subtree core of* $T^{n,l}_{rg}$ *lie on the path from* 1 *to* v'.

Corollary 3.1.9. *Let* v *be the root of the rgood part of* $T^{n,l}_{rg}$ *and let* v' *be the vertex in a heavier branch at* v *with* $\{v, v'\} \in E(T^{n,l}_{rg})$. *Then* $C(T^{n,l}_{rg}) \neq \{v'\}$.

Proof. Let T' be the rgood part of $T_{rg}^{n,l}$ and also let $ht(T') = h$. Suppose $C(T_{rg}^{n,l}) = \{v'\}$. Then $diam(T_{rg}^{n,l}) = 2(h-1)$, which is a contradiction as $diam(T_{rg}^{n,l}) \geqslant 2h-1$. □

3.2 Root containing subtrees

To prove our main result, it is important to know the rooted binary trees which extremize the number of root containing subtrees. In [37], the authors have obtained the rooted binary tree which maximizes the number of root containing subtrees. Here we obtain the rooted binary tree which minimizes the number of root containing subtrees.

Proposition 3.2.1 ([37], Corollary 3.9)**.** *Among all rooted binary trees on n vertices, T_{rg}^{n} maximizes the number of root containing subtrees.*

For a tree T with $u, v \in V(T)$, we denote the number of subtrees of T containing u and v by $f_T(u, v)$.

Lemma 3.2.2. *Let T be a rooted binary tree with root r and x be a pendant vertex in T. Let y be a vertex other than x in the path joining r and x. Then, $f_T(r, y) \geqslant 2f_T(r, x)$ and equality holds if and only if y is adjacent to x.*

Proof. Let x_0 be the vertex adjacent to x in T and let T_0 be the tree $T - x$. Then,

$$f_T(r, x) = f_{T_0}(r, x_0)$$

and

$$f_T(r, y) = f_{T_0}(r, y) + f_T(r, x) = f_{T_0}(r, y) + f_{T_0}(r, x) \geqslant 2f_{T_0}(r, x_0) = 2f_T(r, x).$$

The inequality holds, as any tree containing r and x_0 must contain r and y and equality holds if and only if $y = x_0$. □

We denote the rooted binary tree on n vertices with exactly two vertices at every level (except zero level) by $T^n_{r,2}$.

Theorem 3.2.3. *Among all rooted binary trees on n vertices, the tree $T^n_{r,2}$ uniquely minimizes the number of root containing subtrees.*

Proof. Let T be a rooted binary tree with root r in which there are more than two vertices at some levels. Let x be a pendant vertex of T such that $ht(T) = d(r, x)$. Let y be the vertex nearest to r (y may be same as r) such that every branch at y contains more than two vertices. Then the path joining r and x must contains y. Let y_0, y_1 and y_2 be the vertices adjacent to y. Let the branch at y containing y_0 be the branch which contains r (If $y = r$, then we can take y_1 and y_2 are the only two vertices adjacent to y). Let X and Y be the branches at y containing y_1 and y_2, respectively and let x be in the branch Y. Then $X' = X - y$ is a binary rooted tree with root $y' = y_1$. Let T' be the binary rooted subtree of T with root r, obtained by removing X' from T but keeping y_1 as a pendant vertex of it. Then T can be obtained from T' and X' by identifying y_1 of T' with y' of X'. Then

$$f_T(r) = f_{T'}(r) + f_{T'}(r, y_1)(f_{X'}(y') - 1).$$

Construct a new tree $\hat{T}$ from T' and X' by identifying x of T' with y' of X'. Then $\hat{T}$ is a rooted binary tree with root r and $|V(T)| = |V(\hat{T})|$. Then

$$f_{\hat{T}}(r) = f_{T'}(r) + f_{T'}(r, x)(f_{X'}(y') - 1).$$

So we have

$$f_T(r) - f_{\hat{T}}(r) = (f_{X'}(y') - 1)(f_{T'}(r, y_1) - f_{T'}(r, x)).$$

We have $f_{X'}(y') > 1$ as $|V(X')| \geqslant 3$. Since y_1 is a pendant vertex so $f_{T'}(r, y_1) = f_{T'}(r, y)$. So by Lemma 3.2.2, $f_{T'}(r, y_1) = f_{T'}(r, y) > f_{T'}(r, x)$, hence $f_T(r) - f_{\hat{T}}(r) > 0$. If there are exactly two vertices at every level of $\hat{T}$ then we are done. Otherwise, repeat the above process till we get the rooted binary tree with exactly two vertices at every level (except level zero). □

Corollary 3.2.4. *Let T be a rooted binary tree on n vertices with root r. Then $f_T(r) \geqslant 3 \times 2^{\frac{n-1}{2}} - 2$ and equality holds if and only if $T \cong T^n_{r,2}$.*

Proof. Let r be the root of $T^n_{r,2}$. Suppose u and v are vertices adjacent to r among which u is pendant. Let S_n be the number of subtrees of $T^n_{r,2}$ containing r. We have $S_1 = 1$ and for $n \geqslant 3$,

$$S_n = 2S_{n-2} + 2$$

where number of subtrees containing r but not v is 2 and the number of subtrees containing both r and v is $2S_{n-2}$. We solve this recurrence relation to find the value of S_n. We have

$$\begin{aligned}
S_n &= 2S_{n-2} + 2 \\
&= 2(2S_{n-4} + 2) + 2 = 2^2 S_{n-4} + 2 + 2^2 \\
&\vdots \\
&= 2^{\frac{n-1}{2}} S_1 + 2 + 2^2 + 2^3 + \ldots + 2^{\frac{n-1}{2}} \\
&= 2^{\frac{n-1}{2}} + 2(2^{\frac{n-1}{2}} - 1) \\
&= 3 \times 2^{\frac{n-1}{2}} - 2.
\end{aligned}$$

The result follows from Theorem 3.2.3. □

Let r be the root of T_{rg}^n. It seems difficult to find the value of $f_{T_{rg}^n}(r)$. We will only be able to give a bound for $f_{T_{rg}^n}(r)$ which is solution of a non-linear recurrence relation. Let h be the height of T_{rg}^n and let $m = 2^{h+1} - 1$. For $n \geqslant 3$, $2^h - 1 < n \leqslant m$ and the rooted binary tree T_{rg}^m is complete.

Let A_h be the number of subtrees of T_{rg}^m containing the root r. We have $A_0 = 1$ and for $h \geqslant 1$, let u and v be the vertices adjacent to r. Then

$$A_h = 1 + A_{h-1} + A_{h-1}(1 + A_{h-1}) = (A_{h-1} + 1)^2$$

where the first 1 is for the subtree containing only the single vertex r, the second term A_{h-1} counts the number of subtrees containing r and v but not u and the third term $A_{h-1}(1 + A_{h-1})$ counts the subtrees containing r and u. Then for $h \geqslant 1$, we have

$$A_{h-1} < f_{T_{rg}^n}(r) \leqslant A_h.$$

It will be nice to know the exact value of $f_{T_{rg}^n}(r)$.

3.2.1 Solution to the recurrence $A_h = (A_{h-1} + 1)^2$ for $h \geqslant 1$, $A_0 = 1$

In [2], the authors have established the solution of the following recurrence relation. $x_{n+1} = x_n^2 + g_n$ for $n \geqslant n_0$ with boundary conditions

i) $x_n > 0$

ii) $|g_n| < \frac{1}{4}x_n$ *and* $x_n \geqslant 1$ *for* $n \geqslant n_0$

iii) $|\alpha_n| \geqslant |\alpha_{n+1}|$ *for* $n \geqslant n_0$

where $\alpha_n = \ln(1 + \frac{g_n}{x_n^2})$.

The authors have shown that if $x_n \in \mathbb{Z}$ and $g_n > 0$, then the solution of this recurrence relation is given by $x_n = \lfloor k^{2^n} \rfloor$, where $k = x_0 \exp\left(\sum_{i=o}^{\infty}(2^{-i-1}\alpha_i)\right)$.

We substitute $A_h + 1 = Y_h$ then the recurrence relation $A_h = (A_{h-1}+1)^2$ for $h \geqslant 1$, $A_0 = 1$ translates into $Y_0 = 2$ and $Y_{h+1} = Y_h^2 + 1$ for $h \geqslant 0$. Here $Y_h \in \mathbb{Z}$, $g_h = 1 > 0$ and the relation satisfies the above boundary conditions for $h_0 = 2$. So the solution of this is $Y_h = \lfloor k^{2^h} \rfloor$, where $k = Y_0 \exp(\sum_{i=o}^{\infty}(2^{-i-1}\alpha_i))$ and $\alpha_i = \ln(1 + \frac{1}{Y_i^2})$. So

$$\begin{aligned} k = Y_0 \exp\left(\sum_{i=o}^{\infty}(2^{-i-1}\alpha_i)\right) &= 2\exp\left(\frac{1}{2}\ln(1+\frac{1}{4}) + \frac{1}{4}\ln(1+\frac{1}{25}) + \frac{1}{8}\ln(1+\frac{1}{676}) + \cdots\right) \\ &= 2\exp\left(\frac{1}{2}\ln(\frac{5}{4}) + \frac{1}{4}\ln(\frac{26}{25}) + \frac{1}{8}\ln(\frac{677}{676}) + \cdots\right) = 2.25851845\cdots. \end{aligned}$$

Hence $A_h = \lfloor k^{2^h} \rfloor - 1$ where $k = 2.25851845\cdots$.

3.3 Center, Centroid and Subtree core

In this section, we prove the conjecture posed by Smith et al. (See Section 1.4) and obtain the crg trees which maximize the pairwise distances between the central parts: center, centroid and subtree core. Any crg tree on $n \leqslant 8$ vertices is isomorphic to a binary caterpillar. There are two non-isomorphic binary trees on 10 vertices and both are crg trees. It can be easily checked that (due to symmetry of vertices) both the crg trees on 10 vertices, the center, centroid and subtree core coincide. So throughout this, we consider crg trees on $n \geqslant 12$ vertices.

3.3.1 Center and centroid

Theorem 3.3.1. *Among all binary trees on* n *vertices, the distance between the center and centroid is maximized by a crg tree.*

Proof. Let T be a binary tree on n vertices with $d_T(C, C_d) \geqslant 1$. Let $u \in C(T)$ and $v \in C_d(T)$ such that $d_T(C, C_d) = d(u, v)$. Let $e = \{v, w\} \in E(T)$ such that w lies on the path joining u and v. Let $|V(T_e(v))| = k$. The component $T_e(v)$ is a rooted binary tree with root v. Since $C_d(T) \subseteq T_e(v)$ so by Lemma 3.1.3, $|V(T_e(v))| > |V(T_e(w))|$.

If $T_e(v)$ is a rgood binary tree then rename the tree T as T'. Otherwise, form a new tree T' from T by replacing the component $T_e(v)$ with T_{rg}^k rooted at v. Since $|V(T'_e(w))| < k = |V(T'_e(v))| = |V(T_{rg}^k)|$, so by Lemma 3.1.3, $C_d(T') \subseteq V(T'_e(v))$. By Lemma 3.1.1, $ht(T_e(v)) \geqslant ht(T_{rg}^k)$ and so the $diam(T') \leqslant diam(T)$. If $diam(T') = diam(T)$ then $C(T') = C(T)$. If $diam(T') < diam(T)$ then all the longest path of T' must contain v. So, while moving to T' from T, $C(T')$ is either same as $C(T)$ or moves away from the vertex v as compare to $C(T)$. Hence, $d_{T'}(C, C_d) \geqslant d_T(C, C_d)$.

If $T' \in \Omega_n$ then the result follows. Otherwise let $|V(T'_e(w))| = l$. Construct a new tree T'' from T' by replacing $T'_e(w)$ with $T_{r,2}^l$ rooted at w. Observe that $T'' \in \Omega_n$ and $diam(T'') > diam(T')$. Since the increment occurs in a branch at w not containing v, so while moving to T'' from T', $C(T'')$ moves away from v as compare to $C(T')$. Also, $|V(T''_e(v))| > |V(T''_e(w))|$ and $T''_e(v)$ is same as $T'_e(v)$. So $C_d(T'') = C_d(T')$. Hence $d_{T''}(C, C_d) \geqslant d_{T'}(C, C_d) \geqslant d_T(C, C_d)$. This proves the result. □

Theorem 3.3.2. *Among all crg trees on* $n \geqslant 12$ *vertices, the distance between center and centroid is maximized by the tree* $T_{rg}^{n,l}$, *where* $l = 2\lceil \frac{n}{4} \rceil + 1$.

Proof. Let v be the root of the rgood part of $T_{rg}^{n,l}$ and let $d_{T_{rg}^{n,l}}(C, C_d) = \alpha$. Since n is even, we consider two cases depending on whether n is of the form $4k$ or $4k + 2$.

Case I: $n = 4k$ for some $k \geqslant 3$.

In this case $l = 2\lceil \frac{n}{4} \rceil + 1 = 2k + 1$. In $T_{rg}^{n,l}$, the rgood part has $2k + 1$ vertices and the caterpillar part has $2k$ vertices. Then $\omega(v) = 2k - 1$ and the weight of any other vertex of $T_{rg}^{n,l}$ is greater than $2k - 1$. Following the labelling of vertices of a crg tree mentioned in Section 3.1, we have $C_d(T_{rg}^{n,l}) = \{v\} = \{k + 1\}$. The diameter of the caterpillar part is k and the height of the the rgood part is less than k. So, $C(T_{rg}^{n,l})$ lies in the path from 1 to $k + 1$.

First consider the trees $T_{rg}^{n,l}, T_{rg}^{n,l-2}, \ldots, T_{rg}^{n,5}$. Note that $T_{rg}^{n,5}$ is a binary caterpillar. Then $C_d(T_{rg}^{n,l-i}) = \{k+1\}$ for $0 \leqslant i \leqslant l-5$. In the above sequence of trees, the center lies in the path from 1 to $k + 1$. In $T_{rg}^{n,l-i}$, if the vertex numbered u is the central vertex nearest to $k + 1$, then the central vertex in $T_{rg}^{n,l-i-2}$ nearest to $k + 1$ is either u or $u + 1$. So, $d_{T_{rg}^{n,l-i}}(C, C_d) \geqslant d_{T_{rg}^{n,l-i-2}}(C, C_d)$ for $0 \leqslant i \leqslant l - 7$.

Now consider the sequence of trees $T_{rg}^{n,l}, T_{rg}^{n,l+2}, \ldots, T_{rg}^{n,n-1}$. For $0 \leqslant j \leqslant n - l - 1$, let v_j be the root of the rgood part of $T_{rg}^{n,l+j}$ and v'_j be the vertex in a heavier branch of the rgood part of $T_{rg}^{n,l+j}$ adjacent to v_j. If $d_{T_{rg}^{n,l}}(C, C_d) = \alpha = 0$ then $C(T_{rg}^{n,l}) = \{k+1\}$ or $\{k, k + 1\}$. The height of the rgood part of $T_{rg}^{n,l}$ is k or $k - 1$ depending on $C(T_{rg}^{n,l}) = \{k+1\}$ or $\{k, k+1\}$, respectively. Then the rgood part of $T_{rg}^{n,l}$ has at least $2^{k-1}+1$ vertices and hence $2^{k-1}+1 \leqslant l = 2k+1$. So $k \leqslant 4$. Thus $\alpha = 0$ implies $n \leqslant 16$ and in these cases it can be checked that $d_{T_{rg}^{n,l+j}}(C, C_d) = 0$ for $0 \leqslant j \leqslant n - l - 1$.

If $\alpha \geqslant 1$ then $n \geqslant 20$. If t is the smallest positive integer such that $C_d(T_{rg}^{n,l+t}) = \{v'_t\}$ then $C_d(T_{rg}^{n,l+t+p}) = \{v'_t\}$ for $0 \leqslant p \leqslant n - l - t - 1$. In the tree $T_{rg}^{n,l+2}$, let $e = \{v_2, v'_2\}$. Let B_1 and B_2 be the two components of $T_{rg}^{n,l+2} - e$ containing v_2 and v'_2, respectively. Since $n \geqslant 20$, so $|V(B_1)| > 2k$ and $|V(B_2)| < 2k$. Thus by Lemma 3.1.3, $C_d(T_{rg}^{n,l+2}) \subseteq B_1$ and hence $C_d(T_{rg}^{n,l+2}) = \{v_2\}$. Therefore, $d_{T_{rg}^{n,l+2}}(C, C_d) = \alpha$ or $\alpha - 1$. If $d_{T_{rg}^{n,l+2}}(C, C_d) = \alpha$ then $d_{T_{rg}^{n,l+4}}(C, C_d) = \alpha$ or $\alpha - 1$. If $d_{T_{rg}^{n,l+4}}(C, C_d) = \alpha$ then $C_d(T_{rg}^{n,l+4}) = \{v'_4\}$ and $C_d(T_{rg}^{n,l+j}) = v'_j$ for $4 \leqslant j \leqslant n - l - 1$. Hence the distance between center and centroid of all the trees in the above sequence is at most α. This prove the result for the case $n = 4k$.

Case II: $n = 4k + 2$ for some $k \geqslant 3$.

A similar argument can be given to prove this case. This completes the proof. $\square$

We will now find the distance between center and centroid of $T_{rg}^{n,l}$, for $l = 2\lceil \frac{n}{4} \rceil + 1$. Let h be the height of the rgood part of $T_{rg}^{n,l}$. Then h is the smallest positive integer such that $l \leqslant 2^{h+1} - 1$. This implies $\lceil \frac{n}{4} \rceil \leqslant 2^h - 1$.

The caterpillar part of $T_{rg}^{n,l}$ contains $2\lfloor \frac{n}{4} \rfloor$ vertices. So, the diameter of the caterpillar part is $\lfloor \frac{n}{4} \rfloor$ and hence the root of the rgood part is numbered as $\lfloor \frac{n}{4} \rfloor + 1$. Continuing the labelling of vertices from the root to the center, the central vertex which is nearest to the root of the rgood part is numbered as $\left\lfloor \frac{\lfloor \frac{n}{4} \rfloor + 1 + h}{2} \right\rfloor + 1$. Thus the distance between center and centroid of $T_{rg}^{n,l}$ is $\lfloor \frac{n}{4} \rfloor - \left\lfloor \frac{\lfloor \frac{n}{4} \rfloor + 1 + h}{2} \right\rfloor$, where h is the smallest positive integer such that $\lceil \frac{n}{4} \rceil \leqslant 2^h - 1$. This leads to the following corollary.

Corollary 3.3.3. *Let T be a binary tree on n vertices and let h be the smallest positive integer such that $\lceil \frac{n}{4} \rceil \leqslant 2^h - 1$. Then*

$$d_T(C, C_d) \leqslant \left\lfloor \frac{n}{4} \right\rfloor - \left\lfloor \frac{\lfloor \frac{n}{4} \rfloor + 1 + h}{2} \right\rfloor$$

and equality happens if $T \cong T_{rg}^{n,l}$ where $l = 2\lceil \frac{n}{4} \rceil + 1$.

3.3.2 Center and Subtree core

Theorem 3.3.4. *Among all binary trees on n vertices, the distance between center and subtree core is maximized by a crg tree.*

Proof. Let T be a binary tree on n vertices with $d_T(C, S_c) \geqslant 1$. Let $u \in C(T)$ and $v \in S_c(T)$ such that $d_T(C, S_c) = d(u, v)$. Let $e = \{v, w\} \in E(T)$ such that w lies on the path joining u and v. Let $|V(T_e(v))| = k$. The component $T_e(v)$ is a rooted binary tree with root v. Since $S_c(T) \subseteq V(T_e(v))$ so by Lemma 3.1.6, $f_{T_e(v)}(v) > f_{T_e(w)}(w)$.

If $T_e(v)$ is an rgood binary tree then rename the tree T by T'. Otherwise, form a new tree T' from T by replacing the component $T_e(v)$ with T_{rg}^k rooted at v. By Proposition 3.2.1, $f_{T_{rg}^k}(v) \geqslant f_{T_e(v)}(v) > f_{T_e(w)}(w)$ and hence by Lemma 3.1.6, $S_c(T') \subseteq V(T'_e(v))$. We have by Lemma 3.1.1, $ht(T_e(v)) \geqslant ht(T_{rg}^k)$. So, while moving to T' from T, $C(T')$ is either same as $C(T)$ or moves away from the vertex v as compare to $C(T)$. Hence, $d_{T'}(C, S_c) \geqslant d_T(C, S_c)$.

If $T' \in \Omega_n$ then the result follows. Otherwise, let $|V(T'_e(w))| = l$. Construct a new tree T'' from T' by replacing $T'_e(w)$ with $T_{r,2}^l$ rooted at w. Observe that $T'' \in \Omega_n$. In T'' the length of the longest path is more than the length of the longest path of T' and the increment occurs in a branch at w containing the center. So, while moving to T'' from T', $C(T'')$ moves away from v as compare to $C(T')$. By Proposition 3.2.3, $f_{T_{r,2}^l}(w) < f_{T'_e}(w)$. So $f_{T''_e(v)}(v) > f_{T''_e(w)}(w)$ and hence by Lemma 3.1.6, $S_c(T'') \subseteq V(T''_e(v))$. Thus $d_{T''}(C, S_c) \geqslant d_T(C, S_c)$. This proves the result. □

Theorem 3.3.5. *In any crg tree $T_{rg}^{n,l}$, the centroid lies in the path connecting the center and the subtree core.*

Proof. In a binary caterpillar tree on n vertices the center, centroid and subtree core are same. So we can consider crg trees which are not caterpillar. Let T be a crg non-caterpillar tree, and let T' be the rgood part of T. Let v be the root of T' and let v' be the vertex in a heavier branch of T' such that $\{v, v'\} \in E(T')$. By Corollary 3.1.8, the center, centroid and subtree core of T lie in the path from 1 to v'.

Let w be the centroid vertex of T nearest to v' (w may be same as v'). Let w' be the vertex adjacent to w and lies in the path from 1 to w. Let $e = \{w', w\} \in E(T)$. Then by Lemma 3.1.3, $|V(T_e(w))| \geqslant |V(T_e(w'))|$. If $w = v$ or v' then $T_e(w)$ is a rgood binary tree with root w. By Proposition 3.2.1, $f_{T_e(w)}(w) > f_{T_e(w')}(w')$ and hence by Lemma 3.1.6, $S_c(T) \subseteq V(T_e(w))$. If w is neither v nor v' then $T_e(w')$ is a rooted binary tree in which every level has exactly two vertices(except the zero level). By Proposition 3.2.3, $f_{T_e(w)}(w) > f_{T_e(w')}(w')$ and hence by Lemma 3.1.6, $S_c(T) \subseteq V(T_e(w))$. So, $S_c(T)$ lies in the path between $C_d(T)$ and v'.

Let u be the central vertex of T nearest to the vertex 1. Let u' be the vertex lies in the path from 1 to u (u' may be same as 1) such that $e_1 = \{u', u\} \in E(T)$. By Corollary 3.1.9, u lies in the path from 1 to v and the component $T_{e_1}(u')$ is a rooted binary tree with root u' in which every level has exactly two vertices (except the zero level). Hence $|V(T_{e_1}(u')| < |V(T_{e_1}(u)|$ and by Lemma 3.1.3, $C_d(T) \subseteq V(T_{e_1}(u)$. Thus $C_d(T)$ lies in the path from $C(T)$ to v'. This completes the proof. $\square$

Corollary 3.3.6. *In a crg tree $T_{rg}^{n,l}$, among center, centroid and subtree core, the center is nearest to the vertex* 1.

Proof. We rename the crg tree $T_{rg}^{n,l}$ as T. Let $u \in C(T)$ and $v \in S_c(T)$ such that $d(1, C(T)) = d(1, u)$ and $d(1, S_c) = d(1, v)$. We show that $d(1, v) \geqslant d(1, u)$. Suppose $d(1, v) < d(1, u)$. Let w be the vertex adjacent to u in the path joining 1 and u. Consider the edge $e = \{w, u\}$. Then $v \in V(T_e(w))$. Also, as $u \in C(T)$ is the central vertex nearest to 1, $k = |V(T_e(w))| < |V(T_e(u))|$. Note that the tree $T_e(w)$ is $T_{r,2}^k$. So by Lemma 3.2.3, $f_{T_e(w)}(w) < f_{T_e(u)}(u)$. Hence by Lemma 3.1.6, $v \in V(T_e(u))$, which is a contradiction. $\square$

Let l be an odd integer and let r be the root of T_{rg}^l. We denote the number $f_{T_{rg}^l}(r)$ by R_l.

Lemma 3.3.7. *Let $n \geqslant 12$ be even and let l be the smallest positive odd number such that $R_l > 3 \times 2^{\frac{n-l-1}{2}} - 2$. For an even integer i with $2 \leqslant i \leqslant l-3$, let $e =$*

$\{\frac{n-l+3}{2}, \frac{n-l+5}{2}\} \in E(T_i)$ *where* $T_i = T_{rg}^{n,l-i}$. *Then* $S_c(T_i) \subseteq V(T_{i_e}(\frac{n-l+3}{2}))$ *or* $S_c(T_i) = \{\frac{n-l+3}{2}, \frac{n-l+5}{2}\}$.

Proof. Since $n \geqslant 12$, so $l \geqslant 5$ and T_i is defined for every even integer i with $2 \leqslant i \leqslant l-3$. Also since l is the smallest positive odd integer such that $R_l > 3 \times 2^{\frac{n-l-1}{2}} - 2$, so $R_{l-i} \leqslant R_{l-2} \leqslant 3 \times 2^{\frac{n-l+1}{2}} - 2$.

The component $T_{i_e}(\frac{n-l+5}{2})$ of $T_i - e$ is a binary rooted tree on $l-2$ vertices with root $\frac{n-l+5}{2}$ ($T_{i_e}(\frac{n-l+5}{2})$ is a rgood tree if $i = 2$). By Proposition 3.2.1, $f_{T_{i_e}}(\frac{n-l+5}{2}) \leqslant R_{l-2}$ for $2 \leqslant i \leqslant l-5$. The component $T_{i_e}(\frac{n-l+3}{2})$ of $T_i - e$ is a binary rooted tree on $n-l+2$ vertices with root $\frac{n-l+3}{2}$. By Corollary 3.2.4, $f_{T_{i_e}}(\frac{n-l+3}{2}) = 3 \times 2^{\frac{n-l+1}{2}} - 2$.

Thus we have

$$f_{T_{i_e}}\left(\frac{n-l+3}{2}\right) = 3 \times 2^{\frac{n-l+1}{2}} - 2 \geqslant R_{l-2} \geqslant f_{T_{i_e}}\left(\frac{n-l+5}{2}\right)$$

for $2 \leqslant i \leqslant l-5$. If $S_c(T_i) \neq \{\frac{n-l+3}{2}, \frac{n-l+5}{2}\}$ then $f_{T_{i_e}}(\frac{n-l+3}{2}) > f_{T_{i_e}}(\frac{n-l+5}{2})$. Then by Lemma 3.1.6, $S_c(T_i) \subseteq V(T_{i_e}(\frac{n-l+3}{2}))$. This completes the proof. $\square$

Lemma 3.3.8. *Let* $n \geqslant 12$ *be even and let* l *be the smallest positive odd number such that* $R_l > 3 \times 2^{\frac{n-l-1}{2}} - 2$. *Then* $S_c(T_{rg}^{n,l+j}) = \{v_j\}$ *where* v_j *is the root of the rgood part of* $T_{rg}^{n,l+j}$ *for* $0 \leqslant j \leqslant 2$.

Proof. Since $T_{rg}^{n,5}$ is a binary caterpillar and $n \geqslant 12$, we have $l \geqslant 7$. For $0 \leqslant j \leqslant 2$, let v'_j be the vertex in a heavier branch of of the rgood part of $T_{rg}^{n,l+j}$ with $e_j = \{v_j, v'_j\} \in E(T_{rg}^{n,l+j})$. We have $S_c(T_{rg}^{n,l+j}) \subseteq \{v_j, v'_j\}$ as $R_l > 3 \times 2^{\frac{n-l-1}{2}} - 2$. The component $T_{e_j}(v'_j)$ of $T_{rg}^{n,l+j} - e_j$ is an rgood binary tree with root v'_j and has at most $l-2$ vertices. The component $T_{e_j}(v_j)$ of $T_{rg}^{n,l+j} - e_j$ is an rooted binary tree with root v_j and has at least $n-l+2$ vertices. Also, at level one of $T_{e_j}(v_j)$ there are more than two vertices. Thus we have,

$$f_{T_{e_j}(v'_j)}(v'_j) \leqslant R_{l-2} \leqslant 3 \times 2^{\frac{n-l+1}{2}} - 2 < f_{T_{e_j}(v_j)}(v_j)$$

for $0 \leqslant j \leqslant 2$. Hence by Lemma 3.1.6, $S_c(T_{rg}^{n,l+j}) = \{v_j\}$ for $0 \leqslant j \leqslant 2$. □

Theorem 3.3.9. *Let $n \geqslant 12$ be even and let l be the smallest positive odd number such that $R_l > 3 \times 2^{\frac{n-l-1}{2}} - 2$. Among all crg trees on n vertices, the distance between center and subtree core is maximized by the tree $T_{rg}^{n,l}$.*

Proof. Let v be the root of the rgood part of $T_{rg}^{n,l}$. Then by Lemma 3.3.8, $S_c(T_{rg}^{n,l}) = \{v\}$. Following the labelling of vertices mentioned in Section 3.1, v is labelled as $\frac{n-l+3}{2}$ in $T_{rg}^{n,l}$. Let the vertex numbered as u be the central vertex of $T_{rg}^{n,l}$ nearest to the vertex $\frac{n-l+3}{2}$. Then by Corollary 3.3.6, u lies on the path joining 1 and $\frac{n-l+3}{2}$ and

$$d_{T_{rg}^{n,l}}\left(u, \frac{n-l+3}{2}\right) = d_{T_{rg}^{n,l}}(C, S_c).$$

Let i be an even integer with $2 \leqslant i \leqslant l-3$. Consider the crg tree $T_{rg}^{n,l-i}$. Since the center of a tree is same as the center of every longest path in it, so the central vertex of $T_{rg}^{n,l-i}$ nearest to $\frac{n-l+3}{2}$ is $u+k$ for some $k \geqslant 0$. Also by Lemma 3.3.7, $S_c(T_{rg}^{n,l-i}) = \{\frac{n-l+3}{2}, \frac{n-l+5}{2}\}$ or lies on the path from 1 to $\frac{n-l+3}{2}$. Hence, we have

$$d_{T_{rg}^{n,l-i}}(C, S_c) \leqslant d_{T_{rg}^{n,l-i}}(u, S_c) \leqslant d_{T_{rg}^{n,l-i}}\left(u, \frac{n-l+3}{2}\right) = d_{T_{rg}^{n,l}}(C, S_c)$$

for $2 \leqslant i \leqslant l-3$.

Consider the sequence of trees $T_{rg}^{n,l+j}$ for $0 \leqslant j \leqslant n-l-1$ with j even. Then by Lemma 3.1.6 and Corollary 3.1.8, $S_c(T_{rg}^{n,l+j}) \subseteq \{w, w'\}$ for $0 \leqslant j \leqslant n-l-1$ where w is the root of the rgood part of $T_{rg}^{n,l+j}$ and w' is the vertex in a heavier branch with

$e = \{w, w'\} \in E(T_{rg}^{n,l+j})$. In $T_{rg}^{n,l+j}$, w is numbered as $\frac{n-l-j+3}{2}$. Let $d_{T_{rg}^{n,l}}(C, S_c) = \alpha$. We have two cases :

Case I: $\alpha \geqslant 1$

By Lemma 3.3.8, $d_{T_{rg}^{n,l+2}}(C, S_c) = \alpha$ or $\alpha - 1$. Let j' be the smallest positive even integer such that $d_{T_{rg}^{n,l+j'}}(C, S_c) = 0$. Then $d_{T_{rg}^{n,l+k}}(C, S_c) = 0$ or 1, for $j' \leqslant k \leqslant n-l-1$ and $d_{T_{rg}^{n,l+k}}(C, S_c) \leqslant \alpha$ for $0 \leqslant k \leqslant j' - 2$. Hence $d_{T_{rg}^{n,l+j}}(C, S_c) \leqslant d_{T_{rg}^{n,l}}(C, S_c)$ for $2 \leqslant j \leqslant n - l - 1$.

Case II: $\alpha = 0$

Since n is even, so $n = 4k$ or $4k+2$ for some k. So $l \leqslant 2k+1$ as l is the smallest positive odd number such that $R_l > 3 \times 2^{\frac{n-l-1}{2}} - 2$. It can be checked that $C(T_{rg}^{14,7}) = \{4\}$ and $S_c(T_{rg}^{14,7}) = \{5\}$. So $d_{T_{rg}^{14,7}}(C, S_c) = 1$ and hence for $n = 4k+2$, $k \geqslant 3$, $d_{T_{rg}^{n,l}}(C, S_c) \geqslant 1$. It can also be checked that $C(T_{rg}^{20,11}) = \{5\}$ and $S_c(T_{rg}^{20,11}) = \{6\}$. So $d_{T_{rg}^{20,11}}(C, S_c) = 1$ and hence for $n = 4k$, $k \geqslant 5$, $d_{T_{rg}^{n,l}}(C, S_c) \geqslant 1$.

If $n = 12$ then $l = 7$ and it can be easily checked that $d_{T_{rg}^{12,7}}(C, S_c) = d_{T_{rg}^{12,9}}(C, S_c) = d_{T_{rg}^{12,11}}(C, S_c) = 0$. If $n = 16$ then $l = 9$ and it also can be checked that $d_{T_{rg}^{16,9}}(C, S_c) = d_{T_{rg}^{16,11}}(C, S_c) = d_{T_{rg}^{16,13}}(C, S_c) = d_{T_{rg}^{16,15}}(C, S_c) = 0$. Hence if $d_{T_{rg}^{n,l}}(C, S_c) = 0$ then $d_{T_{rg}^{n,l+j}}(C, S_c) = 0$ for $2 \leqslant j \leqslant n - l - 1$. This completes the proof. □

Corollary 3.3.10. *Let T be a binary tree on $n \geqslant 12$ vertices. Let r be the root of the rooted binary tree T_{rg}^l and let l be the smallest positive integer such that $f_{T_{rg}^l}(r) > 3 \times 2^{\frac{n-l-1}{2}} - 2$. Then*

$$d_T(C, S_c) \leqslant d_{T_{rg}^{n,l}}(C, S_c).$$

3.3.3 Centroid and Subtree core

Theorem 3.3.11. *Among all binary trees on n vertices, the distance between centroid and subtree core is maximized by a crg tree.*

Proof. Consider a binary tree T on n vertices with $d_T(C_d, S_c) \geqslant 1$. Our aim is to construct a crg tree $\tilde{T} \in \Omega_n$ such that $d_{\tilde{T}}(C_d, S_c) \geqslant d_T(C_d, S_c)$. Let $u \in C_d(T)$ and $v \in S_c(T)$ such that $d_T(C_d, S_c) = d(u, v)$. Let u' and v' be the vertices adjacent to u and v respectively, and lie on the path joining u and v. Let $e_1 = \{u, u'\}, e_2 = \{v', v\} \in E(T)$.

Let $|V(T_{e_2}(v))| = k$. The component $T_{e_2}(v)$ is a rooted binary tree with root v. Since $S_c(T) \subseteq V(T_{e_2}(v))$ so by Lemma 3.1.6, $f_{T_{e_2}(v)}(v) > f_{T_{e_2}(v')}(v')$. If $T_{e_2}(v)$ is an rgood binary tree then rename the tree T by T'. Otherwise, form a new tree T' from T by replacing the component $T_{e_2}(v)$ with T^k_{rg} rooted at v. By Proposition 3.2.1, $f_{T^k_{rg}}(v) \geqslant f_{T_{e_2}(v)}(v) > f_{T_{e_2}(v')}(v')$ and hence by Lemma 3.1.6, $S_c(T') \subseteq V(T'_{e_2}(v))$. Since $C_d(T) \subseteq V(T_{e_1}(u))$ so by Lemma 3.1.3, $|V(T_{e_1}(u))| > |V(T_{e_1}(u'))|$. As $d_T(C_d, S_c) \geqslant 1$ and $V(T) = V(T')$ so $C_d(T) = C_d(T')$. Hence, $d_{T'}(C_d, S_c) \geqslant d_T(C_d, S_c)$.

If $T' \in \Omega_n$ then the result follows. Otherwise, let $|V(T'_{e_2}(v'))| = l$. Construct a new tree T'' from T' by replacing $T'_{e_2}(v')$ with $T^l_{r,2}$ rooted at v'. Observe that $T'' \in \Omega_n$. By Proposition 3.2.3, $f_{T^l_{r,2}}(v') < f_{T'_{e_2}}(v')$. So $f_{T''_{e_2}(v)}(v) > f_{T''_{e_2}(v')}(v')$ and hence by Lemma 3.1.6, $S_c(T'') \subseteq V(T''_{e_2}(v))$. Also we can construct T'' from T' step wise such that in each step the centroid is same as the centroid of T' or moves away from v. For that choose a longest path P starting from v' containing the centroid of T in the binary rooted tree $T'_{e_2}(v')$ with root v'. Let x be the end point of the path P. Delete two pendant vertices from same parents, where the parent is not on the path P and add them as pendant vertices at x. Continue this process till $T'_{e_2}(v')$ becomes the tree $T^l_{r,2}$ and we reach the tree T''. In each step of the process, the centroid is either same as the centroid of the tree in the previous step or moves away from v. Hence, $d_{T''}(C_d, S_c) \geqslant d_T(C_d, S_c)$. This completes the proof. $\square$

Theorem 3.3.12. *Let T be a binary tree on $n \geqslant 12$ vertices. Let r be the root of the rooted binary tree T^l_{rg} and let l be the smallest positive integer such that $f_{T^l_{rg}}(r) > 3 \times 2^{\frac{n-l-1}{2}} - 2$. Then*

$$d_T(C_d, S_c) \leqslant \begin{cases} d_{T^{n,l}_{rg}}(C_d, S_c) & \text{if } d_{T^{n,l}_{rg}}(C_d, S_c) \geqslant 1, \\ 1 & \text{otherwise.} \end{cases}$$

Proof. Since n is even, so $n = 4k$ or $4k+2$ for some k. So $l \leqslant 2k+1$ as l is the smallest positive odd number such that $R_l > 3 \times 2^{\frac{n-l-1}{2}} - 2$. Then $C_d(T^{n,l}_{rg})$ lies in the path from 1 to $\frac{n-l+3}{2}$. Let the vertex numbered u be the centroid vertex of $T^{n,l}_{rg}$ nearest to the vertex $\frac{n-l+3}{2}$. Then by Lemma 3.3.8,

$$d_{T^{n,l}_{rg}}\left(u, \frac{n-l+3}{2}\right) = d_{T^{n,l}_{rg}}(C_d, S_c).$$

Let i be an even integer with $2 \leqslant i \leqslant l-3$. Consider the crg tree $T^{n,l-i}_{rg}$. Then the centroid vertex of $T^{n,l-i}_{rg}$ nearest to $\frac{n-l+3}{2}$ is u for $2 \leqslant i \leqslant l-3$. Also by Lemma 3.3.7, $S_c(T^{n,l-i}_{rg}) = \{\frac{n-l+3}{2}, \frac{n-l+5}{2}\}$ or lies on the path from 1 to $\frac{n-l+3}{2}$. So we have

$$d_{T^{n,l-i}_{rg}}(C_d, S_c) = d_{T^{n,l-i}_{rg}}(u, S_c) \leqslant d_{T^{n,l-i}_{rg}}\left(u, \frac{n-l+3}{2}\right) = d_{T^{n,l}_{rg}}(C_d, S_c)$$

for $2 \leqslant i \leqslant l-3$.

Consider the sequence of trees $T^{n,l+j}_{rg}$ for $0 \leqslant j \leqslant n-l-1$ with j even. Then by Lemma 3.1.6 and Corollary 3.1.8, $S_c(T^{n,l+j}_{rg}) \subseteq \{w, w'\}$ for $0 \leqslant j \leqslant n-l-1$ where w is the root of the rgood part of $T^{n,l+j}_{rg}$ and w' is the vertex in a heavier branch with $e = \{w, w'\} \in E(T^{n,l+j}_{rg})$. In $T^{n,l+j}_{rg}$, w is numbered as $\frac{n-l-j+3}{2}$. Let $d_{T^{n,l}_{rg}}(C_d, S_c) = \alpha$. We have two cases :

Case I: $\alpha \geqslant 1$

Let j' be the smallest positive even integer such that $d_{T_{rg}^{n,l+j'}}(C_d, S_c) = 0$. Then $d_{T_{rg}^{n,l+k}}(C_d, S_c) = 0$ or 1, for $j' \leqslant k \leqslant n-l-1$ and $d_{T_{rg}^{n,l+k}}(C_d, S_c) \leqslant \alpha$ for $0 \leqslant k \leqslant j'-2$. Hence

$$d_{T_{rg}^{n,l+j}}(C_d, S_c) \leqslant d_{T_{rg}^{n,l}}(C_d, S_c)$$

for $2 \leqslant j \leqslant n-l-1$.

Case II: $\alpha = 0$

In this case, $d_{T_{rg}^{n,l+j}}(C_d, S_c) = 0$ or 1, for $2 \leqslant j \leqslant n-l-1$.

Hence the result follows from Theorem 3.3.11. $\square$

3.4 Future works

Among all binary trees on n vertices, we have obtained a tree which maximizes the distances between two central parts for the pairs {center, centroid}, {center, subtree core} and {centroid, subtree core}. The trees which maximize the pairwise distances between the characteristic center and any one of the center, centroid and subtree core, over binary trees on n vertices are still not known. We feel that the following is true.

Among all binary trees on n vertices, the pairwise distances between the characteristic center and each one of the center, centroid and subtree core are maximized by some crg tree.

It will be nice to study these maximum distances and justify the truth or fallacy of the above statement.

Chapter 4

The subgraph index of a graph

In this chapter, we characterise the graphs which maximize or minimize the subgraph index among all unicyclic graphs on n vertices and among all graphs on n vertices with fixed number of pendant vertices.

4.1 Some preliminary results

The following lemma is straightforward which shows the effect of a new edge on the subgraph index of a graph.

Lemma 4.1.1. *Let u and v be two non adjacent vertices of a graph G. Let G' be the graph obtained from G by joining u and v with an edge. Then $F(G) < F(G')$.*

It follows from Lemma 4.1.1 that among all connected graphs on n vertices, the subgraph index is maximized by the complete graph K_n and minimized by a tree. Among all trees on n vertices, the subgraph index is maximized by the star $K_{1,n-1}$ and minimized by the path P_n (see [38],Theorem 3.1) with

$$F(K_{1,n-1}) = 2^{n-1} + n - 1 \text{ and } F(P_n) = \binom{n+1}{2}. \tag{4.1.1}$$

Let h_k be the number of connected labelled graphs on k vertices. Then h_k can be obtained by the recurrence relation $k2^{\binom{k}{2}} = \sum_i \binom{k}{i} i h_i 2^{\binom{k-i}{2}}$ (see [46],Theorem 3.10.1). So, $h_1 = 1, h_2 = 1, h_3 = 4, \cdots$ and the sequence $h_k,\ k \geqslant 2$ is strictly increasing. We have

$$F(K_n) = \sum_{i=1}^{n} \binom{n}{i} h_i. \tag{4.1.2}$$

Although there is no routine methods to count the number of connected subgraphs of a graph, the following two lemmas are helpful in counting $F(G)$.

Lemma 4.1.2. *Let u be a cut vertex of G. Let G_1 and G_2 be two subgraphs of G with $G = G_1 \cup G_2$ and $V(G_1) \cap V(G_2) = \{u\}$. Then*

$$F(G) = F(G_1) + F(G_2) - 1 + (f_{G_1}(u) - 1)(f_{G_2}(u) - 1).$$

Lemma 4.1.3. *Let $e = \{u, v\}$ be a bridge in G. Let G_1 and G_2 be the two connected components of $G - e$ containing u and v, respectively. Then*

$$F(G) = F(G_1) + F(G_2) + f_{G_1}(u) f_{G_2}(v).$$

Corollary 4.1.4. *Let G and H be two vertex disjoint graphs having at least 2 vertices each. Let $u, v \in V(G)$ and $w \in V(H)$. Let G_1 and G_2 be the graphs obtained from G and H by identifying the vertex w of H with the vertices u and v of G, respectively. If $f_G(v) \geqslant f_G(u)$ then $F(G_2) \geqslant F(G_1)$ and equality happens if and only if $f_G(v) = f_G(u)$.*

Proof. By Lemma 4.1.2,

$$F(G_1) = F(G) + F(H) - 1 + (f_G(u) - 1)(f_H(w) - 1)$$

and

$$F(G_2) = F(G) + F(H) - 1 + (f_G(v) - 1)(f_H(w) - 1).$$

So

$$F(G_2) - F(G_1) = (f_H(w) - 1)(f_G(v) - f_G(u))$$

and the result follows since $f_H(w) \geqslant 2$. $\square$

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

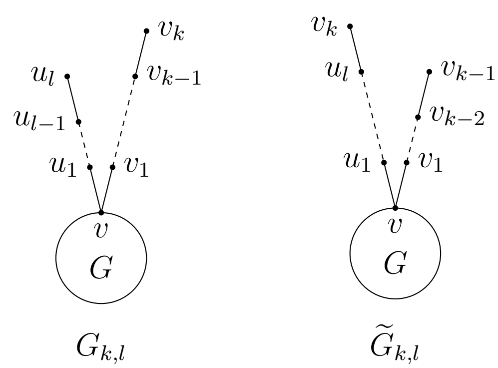


Figure 4.1: Grafting an edge operation

In the path $P_n : v_1v_2 \ldots v_n$,

$$f_{P_n}(v_i) = f_{P_n}(v_{n-i+1}) = i(n + 1 - i), \quad \text{for } i = 1, 2, \ldots, n.$$

So, if n is odd, then

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

and if n is even, then

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

The next result follows from the above observation and Corollary 4.1.4.

Corollary 4.1.5. *If $1 \leqslant k \leqslant l$, then $F(G_{k-1,l+1}) < F(G_{k,l})$.*

Let $v_1, v_2, \ldots, v_k \in V(G)$. By $f_G(v_1, v_2, \ldots, v_k)$, we denote the number of connected subgraphs of G containing $v_1, v_2, \ldots, v_k$. The following result compares the subgraph index of two graphs, where one is obtained from the other by moving a component from one vertex to another vertex.

Lemma 4.1.6. *Let H, X and Y be three pairwise vertex disjoint graphs having at least 2 vertices each, such that $u, v \in V(H)$, $x \in V(X)$ and $y \in V(Y)$. Let G be the graph obtained from H, X, Y by identifying u with x and v with y. Let G^* be the graph obtained from H, X, Y by identifying the vertices u, x, y. If $f_H(u) \geqslant f_H(v)$ then $F(G^*) > F(G)$.*

Proof. Construct the graph G_1 from H and X by identifying u and x and denote the new vertex as w. Then G and G^* are the graphs obtained from G_1 and Y by identifying v with y and w with y, respectively. So, we have

$$f_{G_1}(w) = f_X(x) + f_X(x)(f_H(u) - 1)$$

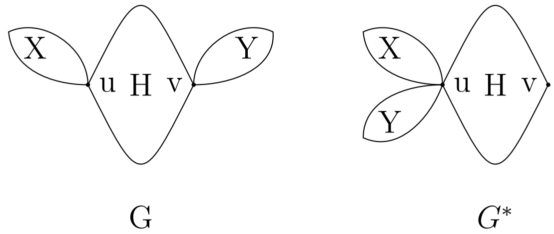


Figure 4.2: Movement of a component from one vertex to other

and

$$f_{G_1}(v) = f_H(v) + f_H(u,v)(f_X(x) - 1).$$

Thus,

$$f_{G_1}(w) - f_{G_1}(v) = (f_X(x) - 1)(f_H(u) - 1 - f_H(u,v)) + (f_X(x) + f_H(u) - 1 - f_H(v)).$$

Since $f_H(u) \geqslant f_H(v)$ and X has at least two vertices, $f_X(x) + f_H(u) - 1 - f_H(v) > 0$. Also as H has at least two vertices, so $f_H(u) - 1 - f_H(u,v) \geqslant 0$. Hence, $f_{G_1}(w) - f_{G_1}(v) > 0$. Since Y has at least 2 vertices, so the result follows from the Corollary 4.1.4. □

The next two corollaries follow from Lemma 4.1.6.

Corollary 4.1.7. *Let $e = \{u, v\}$ be a bridge in G such that neither u nor v be a pendant vertex. Let G' be the graph obtained from G by identifying the vertices u and v (removing the loop) and adding a pendant vertex y at the identified vertex of G'. Then $F(G') > F(G)$.*

Corollary 4.1.8. *Let G be a graph on $n \geqslant 2$ vertices and let $u, v \in V(G)$. For $n_1, n_2 \geqslant 0$, let $G_{uv}(n_1, n_2)$ be the graph obtained from G by attaching n_1 pendant* *vertices at u and n_2 pendant vertices at v. Let $f_G(u) \geqslant f_G(v)$. If $n_1, n_2 \geqslant 1$, then*

$$F(G_{uv}(n_1+n_2,0)) > F(G_{uv}(n_1,n_2)).$$

Lemma 4.1.9. *Let G be a graph on $n \geqslant 3$ vertices. Let $u,v \in V(G)$ such that $f_G(u,v) \geqslant 2$. For $l,k \geqslant 1$, let $G^p_{uv}(l,k)$ be the graph obtained from G by identifying a pendant vertex of the path P_l with u and identifying a pendant vertex of the path P_k with v. Let $f_G(u) \leqslant f_G(v)$. If $l,k \geqslant 2$, then*

$$F(G^p_{uv}(l+k-1,1)) < F(G^p_{uv}(l,k)).$$

Proof. We have

$$\begin{aligned} F(G^p_{uv}(l,k)) &= F(G)+F(P_l)+F(P_k)-2+(f_G(u)-1)(f_{P_l}(u)-1) \\ &\quad + (f_G(v)-1)(f_{P_k}(v)-1)+f_G(u,v)(f_{P_l}(u)-1)(f_{P_k}(v)-1) \\ F(G^p_{uv}(l+k-1,1)) &= F(G)+F(P_{l+k-1})-1+(f_G(u)-1)(f_{P_{l+k-1}}(u)-1) \end{aligned}$$

and the difference

$$\begin{aligned} F(G^p_{uv}(l,k)) - F(G^p_{uv}(l+k-1,1)) &\geqslant F(P_l)+F(P_k)-F(P_{l+k-1})-1 \\ &\quad + (f_G(u)-1)(f_{P_l}(u)-1+f_{P_k}(v)-1-f_{P_{l+k-1}}(u)+1) \\ &\quad + f_G(u,v)(f_{P_l}(u)f_{P_k}(v)-f_{P_l}(u)-f_{P_k}(v)+1) \\ &= l+k-lk-1+f_G(u,v)(lk-l-k+1) \\ &= (f_G(u,v)-1)(lk-l-k+1) \\ &> 0, \text{ as } l,k \geqslant 2 \text{ and } f_G(u,v) \geqslant 2. \end{aligned}$$

This completes the proof. ☐

4.2 Unicyclic graphs

Let v be a vertex of C_n. We need to know the values of $F(C_n)$ and $f_{C_n}(v)$ to count the number of connected subgraphs of unicyclic graphs. In the proof of Theorem 2.1.7, we have seen that $f_{C_n}(v) = 2n + \binom{n-1}{2}$ for any $v \in V(C_n)$. We give the value of $F(C_n)$ in the following lemma.

Lemma 4.2.1. *For $n \geqslant 3$, $F(C_n) = n^2 + 1$.*

Proof. Let $C_n : v_1v_2 \cdots v_nv_1$. The single vertices $v_1, v_2, \ldots, v_n$ are n connected subgraphs of C_n. The cycle C_n itself is one connected subgraph of C_n. Any other connected subgraph of C_n is a path having the end vertices from $\{v_1, v_2, \ldots, v_n\}$. If we chose any two vertices v_i, v_j from $\{v_1, v_2, \ldots, v_n\}$, it corresponds two paths, one in clockwise direction from v_i to v_j and other in anticlockwise direction from v_i to v_j. So the number of such paths are $2\binom{n}{2}$. Thus we have

$$F(C_n) = n + 1 + 2\binom{n}{2} = n^2 + 1.$$

☐

For $n \geqslant 3, \mathcal{U}_n$ denotes the set of all unicyclic graphs on n vertices and $\mathcal{U}_{n,g}$ denotes the set of all unicyclic graphs on n vertices with girth g.

For $3 \leqslant g \leqslant n$, $U_{n,g}(T_1, T_2, \ldots, T_g)$ denotes the unicyclic graph on n vertices containing the cycle $C_g =: 12 \cdots g1$ and trees $T_1, T_2, \ldots, T_g$, where T_i is a tree on $n_i + 1$ vertices containing the only vertex i of C_g with $n_i \geqslant 0$ for $i = 1, 2, \ldots, g$ and $g + \sum n_i = n$. Then clearly, $U_{n,g}(T_1, T_2, \ldots, T_g) \in \mathcal{U}_{n,g}$. For $g < n$, if T_i is a star on $n-g+1$ vertices with i as the center of T_i, for some $i = 1, 2, \ldots, g$, then $U_{n,g}(T_1, T_2, \ldots, T_g) \cong U^p_{n,g}$ and if T_i is a path on $n-g+1$ vertices with i as one of its pendant vertex for some $i = 1, 2, \ldots, g$, then $U_{n,g}(T_1, T_2, \ldots, T_g) \cong U^l_{n,g}$.

Lemma 4.2.2. *Let G be a unicyclic graph on n vertices. Then*

$$F(U_{n,g}(P_{n_1+1}, \cdots, P_{n_g+1})) \leqslant F(G) \leqslant F(U_{n,g}(K_{1,n_1}, \ldots, K_{1,n_g}))$$

where K_{1,n_i} is the star with center at i and P_{n_i+1} is the path with i as one of its pendant vertex. The left equality holds if and only if $G \cong U_{n,g}(P_{n_1+1}, \cdots, P_{n_g+1})$ and the right equality holds if and only if $G \cong U_{n,g}(K_{1,n_1}, \ldots, K_{1,n_g})$.

Proof. Since G is unicyclic, $G \cong U_{n,g}(T_1, T_2, \ldots, T_g)$ for some trees $T_1, T_2, \ldots, T_g$. Suppose, for some $i \in \{1, 2, \ldots, g\}$, T_i is not a star with i as the central vertex. Then the vertex i must be adjacent to a vertex, say v of T_i of degree at least 2. Identify the vertices i and v and add a pendant vertex at i. Continue this operation till T_i becomes K_{1,n_i} with center at i. By Corollary 4.1.7, in each step of this the subgraph index will increase. Continuing this, we get the unicyclic graph $U_{n,g}(K_{1,n_1}, \ldots, K_{1,n_g})$. So, $F(U_{n,g}(T_1, \ldots, T_g)) \leqslant F(U_{n,g}(K_{1,n_1}, \ldots, K_{1,n_g}))$ and the equality happens if and only if $U_{n,g}(T_1, \ldots, T_g) \cong U_{n,g}(K_{1,n_1}, \ldots, K_{1,n_g})$.

To prove the other inequality, suppose T_i is not a path with i as one of its pendant vertex. Then by using the grafting of edges operations, we can make T_i a path with i as one of its pendant vertex. By Corollary 4.1.5, in each step of this, the subgraph index will decrease. Continuing this, we get the unicyclic graph $U_{n,g}(P_{n_1+1}, \ldots, P_{n_g+1})$. This gives us, $F(U_{n,g}(P_{n_1+1}, \ldots, P_{n_g+1})) \leqslant F(U_{n,g}(T_1, \ldots, T_g))$ and the equality holds if and only if $U_{n,g}(T_1, \ldots, T_g) \cong U_{n,g}(P_{n_1+1}, \ldots, P_{n_g+1})$. This completes the proof. $\square$

Now we prove the result which characterises the graph extremizing the subgraph index in $\mathcal{U}_{n,g}$. Note that C_n is the only graph in $\mathcal{U}_{n,n}$.

Theorem 4.2.3. *For $3 \leqslant g < n$, let $G \in \mathcal{U}_{n,g}$. Then*

$$\left(\frac{n-g}{2}\right)(n+g^2+3)+g^2+1 \leqslant F(G) \leqslant n+g^2-g+1+(2^{n-g}-1)\left(2g+\binom{g-1}{2}\right).$$

The left equality holds if and only if $G \cong U^l_{n,g}$ and the right equality holds if and only if $G \cong U^p_{n,g}$.

Proof. By Lemma 4.2.2, $F(G) \leqslant F(U_{n,g}(K_{1,n_1},\ldots,K_{1,n_g}))$ and equality happens if and only if $G \cong U_{n,g}(K_{1,n_1},\ldots,K_{1,n_g})$. If exactly one vertex on the cycle of $U_{n,g}(K_{1,n_1},\ldots,K_{1,n_g})$ has degree greater than 2 then $U_{n,g}(K_{1,n_1},\ldots,K_{1,n_g}) \cong U^p_{n,g}$. Otherwise, let i and j be two vertices of degree greater than 2 on the cycle of $U_{n,g}(K_{1,n_1},\ldots,K_{1,n_g})$. Assume that $f_{U_{n,g}(K_{1,n_1},\ldots,K_{1,n_g})}(i) \geqslant f_{U_{n,g}(K_{1,n_1},\ldots,K_{1,n_g})}(j)$. Move the pendant vertices from the vertex j to the vertex i. Continue this till exactly one vertex on the cycle of $U_{n,g}(K_{1,n_1},\ldots,K_{1,n_g})$ has degree greater than 2. Then by Corollary 4.1.8, $F(U_{n,g}(K_{1,n_1},\ldots,K_{1,n_g}) \leqslant F(U^p_{n,g})$ and equality happens if and only if $U_{n,g}(K_{1,n_1},\ldots,K_{1,n_g}) \cong U^p_{n,g}$.

Let w be the central vertex of $K_{1,m}$. Then $f_{K_{1,m}}(w) = 2^m$. Let u be the vertex in $U^p_{n,g}$ with degree at least 3. Then by Lemma 4.1.2,

$$\begin{aligned} F(U^p_{n,g}) &= F(C_g) + F(K_{1,n-g}) - 1 + (f_{C_g}(u)-1)(f_{K_{1,n-g}}(u)-1) \\ &= g^2+1+2^{n-g}+n-g-1+\left(2g+\binom{g-1}{2}-1\right)(2^{n-g}-1) \\ &= n+g^2-g+1+(2^{n-g}-1)\left(2g+\binom{g-1}{2}\right). \end{aligned} \tag{4.2.1}$$

Similarly, by Lemma 4.2.2, $F(G) \geqslant F(U_{n,g}(P_{n_1+1},\ldots,P_{n_g+1}))$ and equality happens if and only if $G \cong U_{n,g}(P_{n_1+1},\ldots,P_{n_g+1})$. If exactly one vertex on the cycle of

$U_{n,g}(P_{n_1+1},\ldots,P_{n_g+1})$ has degree 3 then $U_{n,g}(P_{n_1+1},\ldots,P_{n_g+1}) \cong U^l_{n,g}$. Otherwise, let i and j be two vertices on the cycle of $U_{n,g}(P_{n_1+1},\ldots,P_{n_g+1})$ of degree 3. Without loss of generality, let $f_{U_{n,g}(P_{n_1+1},\ldots,P_{n_g+1})}(i) \leqslant f_{U_{n,g}(P_{n_1+1},\ldots,P_{n_g+1})}(j)$. Replace both the paths at i and j by a single path at i on n_i+n_j+1 vertices. Continue this till exactly one vertex on the cycle of $U_{n,g}(P_{n_1+1},\ldots,P_{n_g+1})$ has degree 3. Then by Lemma 4.1.9, $F(U_{n,g}(P_{n_1+1},\ldots,P_{n_g+1})) \geqslant F(U^l_{n,g})$ and equality happens if and only if $U_{n,g}(P_{n_1+1},...,P_{n_g+1}) \cong U^l_{n,g}$.

Furthermore, let u be the only degree 3 vertex of $U^l_{n,g}$. Then by Lemma 4.1.2,

$$\begin{aligned} F(U^l_{n,g}) &= F(C_g) + F(P_{n-g+1}) - 1 + (f_{C_g}(u)-1)(f_{P_{n-g+1}}(u)-1) \\ &= g^2+1+\binom{n-g+2}{2} - 1 + \left(2g+\binom{g-1}{2}-1\right)(n-g) \\ &= \left(\frac{n-g}{2}\right)(n+g^2+3)+g^2+1. \end{aligned} \tag{4.2.2}$$

This completes the proof. □

Now we proceed towards finding the graphs which extremize the subgraph index over $\mathcal{U}_n$.

Theorem 4.2.4. *Let $G \in \{U^p_{n,3}, U^p_{n,4}, \ldots, U^p_{n,n-1}\}$. Then $F(G) \leqslant (7\times 2^{n-3})+n$ and equality happens if and only if $G = U^p_{n,3}$.*

Proof. We first compare $F(U^p_{n,g})$ and $F(U^p_{n,g+1})$ for $3 \leqslant g \leqslant n-2$. By (4.2.1), we have

$$F(U^p_{n,g}) = n+g^2-g+1+(2^{n-g}-1)\left(2g+\binom{g-1}{2}\right)$$

and

$$\begin{aligned}F(U^p_{n,g+1}) &= n + (g+1)^2 - (g+1) + 1 + (2^{n-g-1} - 1)\left(2g + 2 + \binom{g}{2}\right)\\ &= n + g^2 + g + 1 + (2^{n-g-1} - 1)\left(2g + 2 + \binom{g}{2}\right).\end{aligned}$$

So, the difference

$$\begin{aligned}F(U^p_{n,g}) - F(U^p_{n,g+1}) &= -2g + (2^{n-g} - 1)\left(2g + \binom{g-1}{2}\right) - (2^{n-g-1} - 1)\left(2g + 2 + \binom{g}{2}\right)\\ &= -(g-1) + 2^{n-g-1}\left[\frac{g(g-1)}{2}\right]\\ &= (g-1)\left[2^{n-g-1}\left(\frac{g}{2}\right) - 1\right]\\ &> 0, \text{ since } g \geqslant 3 \text{ and } n > g.\end{aligned}$$

This implies $U^p_{n,3}$ has the maximum subgraph index in $\{U^p_{n,3}, U^p_{n,4}, \ldots, U^p_{n,n-1}\}$ and the result follows from (4.2.1). $\square$

The following result compares the subgraph index of graphs in $\{U^l_{n,3}, U^l_{n,4}, \ldots, U^l_{n,n-1}\}$.

Theorem 4.2.5. *Let $n \geqslant 5$ and let g_0 be the largest positive integer such that $\frac{3g_0^2 - g_0 + 2}{2g_0} < n$. Let $G \in \{U^l_{n,3}, U^l_{n,4}, \ldots, U^l_{n,n-1}\}$. Then*

$$F(U^l_{n,3}) \leqslant F(G) \leqslant F(U^l_{n,g_0+1})$$

with left equality happens if and only if $G = U^l_{n,3}$ and right equality happens if and only if $G = U^l_{n,g_0+1}$.

Proof. For $3 \leqslant g \leqslant n-2$, by (4.2.2), we have

$$F(U^l_{n,g}) = \left(\frac{n-g}{2}\right)(n + g^2 + 3) + g^2 + 1$$

and

$$F(U^l_{n,g+1}) = \binom{n-g-1}{2}(n+g^2+2g+4)+g^2+2g+2.$$

So the difference

$$\begin{aligned} F(U^l_{n,g+1}) - F(U^l_{n,g}) &= (2g+1)\binom{n-g}{2} - \binom{n+g^2+2g+4}{2} + 2g+1 \\ &= \frac{2gn-(3g^2-g+2)}{2}. \end{aligned}$$

Suppose $2gn-(3g^2-g+2)=0$. Then $3g^2-(2n+1)g+2=0$ which implies $g = \frac{(2n+1)\pm\sqrt{(2n+1)^2-24}}{6}$. But g is an integer so $(2n+1)^2-24$ must be a perfect square. This implies $2n+1=7$ or 5, which is a contradiction as $n \geqslant 5$. So either $F(U^l_{n,g+1}) - F(U^l_{n,g}) > 0$ or $F(U^l_{n,g+1}) - F(U^l_{n,g}) < 0$.

Let g_0 be the largest integer such that $\frac{3g_0^2-g_0+2}{2g_0} < n$. Then among all graphs in $\{U^l_{n,3}, U^l_{n,4}, \ldots, U^l_{n,n-1}\}$, the subgraph index is maximized by the graph U^l_{n,g_0+1} and minimized by the graph $U^l_{n,3}$ or $U^l_{n,n-1}$. But

$$F(U^l_{n,3}) = \binom{n-3}{2}(n+9+3)+9+1$$

and

$$F(U^l_{n,n-1}) = \frac{1}{2}(n+(n-1)^2+3)+(n-1)^2+1.$$

So the difference $F(U^l_{n,n-1}) - F(U^l_{n,3}) = (n-3)(n-4) > 0$ for $n \geqslant 5$. Hence the result follows. $\square$

The graphs $U^l_{4,3}$ and C_4 are the only elements of $\mathcal{U}_4$ and $F(C_4) = 17 < 18 = F(U^l_{4,3})$. For $n=5$ and 6, by Theorem 4.2.3 and Theorem 4.2.5, the subgraph index is minimized by $U^l_{n,3}$ or C_n over $\mathcal{U}_n$. We have $F(C_5) = 26 < 27 = F(U^l_{5,3})$. So, C_5 minimizes the subgraph index over $\mathcal{U}_5$. Also $F(C_6) = 37 = F(U^l_{6,3})$, so both the graphs C_6 and $U^l_{6,3}$ minimizes the subgraph index over $\mathcal{U}_6$. By Lemma 4.2.1, Theorem 4.2.3 and Theorem 4.2.4, $U^p_{n,g}$ maximizes the subgraph index. The following theorem characterizes the graphs which extremize the subgraph index over $\mathcal{U}_n$, $n \geqslant 7$.

Theorem 4.2.6. *Let $n \geqslant 7$ and let $G \in \mathcal{U}_n$. Then*

$$\frac{n^2+9n-16}{2} \leqslant F(G) \leqslant (7 \times 2^{n-3}) + n.$$

The left equality holds if and only if $G \cong U^l_{n,3}$ and the right equality holds if and only if $G \cong U^p_{n,3}$.

Proof. Since $F(U^p_{n,3}) = (7\times 2^{n-3})+n > n^2+1 = F(C_n)$ for $n \geqslant 7$, so by Theorem 4.2.3 and Theorem 4.2.4, the graph $U^p_{n,3}$ uniquely maximizes the subgraph index over $\mathcal{U}_n$. Also by Theorem 4.2.3 and Theorem 4.2.5, the subgraph index is minimized by $U^l_{n,3}$ or C_n over $\mathcal{U}_n$. We have $F(C_n) = n^2+1$ and $F(U^l_{n,3}) = \frac{n^2+9n-16}{2}$. So $F(C_n) - F(U^l_{n,3}) = \frac{n^2-9n+18}{2} > 0$ as $n \geqslant 7$. This completes the proof. $\square$

4.3 Graphs with fixed number of pendant vertices

Let $\mathfrak{H}_{n,k}$ be the class of all connected graphs of order n with k pendant vertices. If $k = n$, then $n = 2$ and $\mathfrak{H}_{n,k} = \{K_2\}$. If $k = n-1$ then $\mathfrak{H}_{n,k} = \{K_{1,n-1} : n \geqslant 3\}$. For $n = 3$, either $k = 0$ (C_3 is the only graph in this case) or $k = 2$ ($K_{1,2}$ is the only graph in this case). So, we assume that $0 \leqslant k \leqslant n-2$ and $n \geqslant 4$.

For $0 \leqslant k \leqslant n-3$ and $n \geqslant 4$, let P^k_n be the graph obtained by adding k pendant vertices at one vertex of the complete graph K_{n-k}. We define a specific subclass of graphs in $\mathfrak{H}_{n,0}$ as follows. Let m_1, m_2 and n be positive integers with $m_1, m_2 \geqslant 3$ and $n \geqslant m_1+m_2-1$. If $n > m_1+m_2-1$, take a path on $n-(m_1+m_2)+2$ vertices and identify one pendant vertex of the path with a vertex of C_{m_1} and another pendant vertex with a vertex of C_{m_2}. If $n = m_1 + m_2 - 1$ then identify one vertex of C_{m_1} with a vertex of C_{m_2}. We denote this graph by $C^n_{m_1,m_2}$.

Figure 4.3: The graphs $C^n_{m_1,m_2}$

We prove the following two results regarding the extremization of the subgraph index over $\mathfrak{H}_{n,k}$.

Theorem 4.3.1. *Let* $0 \leqslant k \leqslant n-2$. *Then*

(i) the graph P^k_n *uniquely maximizes the subgraph index over* $\mathfrak{H}_{n,k}$ *for* $0 \leqslant k \leqslant n-3$. *Furthermore,*

$$F(P^k_n) = (2^k - 1)(F(K_{n-k}) - F(K_{n-k-1})) + F(K_{n-k}) + k.$$

(ii) the tree $T(1, n-3, 2)$ *uniquely maximizes the subgraph index over* $\mathfrak{H}_{n,n-2}$. *Furthermore,*

$$F(T(1, n-3, 2)) = 3(2^{n-3}) + n.$$

Theorem 4.3.2. *Let* $0 \leqslant k \leqslant n-2$ *and let* $G \in \mathfrak{H}_{n,k}$. *Then*

(i) for $2 \leqslant k \leqslant n-2$, $F(G) \geqslant F(T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n-k))$ *and equality happens if and only if* $G \cong T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n-k)$.

(ii) for $k = 1$, $F(G) \geqslant F(U^l_{n,3})$ *and equality happens if and only if* $G \cong U^l_{n,3}$.

(iii) for $k = 0$,

$$F(G) \geqslant \begin{cases} F(C_n), & \text{if } n \leqslant 16 \\ F(C^n_{3,3}), & \text{if } n > 16. \end{cases}$$

Moreover, $F(G) \geqslant \min\{n^2 + 1, \frac{n^2+17n}{2}\}$.

Before proceeding to prove these results, we first see the results regarding extremization of the subgraph index among all trees on n vertices with k pendant vertices. For $2 \leqslant k \leqslant n-1$, let $\mathfrak{T}_{n,k}$ be the subclass of $\mathfrak{H}_{n,k}$ consisting of all trees of order n with k pendant vertices. By Theorem 4.3.1(ii) (we prove later), the tree $T(1, n-3, 2)$ has the maximum subgraph index over $\mathfrak{T}_{n,n-2}$. We next prove this result for $2 \leqslant k \leqslant n-3$. To do this, we first introduce the following tree.

By sG we mean, the graph consisting of s copies of G. Let $T_{n,k}$ be the tree on n vertices that has a vertex v of degree k and $T_{n,k} - v = rP_{q+1} \cup (k-r)P_q$, where $q = \lfloor \frac{n-1}{k} \rfloor$ and $r = n - 1 - kq$. Here, we have $0 \leqslant r < k$. Note that $T_{n,2} \cong P_n$ where v is one of the central vertex of P_n.

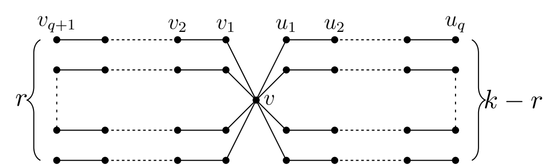


Figure 4.4: The tree $T_{n,k}$

Lemma 4.3.3. *Let $k \geqslant 2$ and $n = kq + 1$. Then* $F(T_{n,k}) = (q+1)(\frac{kq}{2} + (q+1)^{k-1})$.

Proof. Let v be the vertex of degree k and $T_{n,k} - v \cong kP_q$. If $k = 2$, then $T_{n,k}$ is a path on $2q+1$ vertices. So, we have $f_{T_{2q+1,2}}(v) = (q+1)^2$ and $F(T_{2q+1,2}) = \binom{2q+2}{2} = (q+1)(2q+1)$.

Now consider $k \geqslant 3$. Then

$$
\begin{aligned}
f_{T_{n,k}}(v) &= f_{T_{n-q,k-1}}(v) + q f_{T_{n-q,k-1}}(v) \\
&= (q+1) f_{T_{n-q,k-1}}(v) \\
&\vdots \\
&= (q+1)^{k-2} f_{T_{n-(k-2)q,2}}(v) \\
&= (q+1)^{k-2} f_{T_{2q+1,2}}(v) \\
&= (q+1)^{k-2}(q+1)^2 \\
&= (q+1)^k.
\end{aligned}
$$

By Lemma 4.1.3, we have

$$
\begin{aligned}
F(T_{n,k}) &= F(T_{n-q,k-1}) + F(P_q) + q f_{T_{n-q,k-1}}(v) \\
&= F(T_{n-q,k-1}) + \frac{q(q+1)}{2} + q(q+1)^{k-1} \\
&\vdots \\
&= F(T_{2q+1,2}) + (k-2)\left(\frac{q(q+1)}{2}\right) + q(q+1)^2\left[\frac{(q+1)^{k-2}-1}{(q+1)-1}\right] \\
&= (q+1)(2q+1) + (k-2)\left(\frac{q(q+1)}{2}\right) + (q+1)^k - (q+1)^2 \\
&= (q+1)\left(\frac{kq}{2} + (q+1)^{k-1}\right).
\end{aligned}
$$

This completes the proof. □

Lemma 4.3.4. *For $n \geqslant 3$, $F(T_{n,k}) = (q+2)^r(q+1)^{k-r} + \frac{(q+1)(qk+2r)}{2}$ where $q = \lfloor \frac{n-1}{k} \rfloor$ and $r = n-1-kq$.*

Proof. We have $n-1 = kq + r$, with $0 \leqslant r < k$. For $r = 0$, the result follows from Lemma 4.3.3. Now consider $1 \leqslant r < k$. For $k = 2$, $T_{n,k}$ is a path on $2q+2$ vertices and $F(T_{2q+2,2}) = (q+1)(2q+3)$. For $k \geqslant 3$, let v be the vertex of degree k in $T_{n,k}$. Let us rename the tree $T_{r(q+1)+1,r}$ as T_1 and the tree $T_{(k-r)q+1,k-r}$ as T_2. Note that for $r = 1$, $T_1 \cong P_{q+2}$ and for $r = k-1$, $T_2 \cong P_{q+1}$. Then by Lemma 4.1.2, we have

$$\begin{aligned}
F(T_{n,k}) &= F(T_1) + F(T_2) - 1 + (f_{T_1}(v) - 1)(f_{T_2}(v) - 1) \\
&= (q+2)\left(\frac{r(q+1)}{2} + (q+2)^{r-1}\right) + (q+1)\left(\frac{(k-r)q}{2} + (q+1)^{k-r-1}\right) - 1 \\
&+ ((q+2)^r - 1)((q+1)^{k-r} - 1) \\
&= (q+2)^r(q+1)^{k-r} + \frac{(q+1)(qk+2r)}{2}.
\end{aligned}$$

□

Theorem 4.3.5. *For $2 \leqslant k \leqslant n-3$, the tree $T_{n,k}$ uniquely maximizes the subgraph index over $\mathfrak{T}_{n,k}$.*

Proof. If $k = 2$ then P_n is the only tree in $\mathfrak{T}_{n,2}$ and the result is true. So assume $k \geqslant 3$. Let $T \in \mathfrak{T}_{n,k}$ be a tree with maximum subgraph index over $\mathfrak{T}_{n,k}$.

Claim : There is a unique $v \in V(T)$ with $deg(v) \geqslant 3$.

Let there be two vertices $u, v \in V(T)$ with $deg(u) = n_1 \geqslant 3$, $deg(v) = n_2 \geqslant 3$. Let $N_T(u) = \{u_1, u_2, \ldots, u_{n_1}\}$ and $N_T(v) = \{v_1, v_2, \ldots, v_{n_2}\}$ where u_1 and v_1 lie on the path joining u and v (u_1 may be v and v_1 may be u). Let T_1 be the largest subtree of T containing $u, u_2, u_3, \ldots, u_{n_1-1}$ but not u_1, u_{n_1} and T_2 be the largest subtree of T containing $v, v_2, v_3, \ldots, v_{n_2-1}$ but not v_1, v_{n_2}. We rename the vertices $u \in V(T_1)$ and $v \in V(T_2)$ by u' and v', respectively. Let H be the connected component of $T \setminus \{u_2, u_3, \ldots, u_{n_1-1}, v_2, v_3, \ldots, v_{n_2-1}\}$ containing u and v. Then H, T_1 and T_2 are trees having at least 2 vertices each. Without loss of generality, let $f_H(u) \geqslant f_H(v)$. Construct a tree T' from H, T_1 and T_2 by identifying the vertices u, u', v'. Clearly $T' \in \mathfrak{T}_{n,k}$ and by Lemma 4.1.6, $F(T') > F(T)$, which is a contradiction. This proves the claim.

So, the connected components of $T - v$ are all paths and $deg(v) = k$. Suppose $T \ncong T_{n,k}$. Then there exist two paths $P : vv_1 \cdot v_{l_1}$ and $Q : vu_1 \dots u_{l_2}$ attached at v in T with $|l_1 - l_2| = \alpha \geqslant 2$. By grafting an edge operation, we can construct a tree $\tilde{T} \in \mathfrak{T}_{n,k}$ from T such that the difference of the lengths between P and Q in $\tilde{T}$ is $\alpha - 1$. Then by Corollary 4.1.5, $F(\tilde{T}) > F(T)$, which is a contradiction. So, $T_{n,k}$ is the only tree which maximizes the subgraph index over $\mathfrak{T}_{n,k}$.

□

The above result is proved by Zhang et al. in [53] (see Corollary 5.3) but we have given a different proof. We also explained the counting for $F(T_{n,k})$. The following is an important result in the study of minimizing the subgraph index over $\mathfrak{H}_{n,k}$.

Theorem 4.3.6 ([23], Theorem 1)**.** *For $2 \leqslant k \leqslant n-2$, the tree $T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n-k)$ uniquely minimizes the subgraph index over $\mathfrak{T}_{n,k}$. Furthermore,*

$$F\left(T\left(\left\lfloor \frac{k}{2} \right\rfloor, \left\lceil \frac{k}{2} \right\rceil, n-k\right)\right) = \begin{cases} (n-k-1)2^{\frac{k}{2}+1} + 2^k + k + \binom{n-k-1}{2} & \textit{if } k \textit{ is even,} \\ 3(n-k-1)2^{\frac{k-1}{2}} + 2^k + k + \binom{n-k-1}{2} & \textit{if } k \textit{ is odd.} \end{cases}$$

Proof of Theorem 4.3.1: (i) Let $G \in \mathfrak{H}_{n,k}$ and let $v_1, v_2, \dots, v_{n-k}$ be the non-pendant vertices of G. Assume that $G \ncong P_n^k$. It is enough to show that $F(P_n^k) > F(G)$.

If the induced subgraph $G[v_1, v_2, \dots, v_{n-k}]$ is not complete, then form a new graph G' from G by joining all the non-adjacent non-pedant vertices of G with new edges. If the induced subgraph $G[v_1, v_2, \dots, v_{n-k}]$ is complete, the take $G' = G$. Then $G' \in \mathfrak{H}_{n,k}$ and by Lemma 4.1.1, $F(G') \geqslant F(G)$. If $G' \cong P_n^k$ then $G' \neq G$ and in that case $F(G') > F(G)$. Otherwise, G' has at least two vertices of degree greater than or equal to $n-k$. Form a new graph G'' from G' by moving all the pendant vertices to one of the vertex $v_1, v_2, \ldots, v_{n-k}$ following the pattern mentioned in the statement of the Corollary 4.1.8. Then $G'' \cong P_n^k$ and by Corollary 4.1.8, $F(G'') > F(G') \geqslant F(G)$.

For $v \in V(K_n)$, $f_{K_n}(v) = F(K_n) - F(K_{n-1})$. Also we know, $F(K_{1,k}) = 2^k + k$ and $f_{K_{1,k}}(u) = 2^k$ where u is the non-pendant vertex of $K_{1,k}$. Let w be the vertex of P_n^k with which k pendant vertices are adjacent. Then by Lemma 4.1.2 we have

$$\begin{aligned}
F(P_n^k) &= F(K_{n-k}) + F(K_{1,k}) - 1 + (f_{K_{n-k}}(w) - 1)(f_{K_{1,k}}(w) - 1) \\
&= F(K_{n-k}) + F(K_{1,k}) + f_{K_{n-k}}(w) f_{K_{1,k}}(w) - f_{K_{n-k}}(w) - f_{K_{1,k}}(w) \\
&= (2^k - 1)(F(K_{n-k}) - F(K_{n-k-1})) + F(K_{n-k}) + k.
\end{aligned}$$

(ii) Let $G \in \mathfrak{H}_{n,n-2}$. Then G is isomorphic to $T(k,l,2)$ for some $k, l \geqslant 1$. If $k = 1$ or $l = 1$, then $G \cong T(1, n-3, 2)$. If $k, l \geqslant 2$ then form the tree $T(1, n-3, 2)$ from G by moving pendant vertices from one vertex to other following the pattern mentioned in the statement of the Corollary 4.1.8. Then $F(T(1, n-3, 2)) > F(G)$ and by Lemma 4.1.3,

$$F(T(1, n-3, 2)) = 3 + 2^{n-3} + n - 3 + 2^{n-2} = 3(2^{n-3}) + n.$$

This completes the proof.

$\square$

Proof of Theorem 4.3.2 (i) and (ii): (i) Let $G \in \mathfrak{H}_{n,k}, 2 \leqslant k \leqslant n-2$. Suppose $G \ncong T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n-k)$. If G is not a tree, then construct a spanning tree G' from

G by deleting some edges. If G is a tree, take $G' = G$. Then, $F(G') \leqslant F(G)$ and equality holds if $G' = G$. The number of pendant vertices of G' is greater than or equal to k. If G' has k pendant vertices then the result follows from Theorem 4.3.6. Suppose G' has more than k pendant vertices. Since $k \geqslant 2$, G' has at least one vertex of degree greater than 2. Consider a vertex v of G' with $deg(v) \geqslant 3$ and two paths P_{l_1}, P_{l_2} with $l_1 \geqslant l_2$ attached at v. Using grafting of edges operation on G', we will get a new tree $\tilde{G}$ with number of pendant vertices one less than the number of pendant vertices of G' and by Corollary 4.1.5, $F(\tilde{G}) < F(G')$. Continue this process till we get a tree with k pendant vertices from $\tilde{G}$. By Corollary 4.1.5, every step in this process the subgraph index will decrease. So, we will reach a tree of order n with k pendant vertices and the result follows from Theorem 4.3.6.

(ii) Let $G \in \mathfrak{H}_{n,1}$ and $G \ncong U^l_{n,3}$. Since G is connected and has exactly one pendent vertex, it must contain a cycle. Let C_g be a cycle in G. If G has more than one cycle, then construct a new graph G' from G by deleting edges from all cycles other than C_g so that the graph remains connected. If G has exactly one cycle, then take $G' = G$. Clearly $F(G') \leqslant F(G)$ and equality holds if $G' = G$. Now G' is a unicyclic graph on n vertices with girth g. By Theorem 4.2.5, $F(U^l_{n,3}) \leqslant F(G')$ and equality happens if and only if $G' \cong U^l_{n,3}$. As $U^l_{n,3} \in \mathfrak{H}_{n,1}$, so the result follows.

□

The only case left in the problem of minimizing the subgraph index over $\mathfrak{H}_{n,k}$ is when $k = 0$. Upto isomorphism, there are only three connected graphs on 4 vertices without any pendant vertex. It can be easily checked that C_4 has the minimum subgraph index over $\mathfrak{H}_{4,0}$. For the rest of this section, n is at least 5. The next lemma compares the subgraph index of $C^n_{3,3}$ and C_n.

Lemma 4.3.7. *For $n \geqslant 6$, $F(C_n) < F(C^n_{3,3})$ if and only if $n \leqslant 16$.*

Proof. Let v and w be two vertices of $C^6_{3,3}$ with $deg(v) = deg(w) = 3$. Then by Lemma 4.1.3, $F(C^6_{3,3}) = F(C_3) + F(C_3) + f_{C_3}(v)f_{C_3}(w) = 10 + 10 + 49 = 69 > 37 = F(C_6)$. For $n \geqslant 7$, let v_1 be the vertex of one of the 3-cycles with degree 3 and let v_2 be the vertex adjacent to v_1 but not in that 3-cycle of $C^n_{3,3}$. Then by Lemma 4.1.3,

$$\begin{aligned}
F(C^n_{3,3}) &= F(C_3) + F(U^l_{n-3,3}) + f_{C_3}(v_1)f_{U^l_{n-3,3}}(v_2) \\
&= 10 + \binom{n-6}{2}(n+9) + 10 + 7(n+1) \\
&= \frac{n^2+17n}{2}
\end{aligned}$$

So, $F(C^n_{3,3}) - F(C_n) = \frac{n^2+17n}{2} - n^2 - 1 = \frac{17n-n^2-2}{2} > 0$ if and only if $n \leqslant 16$. This completes the proof. $\square$

Lemma 4.3.8. *Let $m_1, m_2 \geqslant 3$ be two integers and let $n = m_1 + m_2 - 1$. Then $F(C_n) < F(C^n_{m_1,m_2})$.*

Proof. Let v be the vertex of degree 4 in $C^n_{m_1,m_2}$. Then by Lemma 4.1.2

$$\begin{aligned}
F(C^n_{m_1,m_2}) &= F(C_{m_1}) + F(C_{m_2}) - 1 + (f_{C_{m_1}}(v) - 1)(f_{C_{m_2}}(v) - 1) \\
&= m_1^2 + 1 + m_2^2 + 1 - 1 + \left(2m_1 + \binom{m_1-1}{2} - 1\right)\left(2m_2 + \binom{m_2-1}{2} - 1\right) \\
&\geqslant m_1^2 + m_2^2 + 1 + 4m_1m_2.
\end{aligned}$$

So, the difference $F(C^n_{m_1,m_2}) - F(C_n) \geqslant 2m_1m_2 + 2m_1 + 2m_2 - 1 > 0$. $\square$

Corollary 4.3.9. *Let $m_1, m_2 \geqslant 3$ be two integers and let $n = m_1 + m_2 - 1$. Let $G \in \mathfrak{H}_{n,0}$ with $C^n_{m_1,m_2}$ as a subgraph of G. Then $F(G) > F(C_n)$.*

Lemma 4.3.10. *Let u be the pendant vertex and v be a non-pendant vertex of the unicyclic graph $U_{n,g}^l$. Then $f_{U_{n,g}^l}(u) < f_{U_{n,g}^l}(v)$.*

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

$$f_{U_{n,g}^l}(u) = f_{P_{n-g}}(u) + f_{C_g}(g).$$

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

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

Since $f_{P_{n-g}}(g+1) = f_{P_{n-g}}(u)$, we have

$$f_{U_{n,g}^l}(v) - f_{U_{n,g}^l}(u) = f_{P_{n-g}}(u)(f_{C_g}(v,g) - 1) > 0.$$

If v is is not on the cycle C_g, then

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

So,

$$f_{U_{n,g}^l}(v) - f_{U_{n,g}^l}(u) = f_{P_{n-g}}(v) - f_{P_{n-g}}(u) + f_{C_g}(g)(f_{P_{n-g}}(g+1,v) - 1) > 0.$$

The last inequality holds because $f_{P_{n-g}}(v) \geqslant f_{P_{n-g}}(u)$ and $f_{P_{n-g}}(g+1,v) > 1$. $\square$

The next corollary follows from Lemma 4.3.10 and Corollary 4.1.4.

Corollary 4.3.11. *Let u be a vertex of G with $V(G) \geqslant 2$. Suppose v is the pendant vertex of $U_{n,g}^l$ and w is a non-pendant vertex of $U_{n,g}^l$. Let G_1 be the graph obtained* *from G and $U^l_{n,g}$ by identifying u with v and G_2 be the graph obtained by identifying u with w. Then $F(G_1) < F(G_2)$.*

Proposition 4.3.12. *Let $G \in \mathfrak{H}_{n,0}$ with at least one cut-vertex. Suppose $C^n_{m_1,m_2}$ with $m_1+m_2-1=n$ is not a subgraph of G. Then $F(G) \geqslant F(C^n_{g_1,g_2})$ for some $g_1, g_2 \geqslant 3$ and the equality holds if and only if $G \cong C^n_{g_1,g_2}$.*

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

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

Let G_1 has some pendant vertices. Then for some $l < n$, $C^l_{g_1,g_2}$ is a subgraph of G_1. By grafting of edges operations (if required), we can form a new graph G_2 from G_1 where G_2 is isomorphic to the graph obtained by attaching paths to different vertices of $C^l_{g_1,g_2}$. Then by Corollary 4.1.5, $F(G_2) < F(G_1)$. If there are paths attached to more than one vertex of $C^l_{g_1,g_2}$ in G_2, then using the graph operation as mentioned in Lemma 4.1.9, form a new graph G_3 from G_2, where G_3 has exactly one path attached to $C^l_{g_1,g_2}$. Then by Lemma 4.1.9, $F(G_3) < F(G_2)$.

Let the path attached to the vertex u in $C^l_{g_1,g_2}$ of G_3. Then we have two cases:

Case-1: $u \in V(C_{g_1}) \cup V(C_{g_2})$

Without loss of generality, assume that $u \in V(C_{g_1})$. Then the induced subgraph of

G_3 containing the vertices of C_{g_1} and the vertices of the path attached to it, is the graph U^l_{p,g_1} for some $p > g_1$. Let v be the pendant vertex of U^l_{p,g_1}. Since the two cycles C_{g_1} and C_{g_2} have at most one vertex in common, so we have two subcases:

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

Let H_1 be the induced subgraph of G_3 containing the vertices $\{V(G_3) \setminus V(U^l_{p,g_1})\} \cup \{w\}$. Clearly H_1 is the cycle C_{g_2}. Then identify the vertex v of U^l_{p,g_1} with the vertex w of H_1 to form a new graph G_4. By Corollary 4.3.11, $F(G_4) < F(G_3)$ and G_4 is the graph $C^n_{g_1,g_2}$.

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

Let H_2 be the induced subgraph of G_3 containing the vertices $V(G_3) \setminus V(U^l_{p,g_1})$. In G_3 exactly one vertex $w_1 \in U^l_{p,g_1}$ adjacent to exactly one vertex w_2 of H_2. Form a new graph G_5 from G_3 by deleting the edge $\{w_1, w_2\}$ and adding the edge $\{v, w_2\}$. By Corollary 4.3.11, $F(G_5) < F(G_3)$ and G_5 is the graph $C^n_{g_1,g_2}$.

Case-2: $u \notin V(C_{g_1}) \cup V(C_{g_2})$

Let w be the pendant vertex of G_3 and let w_3 be a vertex in $C^l_{g_1,g_2}$ of G_3 adjacent to u. Form a new graph G_6 from G_3 by deleting the edge $\{u, w_3\}$ and adding the edge $\{w, w_3\}$. By Corollary 4.3.11, $F(G_6) < F(G_3)$ and G_6 is the graph $C^n_{g_1,g_2}$. This completes the proof. □

Lemma 4.3.13. *Let u be a vertex of G. For $m \geqslant 4$, let G_1 be the graph obtained by identifying the vertex u of G with the pendant vertex of $U^l_{m+1,m}$ and G_2 be the graph obtained by identifying the vertex u with the pendant vertex of $U^l_{m+1,3}$. Then $F(G_2) < F(G_1)$.*

Proof. We have

$$F(G_1) = F(G) + F(U^l_{m+1,m}) - 1 + (f_G(u) - 1)(f_{U^l_{m+1,m}}(u) - 1)$$
$$F(G_2) = F(G) + F(U^l_{m+1,3}) - 1 + (f_G(u) - 1)(f_{U^l_{m+1,3}}(u) - 1).$$

By Theorem 4.2.5, $F(U^l_{m+1,3}) < F(U^l_{m+1,m})$. So, the difference

$$\begin{aligned} F(G_1) - F(G_2) &> (f_G(u) - 1)(f_{U^l_{m+1,m}}(u) - f_{U^l_{m+1,3}}(u)) \\ &= (f_G(u) - 1)\left(1 + 2m + \binom{m-1}{2} - m + 2 - 7\right) \\ &= (f_G(u) - 1)\left(m - 4 + \binom{m-1}{2}\right) \\ &> 0. \end{aligned}$$

□

Corollary 4.3.14. *Let $m_1, m_2 \geqslant 3$ be two integers and let $m_1 + m_2 \leqslant n$. Then $F(C^n_{m_1,m_2}) \geqslant F(C^n_{3,3})$ and equality happens if and only if $m_1 = m_2 = 3$.*

Proposition 4.3.15. *Let G be a 2-connected graph on $n \geqslant 5$ vertices. Then $F(G) \geqslant F(C_n)$ and the equality holds if and only if $G \cong C_n$.*

Proof. Let g be the circumference (length of the longest cycle) of G. Let C_g be a g-cycle in G. Then every connected subgraph of C_g is also a connected subgraph of G. If $g = n$ and G is not isomorphic to C_n, then G has at least $n+1$ edges. In this case clearly $F(G) > F(C_n)$.

If $g = n-1$ then the number of connected subgraphs of C_g is equal to $(n-1)^2+1$. Let v be the vertex of G not on the cycle C_g of G. Since G is 2-connected, so v is adjacent to at least two vertices of C_g. Let u be a vertex of C_g such that $\{u, v\}$ is an edge in G. Then $C_g \cup \{u, v\}$ is a connected subgraph of G. By Lemma 4.2.1, the number of connected subgraphs of $C_g \cup \{u, v\}$ containing $\{u, v\}$ is $2(n-1) + \binom{n-2}{2}$. So, $F(G) > (n-1)^2 + 1 + 2(n-1) + \binom{n-2}{2} > n^2 + 1 = F(C_n)$.

If $g \leqslant n-2$ then at least two vertices of G are not on the cycle C_g. Since G is 2-connected, so for every pair of distinct vertices $u, v \in V(G) \setminus V(C_g)$ there exists at least two distinct paths in G with u and v as pendant vertices. Each of these paths is a connected subgraph of G. Apart from these subgraphs, also for every $v \in V(G) \setminus V(C_g)$ there exists a $w \in V(C_g)$ such that there is a path joining v and w. This path together with C_g gives a subgraph of G with v as a pendant vertex. Thus there are at least $(n-g)(f_{C_g}(w))$ more connected subgraphs in G different from the above mentioned connected subgraphs of G. Thus

$$\begin{aligned}
F(G) &\geqslant F(C_g) + 2\binom{n-g}{2} + (n-g)(f_{C_g}(w)) \\
&= g^2 + 1 + (n-g)(n-g-1) + (n-g)\left(2g + \binom{g-1}{2}\right) \\
&= n^2 + 1 + \frac{g(n-g)}{2}(g-3) > n^2 + 1 = F(C_n).
\end{aligned}$$

The last inequality follows from the fact that g is the circumference of a 2-connected graph on $n \geqslant 5$ vertices. Hence the result follows. □

Proof of Theorem 4.3.2(iii): If G has no cut-vertices, then by Proposition 4.3.15 and Lemma 4.3.7 the result follows. Suppose G has a cut-vertex. If $C^n_{m_1,m_2}$ with $m_1 + m_2 - 1 = n$ is a subgraph of G then by Corollary 4.3.9 and and Lemma 4.3.7 the result follows. If $C^n_{m_1,m_2}$ with $m_1 + m_2 - 1 = n$ is not a subgraph of G then by Proposition 4.3.12, Corollary 4.3.14 and Lemma 4.3.7, the result follows. □

4.4 Future works

We have studied the extremal problems on subgraph index over unicyclic graphs and graphs with fixed number of pendant vertices. Similar problems on the subgraph index can be studied for some other classes of graphs. To be specific, it will be interesting to know the graphs which maximize or minimize the subgraph index over graphs with fixed number of cut vertices. Further, there are no routine methods to count the subgraph index of a graph. Even for many well known graphs the subgraph index is not known. A unified approach to count the number of connected subgraphs of graphs may help to know the subgraph index of various graphs.

Chapter 5

The Wiener index of a graph

In this chapter, we characterize the graphs which extremize the Wiener index among all graphs on n vertices with k pendant vertices and the graph which minimizes the Wiener index among all graphs on n vertices with s cut vertices.

5.1 Some preliminary results

The following lemma is straightforward which shows the effect of a new edge on the Wiener index of a graph.

Lemma 5.1.1. *Let u and v be two non adjacent vertices of G. Let G' be the graph obtained from G by joining u and v by an edge. Then $W(G') < W(G)$.*

It follows from Lemma 5.1.1 that among all connected graphs on n vertices, the Wiener index is uniquely minimized by the complete graph K_n and maximized by some tree. Among all trees on n vertices, the Wiener index is uniquely minimized by the star $K_{1,n-1}$ and uniquely maximized by the path P_n (see [44], Theorem 2.1.14). It is easy to determine the Wiener index of the following graphs(see [44]):

- (i) $W(K_n) = \binom{n}{2}$;
- (ii) $W(P_n) = \binom{n+1}{3}$;
- (iii) $W(K_{1,n-1}) = (n-1)^2$.

The Wiener index of the cycle C_n is (see [30],Theorem 5)

$$W(C_n) = \begin{cases} \frac{1}{8}n^3 & \textit{if } n \textit{ is even,} \\ \frac{1}{8}n(n^2-1) & \textit{if } n \textit{ is odd,} \end{cases} \tag{5.1.1}$$

and for $u \in V(C_n)$

$$D_{C_n}(u) = \begin{cases} \frac{n^2}{4} & \textit{if } n \textit{ is even,} \\ \frac{n^2-1}{4} & \textit{if } n \textit{ is odd.} \end{cases} \tag{5.1.2}$$

The following lemma is useful in counting the Wiener index of graphs with cut vertices.

Lemma 5.1.2 ([3], Lemma 1.1)**.** *Let u be a cut vertex of a graph G. Let G_1 and G_2 be two subgraphs of G with $G = G_1 \cup G_2$ and $V(G_1) \cap V(G_2) = \{u\}$. Then*

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

Corollary 5.1.3. *Let G and H be two vertex disjoint graphs having at least 2 vertices each. Let $u, v \in V(G)$ and $w \in V(H)$. Let G_1 and G_2 be the graphs obtained from G and H by identifying the vertex w of H with the vertices u and v of G, respectively. If $D_G(v) \geqslant D_G(u)$ then $W(G_2) \geqslant W(G_1)$ and equality happens if and only if $D_G(v) = D_G(u)$.*

Proof. By Lemma 5.1.2,

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

and

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

So

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

and the result follows. □

In the path $P_n : v_1 v_2 \cdots v_n$,

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

So, if n is odd, then

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

and if n is even, then

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

Let $G_{k,l}$ be the graph described in Section 4.1. Then the next result follows from the above observation and Corollary 5.1.3.

Corollary 5.1.4 ([24], Lemma 2.4)**.** *If* $1 \leqslant k \leqslant l$, *then* $W(G_{k-1,l+1}) > W(G_{k,l})$.

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

Lemma 5.1.5 ([25], Lemma 2.4)**.** *Let H, X and Y be three pairwise vertex disjoint graphs having at least 2 vertices each. Suppose $u, v \in V(H)$, $x \in V(X)$ and $y \in V(Y)$. Let G be the graph obtained from H, X and Y by identifying u with x and v with y. Let G_1^* be the graph obtained from H, X, Y by identifying the vertices u, x, y and let G_2^* be the graph obtained from H, X, Y by identifying the vertices v, x, y (see Figure 5.1). Then, either $W(G_1^*) < W(G)$ or $W(G_2^*) < W(G)$.*

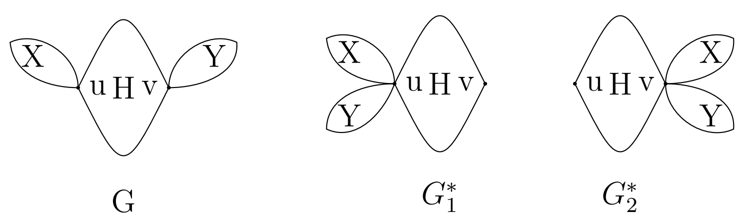


Figure 5.1: Movement of a component from one vertex to other

Let $G_{uv}(n_1, n_2)$ be the graph described in Corollary 4.1.8. Then we have the following corollary.

Corollary 5.1.6. *If $n_1, n_2 \geqslant 1$ then*

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

In [49] Lemma 2.6, the authors have proved the following.

Let G_0 be a connected graph of order $n_0 > 1$ and $u_0, v_0 \in V(G_0)$ be two distinct vertices in G_0. $P_s = u_1u_2 \cdots u_s$ and $P_t = v_1v_2 \cdots v_t$ are two paths of order s and t, respectively. Let G be the graph obtained from G_0, P_s and P_t by adding edges $\{u_0, u_1\}$

and $\{v_0, v_1\}$*. Suppose that* $G_1 = G - \{u_0, u_1\} + \{v_t, u_1\}$ *and* $G_2 = G - \{v_0, v_1\} + \{u_s, v_1\}$*. Then either* $W(G) < W(G_1)$ *or* $W(G) < W(G_2)$ *holds.*

If we take $G_0 = P_{n_0}$ and u_0 and v_0 as two distinct pendant vertices of G_0, then $G_0 \cong G_1 \cong G_2$. So, $W(G_0) \cong W(G_1) \cong W(G_2)$ and hence the statement is not true. We give a proof of the corrected version of this result. Let $G^p_{uv}(l, k)$ be the graph mentioned in Lemma 4.1.9.

Lemma 5.1.7. *Let* u, v *be two vertices of a graph* G *and* G *is not the* u*-*v *path. If* $D_G(u) \geqslant D_G(v)$ *and* $l, k \geqslant 2$*, then*

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

Proof. Let us name the graph $G^p_{u,v}(l, 1)$ as H and let w be the pendant vertex of H corresponding to P_l. Then by Lemma 5.1.2,

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

and

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

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

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

Now

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

and

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

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

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

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

The Wiener index of $U^p_{n,g}$ and $U^l_{n,g}$ are useful for our results and can be found in [49] (see Theorem 1.1). We have

$$W(U^p_{n,g}) = \begin{cases} \frac{g^3}{8} + (n-g)(\frac{g^2}{4} + n - 1) & \textit{if } g \textit{ is even}, \\ \frac{g(g^2-1)}{8} + (n-g)(\frac{g^2-1}{4} + n - 1) & \textit{if } g \textit{ is odd}, \end{cases} \tag{5.1.3}$$

and

$$W(U^l_{n,g}) = \begin{cases} \frac{g^3}{8} + (n-g)(\frac{n^2+ng+3g-1}{6} - \frac{g^2}{12}) & \text{if g is even}, \\ \frac{g(g^2-1)}{8} + (n-g)(\frac{n^2+ng+3g-1}{6} - \frac{g^2}{12} - \frac{1}{4}) & \text{if g is odd}. \end{cases} \tag{5.1.4}$$

We next calculate the Wiener index of some other trees, which we need for the extremal bounds in some of our results. Let $P_{d,m}$ be the path-star tree on $d+m$ vertices. By using Lemma 5.1.2, it is easy to see that

$$W(P_{d,m}) = \binom{d+1}{3} + m^2 + (d-1)m + \frac{d(d-1)m}{2}. \tag{5.1.5}$$

Using the value of $W(P_{d,m})$ and $W(K_{1,l})$ in Lemma 5.1.2, we get

$$W(T(l,m,d)) = \binom{d+1}{3} + l^2 + m^2 + \frac{(d^2+d-2)(m+l)}{2} + (d+1)ml. \qquad (5.1.6)$$

For $k \geqslant 2$, let $T_{n,k}$ be the tree defined in Section 4.3. Let v be the central vertex of $T_{kq+1,k}$. Then

$$D_{T_{kq+1,k}}(v) = k + 2k + \cdots + qk = \frac{kq(q+1)}{2}. \qquad (5.1.7)$$

As $T_{2q+1,2} \cong P_{2q+1}$, in which v is the central vertex of P_{2q+1}, by Lemma 5.1.2

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

Now for $k \geqslant 3$, by Lemma 5.1.2 we have

$$\begin{aligned}
W(T_{kq+1,k}) &= W(T_{(k-1)q+1,k-1}) + W(P_{q+1}) + (k-1)qD_{P_{q+1}}(v) + qD_{T_{(k-1)q+1,k-1}}(v) \\
&= W(T_{(k-1)q+1,k-1}) + \binom{q+2}{3} + (k-1)q^2(q+1) \\
&\vdots \\
&= W(T_{2q+1,2}) + (k-2)\binom{q+2}{3} + (2+3+\cdots+k-1)q^2(q+1) \\
&= 2\binom{q+2}{2} + q^2(q+1) + (k-2)\binom{q+2}{3} + (2+3+\cdots+k-1)q^2(q+1) \\
&= k\binom{q+2}{3} + \frac{q^2(q+1)k(k-1)}{2}. \qquad (5.1.8)
\end{aligned}$$

5.2 Graphs with fixed number of pendant vertices

As in section 4.3, we assume that $0 \leqslant k \leqslant n-2$ and $n \geqslant 4$. The Wiener index and the subgraph index are inversely correlated with each other. In chapter 4, we characterised the graphs which extremize the subgraph index over $\mathfrak{H}_{n,k}$. Here we prove the corresponding results for the Wiener index. We have the following result regarding the maximization of the Wiener index over $\mathfrak{T}_{n,k}$.

Proposition 5.2.1 ([32], Theorem 4)**.** *For $2 \leqslant k \leqslant n-2$, the tree $T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n-k)$ uniquely maximizes the Wiener index over $\mathfrak{T}_{n,k}$.*

We prove the following results.

Theorem 5.2.2. *Let $0 \leqslant k \leqslant n-2$ and let $G \in \mathfrak{H}_{n,k}$. Then*

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

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

(ii) for $k = 1$, $W(G) \leqslant W(U^l_{n,3})$ and equality holds if and only if $G \cong U^l_{n,3}$. Furthermore,

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

(iii) for $k = 0$ and $n \geqslant 7$, $W(G) \leqslant W(C^n_{3,3})$ and equality holds if and only if $G \cong C^n_{3,3}$. Furthermore,

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

Theorem 5.2.3. *Let $0 \leqslant k \leqslant n-2$ and let $G \in \mathfrak{H}_{n,k}$. Then*

(i) for $0 \leqslant k \leqslant n-3$, $W(P^k_n) \leqslant W(G)$ and equality holds if and only if $G \cong P^k_n$.

Furthermore,

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

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

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

Theorem 5.2.4. *Let $2 \leqslant k \leqslant n-2$ and $T \in \mathfrak{T}_{n,k}$. Then $W(T_{n,k}) \leqslant W(T)$ and equality holds if and only if $T \cong T_{n,k}$.*

We now proceed towards proving these results. The following two resullts are useful in that aspect.

Proposition 5.2.5 ([49], Corollary 1.2)**.** *Let $G \in \mathcal{U}_n$, $n \geqslant 5$. Then, $W(G) \leqslant W(U_{n,3}^l)$ and equality holds if and only if $G \cong U_{n,3}^l$.*

Proposition 5.2.6 ([30], Theorem 5)**.** *Let G be a $2-$connected graph with n vertices. Then $W(G) \leqslant W(C_n)$ and equality holds if and only if $G \cong C_n$.*

The following two lemmas compare the Wiener index of C_n with the Wiener index of $C_{3,3}^n$ and C_{m_1,m_2}^n.

Lemma 5.2.7. *For $n \geqslant 6$, $W(C_n) \leqslant W(C_{3,3}^n)$ and equality happens if and only if $n = 6$.*

Proof. By (5.1.4), we have $W(U_{n,3}^l) = \frac{n^3-7n+12}{6}$. If u is the pendant vertex of $U_{n,3}^l$ then

$$D_{U_{n,3}^l}(u) = D_{P_{n-2}}(u) + 2(n-2) = \frac{(n-3)(n-2)}{2} + 2n - 4 = \frac{n^2-n-2}{2}.$$

For $n \geqslant 6$, let u be the cut-vertex common to C_3 and $U^l_{n-2,3}$ of $C^n_{3,3}$. Then by Lemma 5.1.2,

$$\begin{aligned} W(C^n_{3,3}) &= W(C_3) + W(U^l_{n-2,3}) + 2D_{U^l_{n-2,3}}(u) + 2(n-3) \\ &= 3 + \frac{(n-2)^3 - 7(n-2) + 12}{6} + (n-2)^2 - (n-2) - 2 + 2n - 6 \\ &= \frac{n^3 - 13n + 24}{6}. \end{aligned} \tag{5.2.1}$$

By (5.1.1) and (5.2.1), we have

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

Hence the result follows. $\square$

Lemma 5.2.8. *Let $m_1, m_2 \geqslant 3$ be two integers and let $n = m_1 + m_2 - 1$. Then $W(C_n) > W(C^n_{m_1,m_2})$.*

Proof. Let v be the vertex of degree 4 in $C^n_{m_1,m_2}$. First suppose n is even. Then one of m_1 or m_2 is odd and other is even. Without loss of generality, suppose m_1 is odd and m_2 is even. Then by Lemma 5.1.2 and equations (5.1.1) and (5.1.2), we have

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

and

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

The difference is

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

An easy calculation gives

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

which is greater than 0.

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

Case 1: Both m_1 and m_2 are even.

In this case, we have

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

and

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

The difference is

$$\begin{aligned}W(C_n)-W(C^n_{m_1,m_2}) &= \frac{1}{8}\left((m_1-1)m_2^2+(m_2-1)m_1^2-6m_1m_2+2m_1+2m_2\right)\\&\geqslant \frac{1}{8}\left(3(m_1-m_2)^2+2m_1+2m_2\right)\\&> 0.\end{aligned}$$

Case 2: Both m_1 and m_2 are odd.

In this case, we have

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

and the difference is

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

An easy calculation gives

$$W(C_n) - W(C^n_{m_1,m_2}) \begin{cases} > \frac{1}{8}\left(3(m_1-m_2)^2 + 5m_1 + 5m_2 - 4\right) & \text{if } m_1, m_2 \geqslant 5, \\ = \frac{1}{8}(2m_2^2 - 4m_2 + 2) & \text{if } m_1 = 3, \\ = \frac{1}{8}(2m_1^2 - 4m_1 + 2) & \text{if } m_2 = 3, \end{cases}$$

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

Lemma 5.2.9. *Let u be the pendant vertex and v be a non-pendant vertex of the unicyclic graph $U^l_{n,g}$. Then $D_{U^l_{n,g}}(u) > D_{U^l_{n,g}}(v)$.*

Proof. Let v_g be the vertex of degree 3 in $U^l_{n,g}$. Then the path from u to v_g has $n-g+1$ vertices, so

$$D_{U^l_{n,g}}(u) = D_{P_{n-g+1}}(u) + (g-1)(n-g) + D_{C_g}(v_g). \tag{5.2.2}$$

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

$$D_{U^l_{n,g}}(v) = D_{C_g}(v) + d(v, v_g)(n-g) + D_{P_{n-g+1}}(v_g).$$

Since $D_{P_{n-g+1}}(u) = D_{P_{n-g+1}}(v_g)$, so

$$D_{U^l_{n,g}}(u) - D_{U^l_{n,g}}(v) = (n-g)(g-1-d(v,v_g)) > 0.$$

If v is not on the cycle C_g of $U^l_{n,g}$, then

$$D_{U^l_{n,g}}(v) = D_{P_{n-g+1}}(v) + d(v, v_g)(g-1) + D_{C_g}(v_g).$$

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

$$D_{U^l_{n,g}}(u) - D_{U^l_{n,g}}(v) > (g-1)(n-g-d(v,v_g)) > 0.$$

This completes the proof.

□

The next corollary follows from Lemma 5.2.9 and Corollary 5.1.3.

Corollary 5.2.10. *Let u be a vertex of G with $|V(G)| \geqslant 2$. Suppose v is the pendant vertex of $U^l_{n,g}$ and w is a non-pendant vertex of $U^l_{n,g}$. Let G_1 and G_2 be the graphs obtained from G and $U^l_{n,g}$ by identifying u of G with the vertices v and w of $U^l_{n,g}$, respectively. Then $W(G_1) > W(G_2)$.*

Lemma 5.2.11. *Let u be a vertex of G. For $m \geqslant 4$, let G_1 be the graph obtained by identifying the vertex u of G with the pendant vertex of $U^l_{m+1,m}$ and G_2 be the graph obtained by identifying the vertex u with the pendant vertex of $U^l_{m+1,3}$. Then $W(G_2) > W(G_1)$.*

Proof. By Lemma 5.1.2, we have

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

and

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

By Proposition 5.2.5, $W(U^l_{m+1,3}) > W(U^l_{m+1,m})$. So, the difference is

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

By (5.2.2), we have $D_{U^l_{m+1,3}}(u) = \frac{(m-1)(m+2)}{2}$ and

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

So,

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

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

Corollary 5.2.12. *Let $m_1, m_2 \geqslant 3$ be two integers and let $m_1 + m_2 \leqslant n$. Then $W(C^n_{3,3}) \geqslant W(C^n_{m_1,m_2})$ and equality happens if and only if $m_1 = m_2 = 3$.*

Proof of Theorem 5.2.2: (i) Let $G \in \mathfrak{H}_{n,k}$, $2 \leqslant k \leqslant n-2$. Suppose G is not isomorphic to $T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n-k)$. If G is a tree then by Proposition 5.2.1, $W(G) < W(T(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil, n-k))$.

Suppose G is not a tree. Construct a spanning tree G' from G by deleting some edges. Then by Lemma 5.1.1, $W(G') > W(G)$. The number of pendant vertices of G' is greater than or equal to k. Suppose G' has more than k pendant vertices. Since $k \geqslant 2$, G' has at least one vertex of degree greater than 2 and at least two paths attached to it. Consider a vertex v of G' with $deg(v) \geqslant 3$ and two paths P_{l_1}, P_{l_2}, $l_1 \geqslant l_2$ attached at v. Using grafting of edges operation on G', we get a new tree $\tilde{G}$ with number of pendant vertices one less than the number of pendant vertices of G' and by Corollary 5.1.4, $W(\tilde{G}) > W(G')$. Continue this process till we get a tree with k pendant vertices from $\tilde{G}$. By Corollary 5.1.4, every step in this process the Wiener index will increase. So, we will reach at a tree T of order n with k pendant vertices. By Proposition 5.2.1, we have

$W(T(\lfloor\frac{k}{2}\rfloor, \lceil\frac{k}{2}\rceil, n-k)) \geqslant W(T) > W(G)$. Hence $T(\lfloor\frac{k}{2}\rfloor, \lceil\frac{k}{2}\rceil, n-k)$ uniquely maximizes the Wiener index over $\mathfrak{H}_{n,k}$.

Now by replacing d, l and m with $n-k$, $\lfloor\frac{k}{2}\rfloor$ and $\lceil\frac{k}{2}\rceil$, respectively in (5.1.6), we get the value of $W\left(T(\lfloor\frac{k}{2}\rfloor, \lceil\frac{k}{2}\rceil, n-k)\right)$ as in the statement. This completes the proof.

(ii) Let $G \in \mathfrak{H}_{n,1}$. Suppose G is not isomorphic to $U^l_{n,3}$. Since G is connected and has exactly one pendent vertex, it must contain a cycle. Let C_g be a cycle in G. If G is a unicyclic graph then by Proposition 5.2.5, $W(U^l_{n,3}) > W(G)$. If G has more than one cycle, then construct a new graph G' from G by deleting edges from all cycles other than C_g so that the graph remains connected. Then by Lemma 5.1.1, $W(G') > W(G)$ and G' is a unicyclic graph on n vertices with girth g. By Proposition 5.2.5, $W(U^l_{n,3}) \geqslant W(G') > W(G)$. Hence $U^l_{n,3}$ uniquely maximizes the Wiener index over $\mathfrak{H}_{n,1}$. We get the value of $W(U^l_{n,3})$ from (5.1.4) and this completes the proof.

(iii) Let $n \geqslant 7$ and let $G \in \mathfrak{H}_{n,0}$. Suppose G is not isomorphic to $C^n_{3,3}$. Then we have two cases:

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

Since $C^n_{m_1,m_2}$ is a subgraph of G, by deleting some edges(if required) from G, we get $C^n_{m_1,m_2} \in \mathfrak{H}_{n,0}$ and by Lemma 5.1.1, $W(G) \leqslant W(C^n_{m_1,m_2})$. Again by Lemma 5.2.7 and Lemma 5.2.8, we have

$$W(G) \leqslant W(C^n_{m_1,m_2}) < W(C_n) < W(C^n_{3,3}).$$

Case 2: There are no integers $m_1, m_2 \geqslant 3$ with $n = m_1 + m_2 - 1$ such that

$C^n_{m_1,m_2}$ is a subgraph of G.

If G is a two connected graph then by Proposition 5.2.6 and Lemma 5.2.7, $W(G) \leqslant W(C_n) < W(C^n_{3,3})$. So let G has at least one cut vertex.

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

If G has exactly $n + 1$ edges, then there is no common vertex between C_{g_1} and C_{g_2} and $G \cong C^n_{g_1,g_2}$. As G is not isomorphic to $C^n_{3,3}$, so by Corollary 5.2.12, $W(G) < W(C^n_{3,3})$.

Now let $|E(G)| \geqslant n + 2$. Suppose $|E(G)| = n + k$, where $k \geqslant 2$. Choose $k - 1$ edges $\{e_1, \ldots, e_{k-1}\} \subset E(G)$ such that $e_i \notin E(C_{g_1}) \cup E(C_{g_2}), \;\; i = 1, \ldots, k - 1$ and $G \setminus \{e_1, \ldots, e_{k-1}\}$ is connected. Let $G_1 = G \setminus \{e_1, \ldots, e_{k-1}\}$ (G_1 may have some pendant vertices). Then by Lemma 5.1.1, $W(G_1) > W(G)$. If G_1 has no pendant vertices then $G_1 \cong C^n_{g_1,g_2}$ for some $g_1, g_2 \geqslant 3$. By Corollary 5.2.12, $W(G) < W(G_1) \leqslant W(C^n_{3,3})$.

Suppose G_1 has some pendant vertices. Then for some $p < n$, $C^p_{g_1,g_2}$ is a subgraph of G_1. By grafting of edges operations (if required), we can form a new graph G_2 from G_1 where G_2 is a connected graph on n vertices obtained by attaching paths to different vertices of $C^p_{g_1,g_2}$. Then by Corollary 5.1.4, $W(G_2) \geqslant W(G_1)$. If there are paths attached to more than one vertices of $C^p_{g_1,g_2}$ in G_2, then using the graph operation as mentioned in Lemma 5.1.7, form a new graph G_3 from G_2, where G_3 has exactly one path attached to $C^p_{g_1,g_2}$. Then by Lemma 5.1.7, $W(G_3) \geqslant W(G_2)$.

Let u be the vertex on $C^p_{g_1,g_2}$ of G_3 at which the path is attached. Then we have two cases:

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

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

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

Let H_1 be the induced subgraph of G_3 containing the vertices $\{V(G_3) \backslash V(U^l_{p,g_1})\} \cup \{w\}$. Clearly H_1 is the cycle C_{g_2}. Then identify the vertex v of U^l_{p,g_1} with the vertex w of H_1 to form a new graph G_4. By Corollary 5.2.10, $W(G_4) > W(G_3)$ and G_4 is the graph $C^n_{g_1,g_2}$. By Corollary 5.2.12, $W(G) < W(G_4) \leqslant W(C^n_{3,3})$.

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

Let H_2 be the induced subgraph of G_3 containing the vertices $V(G_3) \setminus V(U^l_{p,g_1})$. In G_3 exactly one vertex $w_1 \in U^l_{p,g_1}$ adjacent to exactly one vertex w_2 of H_2. Form a new graph G_5 from G_3 by deleting the edge $\{w_1, w_2\}$ and adding the edge $\{v, w_2\}$. By Corollary 5.2.10, $W(G_5) > W(G_3)$ and G_5 is the graph $C^n_{g_1,g_2}$. Again by Corollary 5.2.12, we have $W(G) < W(G_5) \leqslant W(C^n_{3,3})$.

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

Let w be the pendant vertex of G_3 and let w_3 be a vertex on $C^p_{g_1,g_2}$ of G_3 adjacent to u. Form a new graph G_6 from G_3 by deleting the edge $\{u, w_3\}$ and adding the edge $\{w, w_3\}$. By Corollary 5.2.10, $W(G_6) > W(G_3)$ and G_6 is the graph $C^n_{g_1,g_2}$. Again by Corollary 5.2.12, we have $W(G) < W(G_6) \leqslant W(C^n_{3,3})$. Hence $C^n_{3,3}$ uniquely maximizes the Wiener index over $\mathfrak{H}_{n,0}$ for $n \geqslant 7$.

By (5.2.1), we have $W(C^n_{3,3}) = \frac{n^3-13n+24}{6}$. This completes the proof.

$\square$

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

Proof of Theorem 5.2.3: (i) Let $G \in \mathfrak{H}_{n,k}$, $0 \leqslant k \leqslant n-3$ and let $v_1, v_2, \ldots, v_{n-k}$ be the non-pendant vertices of G. Suppose G is not isomorphic to P^k_n. If the induced subgraph $G[v_1, v_2, \ldots, v_{n-k}]$ is complete, then name G as G', otherwise, form G' from G by joining all the non-adjacent non-pendant vertices of G with new edges. Then $G' \in \mathfrak{H}_{n,k}$ and by Lemma 5.1.1, $W(G') \leqslant W(G)$ (equality holds if and only if $G' \cong G$). If $G' \cong P^k_n$ then $W(P^k_n) < W(G)$. Otherwise, G' has at least two vertices of degree greater than or equal to $n-k$. Form a new graph G'' from G' by moving all the pendant vertices to one of the vertex $v_1, v_2, \ldots, v_{n-k}$. Then $G'' \cong P^k_n$ and by Corollary 5.1.6, $W(P^k_n) = W(G'') < W(G') \leqslant W(G)$. Hence for $0 \leqslant k \leqslant n-3$, P^k_n uniquely minimizes the Wiener index over $\mathfrak{H}_{n,k}$.

Let $u \in V(P^k_n)$ be the vertex of degree $n-1$. Then by Lemma 5.1.2, we have

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

(ii) Let $G \in \mathfrak{H}_{n,n-2}$. Suppose G is not isomorphic to $T(1, n-3, 2)$. Then G is isomorphic to a tree $T(k, l, 2)$ for some $k, l \geqslant 2$. Now form the tree $T(1, n-3, 2)$ from G by moving all but one pendant vertices from one end of P_2 to the other end. Then by Corollary 5.1.6, $W(T(1, n-3, 2)) < W(G)$ and by taking $d = 2, l = 1$ and $k = n - 3$ in (5.1.6), we have $W(T(1, n-3, 2)) = n^2 - n - 2$.

□

Proof of Theorem 5.2.4. The path P_n is the only tree in $\mathfrak{T}_{n,2}$ and hence the result is true for $k = 2$. So, assume $3 \leqslant k \leqslant n-3$ and let T be the tree with minimum Wiener index in $\mathfrak{T}_{n,k}$.

Claim: There is a unique vertex v in T with $deg(v) \geqslant 3$.

Let there be two vertices $u, v \in V(T)$ with $deg(u) = n_1 \geqslant 3$, $deg(v) = n_2 \geqslant 3$. Let $N_T(u) = \{u_1, u_2, \ldots, u_{n_1}\}$ and $N_T(v) = \{v_1, v_2, \ldots, v_{n_2}\}$ where u_1 and v_1 lie on the path joining u and v (u_1 may be v and v_1 may be u). Let T_1 be the largest subtree of T containing $u, u_2, u_3, \ldots, u_{n_1-1}$ but not u_1, u_{n_1} and T_2 be the largest subtree of T containing $v, v_2, v_3, \ldots, v_{n_2-1}$ but not v_1, v_{n_2}. We rename the vertices $u \in V(T_1)$ and $v \in V(T_2)$ by u' and v', respectively. Let H be the connected component of $T \setminus \{u_2, u_3, \ldots, u_{n_1-1}, v_2, v_3, \ldots, v_{n_2-1}\}$ containing u and v. Then H, T_1 and T_2 are trees with at least two vertices each. Construct two trees T' and T'' from H, T_1 and T_2 by identifying the vertices u, u', v' and v, u', v', respectively. Clearly both $T', T'' \in \mathfrak{T}_{n,k}$ and by Lemma 5.1.5, either $W(T') < W(T)$ or $W(T'') < W(T)$, which is a contradiction. This proves the claim.

So, the connected components of $T - v$ are all paths and $deg(v) = k$. Suppose $T \ncong T_{n,k}$. Then there exist two paths $P : vv_1 \cdots v_{l_1}$ and $Q : uu_1 \cdots u_{l_2}$ attached at v in T with $|l_1 - l_2| = \alpha \geqslant 2$. By grafting an edge operation, we can construct a tree $\tilde{T}$ from T such that the difference of the lengths between P and Q in $\tilde{T}$ is $\alpha - 1$. Then by Corollary 5.1.4, $W(\tilde{T}) < W(T)$, which is a contradiction. So, $T_{n,k}$ is the only tree which minimizes the Wiener index over $\mathfrak{T}_{n,k}$. □

For $r = 0$, $n = kq + 1$ and hence by (5.1.8),

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

For $1 \leqslant r < k$, by Lemma 5.1.2, we have

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

where v is the vertex of $T_{n,k}$ with $T_{n,k} - v = rP_{q+1} \cup (k-r)P_q$. Thus by using (5.1.7) and (5.1.8) the value of $W(T_{n,k})$ can be obtained.

5.3 Graphs with fixed number of cut vertices

We denote the set of all connected graphs on n vertices with s cut vertices by $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. Any graph on n vertices has at most $n-2$ cut vertices. The path P_n is the only graph on n vertices with $n-2$ cut vertices. Hence for $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$, we consider $0 \leqslant s \leqslant n-3$. Let $\mathfrak{C}^{\mathfrak{t}}_{\mathfrak{n},\mathfrak{s}}$ be the set of all trees on n vertices with s cut vertices. In a tree, every vertex is either a pendant vertex or a cut vertex. So, $\mathfrak{C}^{\mathfrak{t}}_{\mathfrak{n},\mathfrak{s}} = \mathfrak{T}_{n,n-s}$. Hence the next result follows from Proposition 5.2.1 and Theorem 5.2.4.

Theorem 5.3.1. *For $0 \leqslant s \leqslant n-3$, the tree $T(\lfloor \frac{n-s}{2} \rfloor, \lceil \frac{n-s}{2} \rceil, s)$ uniquely maximizes the Wiener index and the tree $T_{n,n-s}$ uniquely minimizes the Wiener index over $\mathfrak{C}^{\mathfrak{t}}_{\mathfrak{n},\mathfrak{s}}$.*

For $2 \leqslant m \leqslant n$, let $v_1, v_2, \ldots, v_m$ be the vertices of the complete graph K_m. For $i = 1, 2, \ldots, m$ consider the paths P_{l_i}, $l_i \geqslant 1$ such that $l_1 + l_2 + \cdots + l_m = n$. By identifying a pendant vertex of the path P_{l_i} with the vertex v_i (if $l_i = 1$, then identify the single vertex with v_i), for $i = 1, 2, \ldots, m$, we obtain a graph on n vertices with $n-m$ cut vertices. We denote this graph by $K^n_m(l_1, l_2, \ldots, l_m)$. In this section, we obtain the graph which minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. We prove the following result.

Theorem 5.3.2. *For $0 \leqslant s \leqslant n-3$, the graph $K_{n-s}^{n}(l_1, l_2, \ldots, l_{n-s})$ with $|l_i - l_j| \leqslant 1$ for all $i, j \in \{1, 2, \ldots, n-s\}$ uniquely minimizes the Wiener index over $\mathfrak{C}_{n,s}$.*

To prove our result, we develop some theory about the Wiener index of graphs in $\mathfrak{C}_{n,s}$. First we recall the definition of the block graph of a graph.

Let G be a graph. The *block graph* B_G of G is the graph with $V(B_G)$ as the set of blocks of G and two vertices of B_G are adjacent whenever the corresponding blocks in G contain a common cut vertex of G. We call a block B in G, a *pendant block* if there is exactly one cut vertex of G in B. The block corresponding to a central vertex in B_G is called a *central block* of G. Two blocks in G are said to be *adjacent blocks* if they share a common cut vertex.

Lemma 5.3.3. *Let G be a graph which minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. Then every block of G is a complete graph.*

Proof. Let B be a block of G which is not complete. Then there are at least two non adjacent vertices in B. Let u and v be two non adjacent vertices in B. Form a new graph G' from G by joining the edge $\{u, v\}$. Clearly $G' \in \mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$ and by Lemma 5.1.1, $W(G') < W(G)$, which is a contradiction. $\square$

Lemma 5.3.4. *Let G be a graph which minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. Then every cut vertex of G is shared by exactly two blocks.*

Proof. Let c be a cut vertex in G shared by more than two blocks say $B_1, B_2, \ldots, B_k$, $k \geqslant 3$. Construct a new graph G' from G by joining all the non adjacent vertices of $\bigcup_{i=2}^{k} B_i$. Then $G' \in \mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$ and by Lemma 5.1.1, $W(G') < W(G)$, which is a contradiction. $\square$

Lemma 5.3.5. *Let $m \geqslant 3$. For $i, j \in \{1, 2, \ldots, m\}$, if $l_i \leqslant l_j - 2$, then*

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

Proof. Let u be the pendant vertex of $K_m^n(l_1, \ldots, l_i+1, \ldots, l_j-1, \ldots, l_m)$ on the path P_{l_i+1} and v be the pendant vertex of $K_m^n(l_1, \ldots, l_i, \ldots, l_j, \ldots, l_m)$ on the path P_{l_j}. Let w_1 and w_2 be the vertices adjacent to u and v, respectively. Then using Lemma 5.1.2 we have

$$\begin{aligned} &W(K_m^n(l_1, \ldots, l_i + 1, \ldots, l_j - 1, \ldots, l_m)) - W(K_m^n(l_1, \ldots, l_i, \ldots, l_j, \ldots, l_m)) \\ &= D_{K_m^{n-1}(l_1, \ldots, l_i, \ldots, l_j - 1, \ldots, l_m)}(w_1) - D_{K_m^{n-1}(l_1, \ldots, l_i, \ldots, l_j - 1, \ldots, l_m)}(w_2) < 0, \end{aligned}$$

since $l_i < l_j - 1$ and $m \geqslant 3$. □

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

Lemma 5.3.6. *Let G be a graph which minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. If $s \geqslant 2$, then every pendant block of G is K_2.*

Proof. By Lemma 5.3.3, all the blocks in G are complete. Suppose B is a pendant block of G which is not K_2. Let $V(B) = \{v_1, v_2, \ldots, v_m\}$ with $m \geqslant 3$. Assume v_1 is the cut vertex of G in B which is shared by another block B' with $V(B') = \{v_1 = u_1, u_2, \ldots, u_r\}$ and $r \geqslant 2$. Construct a new graph G' from G as follows: Delete the edges $\{v_2, v_j\}, j = 3, 4, \ldots, m$ and add the edges $\{v_j, u_i\}, j = 3, 4, \ldots, m$ and $i = 2, 3, \ldots r$. When G changes to G' the only type of distances which increase are $d(v_2, v_j)$, $j = 3, 4, \ldots, m$. Each such distance increases by one and hence the total increment in distances for v_j, $j = \{3, \ldots, m\}$ is exactly $m-2$. The distance $d(v_j, u_i), j = 3, 4, \ldots, m; i = 2, 3, \ldots r$ decreases by one. Since $r \geqslant 2$, the total distance decreases by such pair of vertices is at least $m-2$. Since $s \geqslant 2$ there exists a vertex w belonging to some other block B'' such that $d(v_j, w), j = 3, 4, \ldots m$ decreases by one. So $W(G') < W(G)$, which is a contradiction. □

Lemma 5.3.7. *Let G be a graph which minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. If $s \geqslant 2$ then all non-central blocks of G are K_2.*

Proof. Since G minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$, by Lemma 5.3.3 and Lemma 5.3.6, all blocks of G are complete and all pendant blocks are K_2. Assume that G has a non-pendant non-central block which is not K_2. By Lemma 5.3.4, every cut vertex of G is shared by exactly two blocks. Let B be a central block in G. Let B_1 be a non-central non-pendant block with at least 3 vertices and a cut vertex (of G) $c_1 \in V(B_1)$ such that a path P_l is attached to B_1 at c_1. Since B_1 is a non-pendant block, so there is a cut vertex (of G) $c_2 \in V(B_1)$ different from c_1, shared by another block B_2 such that the vertices corresponding to the blocks B_1, B_2 and B (starting from B_1) in the tree B_G lie on a path.

Let $V(B_1) = \{c_1 = u_1, u_2, \ldots, u_{m_1} = c_2\}$ and $V(B_2) = \{v_1, v_2, \ldots, v_{m_2} = c_2\}$. Construct a new graph G' from G as follow: Delete the edges $\{c_1, u_i\}$ for all $u_i \in V(B_1) \setminus \{c_1, c_2\}$ and add the edges $\{u_i, v_j\}$ for all $u_i \in V(B_1) \setminus \{c_1, c_2\}$ and $v_j \in V(B_2) \setminus \{c_2\}$.

For $i = 2, \ldots, m_1 - 1$, let H_i be the maximal connected component of G containing exactly one vertex u_i of B_1. Let $P_l : t_1 t_2 \cdots t_l$ be the path with t_1 identified with c_1. When G changes to G', the only type of distances which increase in G' are $d_{G'}(u, t_j)$ where $u \in \bigcup_{i=2}^{m_1-1} V(H_i)$ and $j = 1, 2, \ldots, l$. Each such distance increases by one in G'. For any other pair of vertices, the distance between them either decreases or remains the same. Since B_1 is not a central block, for each $t_j, j = 1, 2, \ldots, l$ there exists a vertex $t'_j \in V(G) \setminus \left(\bigcup_{i=2}^{m_1-1} V(H_i) \cup \{t_1, t_2, \ldots, t_l, v_1, v_2, \ldots, v_{m_2}\}\right)$ such that $d_{G'}(u, t'_j)$ decreases by one where $u \in \bigcup_{i=2}^{m_1-1} V(H_i)$. So, the increment in distances by the pairs u, t_j are neutralized by the pairs u, t'_j. Apart from this, at least the distances $d_{G'}(u_i, v_j)$ for $i = 2, 3, \ldots, m_1 - 1$ and $j = 1, 2, \ldots, m_2 - 1$ decreases by one. So $W(G') < W(G)$, which is a contradiction. Hence for $s \geqslant 2$, all non-central blocks of G are K_2. $\square$

Proof of Theorem 5.3.2: Let G be a graph which minimizes the Wiener index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$.

Claim: $G \cong K^n_{n-s}(l_1, \ldots, l_{n-s})$ for some $l_1, l_2, \ldots, l_{n-s}$.

By Lemma 5.3.3 and Lemma 5.3.4, every block of G is complete and every cut vertex of G is shared by exactly two blocks.

If $s = 0$, then G has exactly one block. So $G \cong K_n \cong K^n_n(1, 1, \cdots, 1)$.

If $s = 1$, then G has exactly two complete blocks with a common vertex w (say). Let B_1 and B_2 be the two blocks of G. If any of B_1 or B_2 is K_2 then $G \cong K^n_{n-1}(2, 1, \ldots, 1)$. Suppose neither of B_1 or B_2 is complete. Then $|V(B_1)|, |V(B_2)| \geqslant 3$. Let $V(B_1) = \{u_1, u_2, \ldots, u_{m_1} = w\}$ and $V(B_2) = \{v_1, v_2, \ldots, v_{m_2} = w\}$ with $m_1, m_2 \geqslant 3$. Construct a new graph G' from G as follow: Delete the edges $\{u_1, u_i\}, i = 2, 3, \ldots, m_1 - 1$ and add the edges $\{u_i, v_j\}, i = 2, 3, \ldots, m_1 - 1; j = 1, 2, \ldots, m_2 - 1$. Clearly $G' \in \mathfrak{C}_{\mathfrak{n},1}$. Then, the only type of distances which increase are $d(u_1, u_j), j = 2, 3, \ldots u_{m_1-1}$ and each such distance increases by one. So total increment in distance is exactly $m_1 - 2$. Also each distance $d(u_i, v_j),\ i = 2, 3, \ldots, m_1 - 1; j = 2, 3, \ldots m_2 - 1$ decreases by one. The total decrement is $(m_1 - 2)(m_2 - 1)$. Since $m_1, m_2 \geqslant 3$, so $W(G') < W(G)$, which is a contradiction. Hence $G \cong K^n_{n-1}(2, 1, \ldots, 1)$.

If $s \geqslant 2$, then G has $s + 1$ blocks and also G has either one central block or two adjacent central blocks. By Lemma 5.3.7, all non-central blocks of G are K_2. If G has exactly one central block, then $G \cong K^n_{n-s}(l_1, \ldots, l_{n-s})$ for some $l_1, l_2, \ldots, l_{n-s}$. Suppose G has two central blocks and G is not isomorphic to $K^n_{n-s}(l_1, \ldots, l_{n-s})$ for any $l_1, l_2, \ldots, l_{n-s}$. Then each of the central blocks of G has at least 3 vertices. Let B_1 and B_2 be the two central blocks with a common vertex w. Let $V(B_1) = \{u_1, u_2, \ldots, u_{m_1} = w\}$ and $V(B_2) = \{v_1, v_2, \ldots, v_{m_2} = w\}$ with $m_1, m_2 \geqslant 3$. Let $H_1(H_2)$ be the maximal connected component of G containing exactly one vertex w of $B_2(B_1)$. Let $P_l : wu_1t_3 \cdots t_l$ be the longest path in H_1 starting at w containing u_1 such that non of the vertices $t_3, \ldots, t_l$ belong to B_1. Take w as t_1 and u_1 as t_2 in P_l. Since B_1 and B_2 are central blocks, so there exists a path $P'_l : t'_1t'_2 \cdots t'_l$ on l vertices in H_2 starting at $w = t'_1$ and containing exactly two vertices of B_2. Construct a new graph G' from G as follow: Delete the edges $\{u_1, u_i\}, i = 2, 3, \ldots, m_1 - 1$ and add the edges $\{u_i, v_j\}, i = 2, 3, \ldots, m_1 - 1; j = 1, 2, \ldots, m_2 - 1$. Clearly $G' \in \mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. The only type of distances which increase in G' are $d_{G'}(u, t_j)$ where $u \in V(H_1) \setminus V(P_l)$ and $j = 2, \ldots, l$ also each such distance increases by one. The distance $d_{G'}(u, t'_j)$ decreases by one where $u \in V(H_1) \setminus V(P_l)$ and $j = 2, \ldots, l$. So, the increment in distances by the pairs $\{u, t_j\}$ are neutralized by the pairs $\{u, t'_j\}$. Since $m_2 \geqslant 3$, there exist at least one vertex w' in B_2 which is not in P'_l. For each $u \in V(H_1) \setminus V(P_l)$, the distance $d_{G'}(u, w')$ decreases by one. So, $W(G') < W(G)$, which is a contradiction. Hence $G \cong K^n_{n-s}(l_1, \ldots, l_{n-s})$ for some $l_1, l_2, \ldots, l_{n-s}$. This proves the claim.

Suppose $|l_i - l_j| \geqslant 2$ for some $i, j \in \{1, 2, \ldots n - s\}$. Without loss of generality assume that $l_1 \leqslant l_2 - 2$. Then, by Lemma 5.3.5, $W(K^n_{n-s}(l_1 + 1, l_2 - 1, \ldots, l_{n-s})) < W(K^n_{n-s}(l_1, l_2, \ldots, l_{n-s}))$, which is a contradiction. So, $|l_i - l_j| \leqslant 1$ for all $i, j \in \{1, 2, \ldots, n - s\}$ and this completes the proof. □

5.4 Future works

Though the Wiener index is the oldest known graphical index, there are still some classes of graphs in which the graphs maximizing or minimizing the Wiener index are not known. Over graphs with fixed number of cut vertices, we only obtained the graph which minimizes the Wiener index. In this class, the graph which maximizes the Wiener index is still unknown. Further, it is observed that, in the study of the extremal problems for many classes of graphs, the Wiener index has a reverse correlation with the subgraph index. But in [38], the authors have given an example of two trees T_1 and T_2 such that $W(T_1) > W(T_2)$ and $F(T_1) > F(T_2)$. A detailed study may be needed to say anything concretely regarding the relation between the Wiener index and the subgraph index of graphs.

Chapter 6

The total eccentricity index of a graph

In this chapter, we obtain the graphs which maximize the total eccentricity index over graphs with fixed number of pendant vertices and the graphs which minimize the total eccentricity index over graphs with fixed number of cut vertices. Further, over graphs with s cut vertices, we obtain the graphs maximizing the total eccentricity index for $s = 0, 1, n-3, n-2$ and propose a conjecture for $2 \leqslant s \leqslant n-4$.

6.1 Some preliminary results

The following lemma is straightforward which shows the effect of a new edge on the total eccentricity index of a graph.

Lemma 6.1.1. *Let u and v be two non-adjacent vertices of a graph G. Let G' be the graph obtained from G by joining u and v with an edge. Then $\varepsilon(G) \geqslant \varepsilon(G')$.*

Lemma 6.1.2 ([18], Theorem 2.1 and [40], Lemma 4.5)**.** *Let $G_{k,l}$ be the graph defined in Section 4.1. If $1 \leqslant k \leqslant l$, then $\varepsilon(G_{k-1,l+1}) > \varepsilon(G_{k,l})$.*

In a graph G, a vertex u is called an eccentric vertex of v if $e(v) = d(v, u)$. In the following lemma, we compare the total eccentricity index of two graphs, where one graph is obtained from the other by some graph perturbation.

Lemma 6.1.3. *Consider two connected graphs H_1 and H_2 with $|V(H_1)|, |V(H_2)| \geqslant 2$ and a path $P : v_1v_2 \cdots v_d$ with $d \geqslant 2$. Suppose $u \in V(H_1)$ and $v \in V(H_2)$. Let G be the graph obtained from H_1, H_2 and P by identifying the vertices u and v with v_1 and let G' be the graph obtained from H_1, H_2 and P by identifying the vertices u with v_1 and v with v_d (See Figure 6.1). Then $\varepsilon(G') > \varepsilon(G)$.*

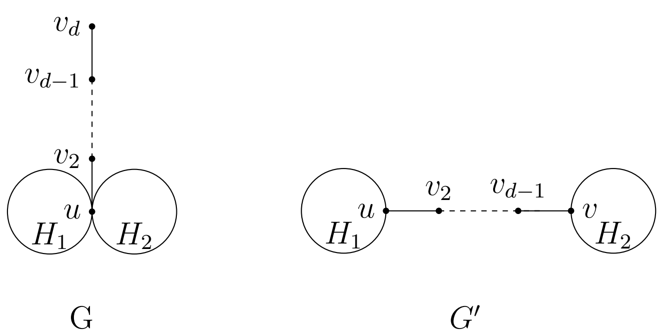


Figure 6.1: The graphs G and G'

Proof. Let $x, y \in V(H_1)$. Then from the construction of both G and G' (see Figure 6.1), it is clear that the length of all the shortest paths between x and y remain unchanged in both G and G'. So, $d_{G'}(x, y) = d_G(x, y)$. Similarly, for any two vertices either in H_2 or in P, the distance between them remain unchanged in both G and G'. Now take one vertex in H_i, $i = 1, 2$ and the other vertex is in P. Without loss of generality, suppose $z \in V(H_1)$ and $w \in V(P)$. Then

$$\begin{aligned} d_{G'}(z,w) &= d_{G'}(z,u) + d_{G'}(u,w) \\ &= d_G(z,u) + d_G(u,w) \\ &= d_G(z,w). \end{aligned}$$

Finally suppose $a \in V(H_1)$ and $b \in V(H_2)$. Then $d_{G'}(a,b) = d_{G'}(a,u) + d_{G'}(u,v) + d_{G'}(v,b) > d_{G'}(a,u) + d_{G'}(v,b) = d_G(a,u) + d_G(u,b) = d_G(a,b)$. So, while moving from G to G', the eccentricity of each vertex either increases or remains same. Now it is enough to find a vertex x_0 belong to both $V(G)$ and $V(G')$ such that $e_{G'}(x_0) > e_G(x_0)$.

Without loss of generality, take $diam(H_1) = D_1 \geqslant diam(H_2) = D_2$. Let $x_0 \in V(H_2)$ be a vertex farthest from v. Then $d_{H_2}(x_0, v) \geqslant \frac{D_2}{2}$. Similarly, there exists $y_0 \in V(H_1)$ farthest from u such that $d_{H_1}(y_0, u) \geqslant \frac{D_1}{2}$. Then $d_G(x_0, y_0) = d_G(x_0, u) + d_G(u, y_0) \geqslant D_2$. So, an eccentric vertex of x_0 in G lies outside H_2. Therefore, $e_G(x_0) = d_G(x_0, v_d)$ or $e_G(x_0) = d_G(x_0, y_0)$. But $e_{G'}(x_0) = d_{G'}(x_0, v) + d_{G'}(v, u) + d_{G'}(u, y_0) > e_G(x_0)$. Hence $\varepsilon(G') > \varepsilon(G)$. □

Corollary 6.1.4 ([11], Corollary 1 and [40], Proposition 4.3)**.** *Among all trees on n vertices, the total eccentricity index is maximised by the path and minimised by the star.*

An easy calculation gives $\varepsilon(K_{1,n-1}) = 2n-1$ and $\varepsilon(P_n) = \lfloor \frac{3n^2-2n}{4} \rfloor$. Since $\varepsilon(K_n) = n$, so for any connected graph G with n vertices,

$$n \leqslant \varepsilon(G) \leqslant \left\lfloor \frac{3n^2-2n}{4} \right\rfloor.$$

Lemma 6.1.5. *Let B and B' be two blocks in G. Suppose $d(B,B')$ is maximum among all pairs of blocks in G. Then both B and B' are pendant blocks.*

Proof. Suppose B is not a pendant block. Then B contains at least two cut vertices of G. Let u and v be two cut vertices of G in B such that $d(B, B') = d(\{u\}, B')$. Since v is a cut vertex of G there exists a block B'' (other than B and B') containing v. Then $d(B'', B') = d(\{v\}, B') = d(v, u) + d(\{u\}, B') > d(B, B')$, which is a contradiction. Hence B is a pendant block of G. Similarly, we can show that B' is also a pendant block of G. □

Lemma 6.1.6. *Let B be a block in G. Suppose $|V(B)| = r \geqslant 3$ and at most one vertex of B is a cut vertex in G. Let G' be the graph obtained from G by replacing B with the cycle C_r. Then $\varepsilon(G') \geqslant \varepsilon(G)$.*

Proof. Since $|V(B)| \geqslant 3$ and B is a block in G, so B must contain a cycle. Let $x \in V(G)$ and y be an eccentric vertex of x in G.

First suppose G has no cut vertex. Then $G = B$ and $G' = C_r$. Let $C_l : v_1v_2 \dots v_lv_1$ be a largest cycle in B. Since G has no cut vertex, so there exists a cycle C_k containing both x and y. As C_l is a largest cycle of G, so $k \leqslant l$. Therefore, $e_G(x) \leqslant \lfloor \frac{k}{2} \rfloor \leqslant \lfloor \frac{l}{2} \rfloor \leqslant \lfloor \frac{r}{2} \rfloor$. But the eccentricity of any vertex of G' is $\lfloor \frac{r}{2} \rfloor$. Hence the result follows for this case.

Now suppose $w \in V(B)$ is the cut vertex in G. Let $C_m : wv_2 \dots v_mw$ be a largest cycle in B containing w. Delete the vertices of B not in C_m and insert those $r - m$ vertices between $v_{\lceil \frac{m}{2} \rceil}$ and $v_{\lceil \frac{m}{2} \rceil + 1}$ to form G' from G. Let $S = (V(G) \setminus V(B)) \cup \{w\} \subseteq V(G)$. Since $(V(G) \setminus V(B)) \cup \{w\} = (V(G') \setminus V(C_r)) \cup \{w\}$ so $S \subseteq V(G')$.

First suppose $x \in S \subseteq V(G)$. If $y \in S$ then $e_G(x) = d_G(x, y) = d_{G'}(x, y) \leqslant e_{G'}(x)$. If $y \in V(G) \setminus S$, then $e_G(x) = d_G(x, y) = d_G(x, w) + d_G(w, y) \leqslant d_{G'}(x, w) + \lfloor \frac{r}{2} \rfloor = e_{G'}(x)$.

Now suppose $x \in V(G) \setminus S = V(G') \setminus S$. If $y \in V(G) \setminus S$, $e_G(x) = d_G(x, y) \leqslant$

$\lfloor \frac{r}{2} \rfloor \leqslant e_{G'}(x)$. If $y \in S$, then $e_G(x) = d_G(x,y) = d_G(x,w) + d_G(w,y)$. In G', if $x \in \{v_2, \ldots, v_m\}$ then $d_G(x,w) \leqslant d_{G'}(x,w)$ and hence $e_G(x) = d_G(x,w) + d_G(w,y) \leqslant d_{G'}(x,w) + d_{G'}(w,y) = d_{G'}(x,y) \leqslant e_{G'}(x)$. In G', if $x \notin \{v_2, \ldots, v_m\}$ then $d_{G'}(x,w) \geqslant \lfloor \frac{m}{2} \rfloor$. Since C_m is the largest cycle in B containing w, so $d_G(x,w) \leqslant \lfloor \frac{m}{2} \rfloor \leqslant d_{G'}(x,w)$. Therefore, $e_G(x) = d_G(x,w) + d_G(w,y) \leqslant d_{G'}(x,w) + d_{G'}(w,y) = d_{G'}(x,y) \leqslant e_{G'}(x)$. This completes the proof. $\square$

6.2 Graphs with fixed number of pendant vertices

As in previous chapters, we take $0 \leqslant k \leqslant n-2$ and $n \geqslant 4$. Note that all the elements of $\mathfrak{H}_{n,n-2}$ are of the form $T_{l,n-l-2,2}$, where $1 \leqslant l \leqslant n-3$. It is easy to check that the total eccentricity index of $T_{l,n-l-2,2}$ is same for any l, $1 \leqslant l \leqslant n-3$. So, we take $0 \leqslant k \leqslant n-3$.

We are familiar with the tree $T_{n,k}$. Here we define a new tree belonging to $\mathfrak{T}_{n,k}$. For $k \geqslant 2$ with $k|n-2$, let $T^t_{n,k}$ be the tree having two adjacent vertices u and v with degree $t+1$ and $k-t+1$, respectively, such that $T^t_{n,k} - u - v = kP_{\frac{n-2}{k}}$. Note that $T^t_{n,k} \in \mathfrak{T}_{n,k}$.

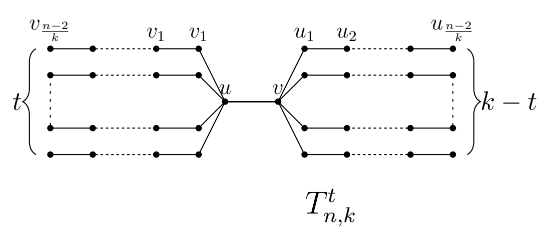


Figure 6.2: The tree $T^t_{n,k}$

In [40], the authors have studied the total eccentricity index (in terms of average eccentricity) of trees over $\mathfrak{T}_{n,k}$ and proved the following results.

Proposition 6.2.1 ([40], Proposition 4.7). *Let $T \in \mathfrak{T}_{n,k}$. Then*

$$\varepsilon(T) \leqslant \varepsilon(T(l, k-l, n-k)), \quad \textit{for any } 1 \leqslant l \leqslant k-1,$$

and

$$\varepsilon(T) \geqslant \begin{cases} \varepsilon(T_{n,k}) & \textit{if } k \nmid n-2, \\ \varepsilon(T^t_{n,k}) & \textit{if } k \mid n-2, \end{cases} \quad \textit{for any } 1 \leqslant t \leqslant k-1.$$

Since $\varepsilon(P_n)$ is known, the value of $\varepsilon(T(l, m, d))$ can be easily calculated. We have

$$\varepsilon(T(l, k-l, n-k)) = \left\lfloor \frac{3n^2 - k^2 - 2nk + 2(n+k)}{4} \right\rfloor.$$

The values of $\varepsilon(T_{n,k})$ and $\varepsilon(T^t_{n,k})$ are given in [40].

In [41] and [50], the authors have studied the total eccentricity index (in terms of average eccentricity) of unicyclic graphs and proved the following results.

Proposition 6.2.2 ([41], Theorem 3.3 and [50], Theorem 2.3). *Let H be a unicyclic graph on $n \geqslant 5$ vertices. Then*

$$2n - 1 \leqslant \varepsilon(H) \leqslant \left\lfloor \frac{3n^2 - 4n - 3}{4} \right\rfloor.$$

Furthermore, the left equality happens if and only if $H \cong U^p_{n,3}$ and the right equality happens if and only if $H \cong U^l_{n,3}$.

The authors have proved the Proposition 6.2.2 for $n \geqslant 6$. A simple calculation shows that the result is also true for $n = 5$. So, we modified the statement in Proposition 6.2.2 by taking $n \geqslant 5$. It is clear that K_n uniquely minimizes the total eccentricity index over $\mathfrak{H}_{n,0}$. For $1 \leqslant k \leqslant n-3$, we have the following result due to Tang and West.

Theorem 6.2.3 ([42], Theorem 3.4). *Let $G \in \mathfrak{H}_{n,k}$, $n \geqslant 3$ and $1 \leqslant k \leqslant n-3$, . Then $\varepsilon(G) \geqslant 2n-1$ and the equality happens if $G \cong P_n^k$.*

Now we prove some lemmas to prove the corresponding maximization result over $\mathfrak{H}_{n,k}$.

Lemma 6.2.4. *Let H be a graph with at least two vertices and $u \in V(H)$. Let G be the graph obtained by joining an edge between u and the pendant vertex of $U_{r,g}^l$ with $g \geqslant 4$. Let G' be the graph obtained by joining an edge between u and the pendant vertex of $U_{r,3}^l$. Then $\varepsilon(G) < \varepsilon(G')$.*

Proof. Let $V(U_{r,g}^l) = \{v_1, v_2, \ldots, v_r\}$ where $v_1 v_2 \cdots v_{r-g}$ is the path P_{r-g}, $v_{r-g+1}v_{r-g+2} \cdots v_r v_{r-g+1}$ is the cycle C_g and v_{r-g} is adjacent to v_{r-g+1}. We form G' from G by naming the vertices of $U_{r,3}^l$ as following: $v_1 v_2 \cdots v_{r-3}$ is the path P_{r-3}, $v_{r-2}v_{r-1}v_r v_{r-2}$ is the cycle C_3 and v_{r-3} is adjacent to v_{r-2}. Note that $V(G) = V(G')$. We will prove that for any $v \in V(G) = V(G')$, $e_G(v) \leqslant e_{G'}(v)$ and strict inequality occurs for atleast one vertex.

Suppose $v \in V(G) = V(G')$. Let v' be an eccentric vertex of v in G. Following are the three cases.

Case-I: $v \in V(H)$.

If $v' \in V(H)$, then $e_G(v) = d_G(v, v') = d_{G'}(v, v') \leqslant e_{G'}(v)$. If $v' \notin V(H)$, then v_{r-1} is an eccentric vertex of v in G'. So, $e_G(v) = d_G(v, v') = d_G(v, u) + d_G(u, v') \leqslant d_{G'}(v, u) + r - 1 = e_{G'}(v)$.

Case-II: $v \in \{v_1, v_2, \cdots, v_{r-1}\}$.

We have $d_G(v_i, u) \leqslant d_{G'}(v_i, u)$ for $1 \leqslant i \leqslant r-1$. If $v' \in V(H)$, then $e_G(v) = d_G(v, v') = d_G(v, u) + d_G(u, v') \leqslant d_{G'}(v, u) + d_{G'}(u, v') = d_{G'}(v, v') \leqslant e_{G'}(v)$. If

$v' \notin V(H)$, then v' is in the cycle C_g. So,

$$e_G(v_i) = \begin{cases} r-g-i+1+\lfloor \frac{g}{2} \rfloor & \text{if } 1 \leqslant i \leqslant r-g, \\ \lfloor \frac{g}{2} \rfloor & \text{if } r-g+1 \leqslant i \leqslant r-1. \end{cases}$$

Thus, for $1 \leqslant i \leqslant r-g$, v_{r-1} is an eccentric vertex of v_i in G'. So, we have $e_G(v_i) = r-g-i+1+\lfloor \frac{g}{2} \rfloor = r-i-(g-\lfloor \frac{g}{2} \rfloor -1) \leqslant r-i-1 = e_{G'}(v_i)$. The last inequality holds since $g \geqslant 4$. For $r-g+1 \leqslant i \leqslant r-1$, $e_G(v_i) = \lfloor \frac{g}{2} \rfloor \leqslant e_{G'}(v_i)$, since v_i lies on a path in G' of length at least g.

Case-III: $v = v_r$.

Let z be a vertex of H farthest from u. In this case, $e_G(v_r) = \max\{r-g+2+d(u,z), \lfloor \frac{g}{2} \rfloor\}$. Since $g \geqslant 4$ so $r-1 > \max\{r-g+2, \lfloor \frac{g}{2} \rfloor\}$ and hence $e_G(v_r) < r-1+d(u,z) = e_{G'}(v_r)$.

Therefore, $\varepsilon(G) < \varepsilon(G')$ and this completes the proof. $\square$

Lemma 6.2.5. *For $n \geqslant 7$, $\varepsilon(C^n_{3,3}) > \varepsilon(C_n)$.*

Proof. We have

$$\varepsilon(P_n) = \begin{cases} \frac{3n^2-2n}{4} & \text{if } n \text{ is even,} \\ \frac{3n^2-2n-1}{4} & \text{if } n \text{ is odd,} \end{cases}$$

and it is easy to check that

$$\varepsilon(C_n) = \begin{cases} \frac{n^2}{2} & \text{if } n \text{ is even,} \\ \frac{n^2-n}{2} & \text{if } n \text{ is odd.} \end{cases}$$

Also

$$\varepsilon(C^n_{3,3}) = \varepsilon(P_{n-2}) + 2(n-3).$$

So,

$$\varepsilon(C^n_{3,3}) = \begin{cases} \frac{3}{4}n^2 - \frac{3}{2}n - 2 & \text{if } n \text{ is even,} \\ \frac{3}{4}n^2 - \frac{3}{2}n - \frac{9}{4} & \text{if } n \text{ is odd.} \end{cases}$$

Hence

$$\varepsilon(C^n_{3,3}) - \varepsilon(C_n) = \begin{cases} \frac{n^2}{4} - \frac{3}{2}n - 2 & \text{if } n \text{ is even,} \\ \frac{n^2}{4} - n - \frac{9}{4} & \text{if } n \text{ is odd.} \end{cases}$$

$$> 0, \text{ for } n \geqslant 7.$$

□

Lemma 6.2.6. *Let $m_1, m_2 \geqslant 3$ and $n = m_1+m_2-1$. For $n \geqslant 7$, $\varepsilon(C^n_{3,3}) > \varepsilon(C^n_{m_1,m_2})$.*

Proof. Without loss of generality assume that $m_1 \leqslant m_2$. As $n \geqslant 7$, so $m_2 \geqslant 4$. If $m_2 = 4$, then $C^n_{m_1,m_2} = C^7_{4,4}$ and $\varepsilon(C^7_{4,4}) = 22 < 24 = \varepsilon(C^n_{3,3})$.

Suppose $n \geqslant 8$. Then $m_2 \geqslant 5$. Let $C_{m_2} : v_1v_2 \cdots v_{m_2}v_1$ be the subgraph of $C^n_{m_1,m_2}$ with $\deg(v_1) = 4$. Delete the edge $\{v_{\lceil \frac{m_2}{2} \rceil}, v_{\lceil \frac{m_2}{2} \rceil+1}\}$ from $C^n_{m_1,m_2}$ to get a new graph G. By Lemma 6.1.1, $\varepsilon(C^n_{m_1,m_2}) \leqslant \varepsilon(G)$. Note that in G there are two paths ($v_1v_2 \ldots v_{\lceil \frac{m_2}{2} \rceil}$ and $v_1v_{m_2} \ldots v_{\lceil \frac{m_2}{2} \rceil+1}$) attached at v_1 each of length at least 2. By grafting of edges operation we can get a new graph G' from G where G' is the graph in which two paths, one of length 1 and other of length $m_2 - 2$ are attached at a vertex v_1 of C_{m_1}. Then by Lemma 6.1.2, $\varepsilon(G) < \varepsilon(G')$.

Let $P : v_1v_2$ and $P' : v_1v_{m_2}v_{m_2-1} \cdots v_3$ be the paths attached at v_1 in G'. Observe that if v_2 is an eccentric vertex of some $x \in V(G')$ then $m_1 = 3$ and the two vertices of C_3 other than v_1 are also the eccentric vertices of x. So, we will not consider v_2 as an eccentric vertex of any vertex of G'. Construct a new graph G'' from G' by deleting the edge $\{v_1, v_2\}$ and adding the edges $\{v_2, v_4\}$ and $\{v_2, v_3\}$.

For any $x \in V(G') \setminus \{v_2\}$, $e_{G'}(x) = e_{G''}(x)$. Let $w \in V(C_{m_1})$ be a vertex farthest from v_1. Then $e_{G''}(v_2) = d_{G''}(v_2, v_1) + d_{G''}(v_1, w) = m_2 - 2 + d_{G''}(v_1, w) = m_2 - 2 + d_{G'}(v_1, w) \geqslant \max\{m_2 - 1, 1 + d_{G'}(v_1, w)\} = e_{G'}(v_2)$ and hence $\varepsilon(C^n_{m_1,m_2}) < \varepsilon(G') \leqslant \varepsilon(G'')$. Note that $G'' \cong C^n_{m_1,3}$. If $m_1 \geqslant 4$, then the result follows from Lemma 6.2.4. □

We now prove the maximization result on the total eccentricity index over $\mathfrak{H}_{n,k}$.

Theorem 6.2.7. *Let $G \in \mathfrak{H}_{n,k}$ and $0 \leqslant k \leqslant n-3$. Then*

(i) for $2 \leqslant k \leqslant n-3$, $\varepsilon(G) \leqslant \left\lfloor \dfrac{3n^2 - k^2 - 2nk + 2(n+k)}{4} \right\rfloor$ and equality is attained by the trees $T(l, k-l, n-k)$ for any $1 \leqslant l \leqslant k-1$.

(ii) for $k = 1$, $\varepsilon(G) \leqslant \left\lfloor \frac{3n^2-4n-3}{4} \right\rfloor$ and equality holds if and only if $G \cong U^l_{n,3}$.

(iii) For $n \geqslant 7$ and $k = 0$, $\varepsilon(G) \leqslant \left\lfloor \frac{3n^2-6n-8}{4} \right\rfloor$ and equality holds if and only if $G \cong C^n_{3,3}$.

Proof. (i) Suppose $G \ncong T(l, k-l, n-k)$ for any $1 \leqslant l \leqslant k-1$. If G is not a tree, construct a spanning tree G' from G by deleting some edges. If G is a tree, then take G' same as G. By Lemma 6.1.1, $\varepsilon(G) \leqslant \varepsilon(G')$. While constructing G' from G, the number of pendant vertices may increase in G'. Suppose G' has more than k pendant vertices. Since $k \geqslant 2$, G' has at least one vertex of degree greater than 2 and at least two paths attached to it. Consider a vertex v of G' with $deg(v) \geqslant 3$ and two paths P_{l_1}, P_{l_2}, $l_1 \geqslant l_2$ attached at v. Using grafting of edges operation on G', we get a new tree $\tilde{G}$ with number of pendant vertices one less than the number of pendant vertices of G' and by Lemma 6.1.2, $\varepsilon(G') < \varepsilon(\tilde{G})$. Continue this process till we get a tree with k pendant vertices from $\tilde{G}$. By Lemma 6.1.2, every step in this process the total eccentricity index will increase. So, we will reach at a tree T of order n with k pendant vertices. If

G' has k pendant vertices then take T as G'. Thus $\varepsilon(G') \leqslant \varepsilon(T)$. By Proposition 6.2.1, $\varepsilon(T) \leqslant \varepsilon(T(l, k-l, n-k))$ for any $1 \leqslant l \leqslant k-1$. Now the result follows as $\varepsilon(T(l, k-l, n-k)) = \left\lfloor \dfrac{3n^2 - k^2 - 2nk + 2(n+k)}{4} \right\rfloor$ for any $1 \leqslant l \leqslant k-1$.

(ii) Suppose G is not isomorphic to $U^l_{n,3}$. Since G is connected and has exactly one pendent vertex, it must contain a cycle. Let C_g be a cycle in G. If G is a unicyclic graph then by Proposition 6.2.2, $\varepsilon(G) \leqslant \lfloor \frac{3n^2-4n-3}{4} \rfloor$ with equality if and only if $G \cong U^l_{n,3}$. If G has more than one cycle, then construct a new graph G' from G by deleting edges from all cycles other than C_g, so that the graph remains connected and $G' \ncong U^l_{n,3}$. Then, by Lemma 6.1.1, $\varepsilon(G) \leqslant \varepsilon(G')$ and G' is a unicyclic graph on n vertices with girth g. By Proposition 6.2.2, $\varepsilon(G) \leqslant \varepsilon(G') \leqslant \lfloor \frac{3n^2-4n-3}{4} \rfloor$ and equality holds if and only if $G \cong U^l_{n,3}$.

(iii) Let $G \ncong C^n_{3,3}$. First suppose G has no cut vertex. Then G has exactly one block, which is G itself. By Lemma 6.1.6, $\varepsilon(G) \leqslant \varepsilon(C_n)$ and the result follows from Lemma 6.2.5.

Now suppose G has at least one cut vertex. Then G has at least two blocks. Let H_1 and H_2 be two blocks such that distance between them is maximum among all pair of blocks in G. Suppose $|V(H_1)| = n_1$ and $|V(H_2)| = n_2$.

First suppose $d(H_1, H_2) = 0$. Then there is exactly one cut vertex w in G and every block is a pendant block with at least 3 vertices. Replace each block by a cycle on same number of vertices to get a new graph G'. Then by Lemma 6.1.6, $\varepsilon(G) \leqslant \varepsilon(G')$. If there are exactly two cycles in G', then the result follows by Lemma 6.2.6. If there are more than two cycles in G', then keep two cycles say C_{n_1} and C_{n_2} unchanged and from all other cycles delete an edge with an end point w to get a new graph G''. Clearly $\varepsilon(G'') \geqslant \varepsilon(G)$ but number of pendant vertices in G'' is more than that of G. If there are more than one path attached at w in G'', then sequentially apply grafting an edge operation to G'' to obtain a new graph $\tilde{G}$ such that $\tilde{G}$ has exactly one path attached at w. If exactly one path is attached at w in G', then take $\tilde{G}$ as G''. By Lemma 6.1.2, $\varepsilon(\tilde{G}) \geqslant \varepsilon(G'')$. Note that $\tilde{G} \in \mathfrak{H}_{n,1}$ and is isomorphic to the graph obtained by identifying a vertex x of C_{n_1}, a vertex y of C_{n_2} and a pendant vertex z of the path $P_{n+2-n_1-n_2}$. Let v be the pendant vertex of $\tilde{G}$. Construct a new graph $\bar{G}$ from $\tilde{G}$ by identifying x with v and y with z. Then $\bar{G}$ has zero pendant vertex and by Lemma 6.1.3, $\varepsilon(\bar{G}) > \varepsilon(\tilde{G})$. Now the result follows from Lemma 6.2.4.

Now suppose $d(H_1, H_2) \geqslant 1$. Replace the blocks (if required) H_1 and H_2 by two cycles C_{n_1} and C_{n_2} respectively to form a new graph G' from G. Clearly $G' \in \mathfrak{H}_{n,0}$ and by Lemma 6.1.6, $\varepsilon(G') \geqslant \varepsilon(G)$. If G' is isomorphic to $C^n_{n_1,n_2}$ then the result follows from Lemma 6.2.4. Otherwise, there must be some blocks in G' other than C_{n_1} and C_{n_2} with at least three vertices. Remove edges say $\{e'_1, \ldots, e'_p\}$ from all such blocks to form a new graph G'' such that G'' is connected and there are no cycles other than C_{n_1} and C_{n_2}. We can choose the edges $\{e'_1, \ldots, e'_p\}$ such that G'' is not isomorphic to $C^n_{n_1,n_2}$. Then by Lemma 6.1.1, $\varepsilon(G'') \geqslant \varepsilon(G')$.

Let $P : v_1 v_2 \ldots v_k$ be the path in G'' joining C_{n_1} and C_{n_2} where $v_1 \in V(C_{n_1})$ and $v_k \in V(C_{n_2})$. Let v_0 and v'_0 be the two vertices on C_{n_1} adjacent with v_1, and let v_{k+1} and v'_{k+1} be the two vertices on C_{n_2} adjacent with v_k. Consider the edges $e_i = \{v_i, v_{i+1}\}$ for $i = 1, 2, \ldots, k-1$,$e_0 = \{v_1, v_0\}$, $e'_0 = \{v_1 v'_0\}$, $e_k = \{v_k, v_{k+1}\}$ and $e'_k = \{v_k, v'_{k+1}\}$ in G''.

Since $G'' \ncong C^n_{n_1,n_2}$ and contains exactly two cycles there are some non trivial trees attached at v_i for some $i = 1, 2, \ldots, k$. Let T_i be the tree attached at v_i for $i = 1, 2, \ldots, k$. Note that for $i = 2, \ldots, k-1$, T_i is the component containing

v_i in $G'' \setminus \{e_{i-1}, e_{1+1}\}$, T_1 is the component containing v_1 in $G'' \setminus \{e_1, e_0, e'_0\}$ and T_k is the component containing v_k in $G'' \setminus \{e_{k-1}, e_k, e'_k\}$.

Suppose some T_i's, $i = 1, \ldots, k$ are neither trivial trees nor paths with v_i as a pendant vertex. Then form $\tilde{G}$ from G'' by sequentially applying grafting of edges operations on those trees such that all T_i, $i = 1, \ldots, k$ become paths with v_i as a pendant vertex. If all T_i, $i = 1, \ldots, k$ are either trivial or paths with v_i as a pendant vertex then take $\tilde{G}$ as G''. By Lemma 6.1.2, $\varepsilon(\tilde{G}) \geqslant \varepsilon(G'')$.

Let v_i be the vertex nearest to v_1 in $\tilde{T}$ such that $deg(v_i) \geqslant 3$ (strict inequality occurs only when $v_i = v_1$ or v_k, in these cases $d(v_i) = 4$) and suppose w_i is the pendant vertex of the path P_i attached at v_i. If $v_i = v_1$, delete the edge $\{v_1, v_2\}$ and add the edge $\{w_1, v_2\}$ and if $v_i \neq v_1$, then delete the edge $\{v_i, v_{i-1}\}$ and add the edge $\{v_{i-1}, w_i\}$. Repeat this till $\deg(v_1) = \deg(v_k) = 3$ and $\deg(v_i) = 2$ for $i = 2, \ldots, k-2$. . This way we get the graph $C^n_{n_1,n_2}$ from $\tilde{G}$ and by Lemma 6.1.3, $\varepsilon(C_{n_1,n_2}) > \varepsilon(\tilde{G})$. Now the result follows from Lemma 6.2.4.

□

For $3 \leqslant n \leqslant 6$, it can be easily checked that C_n uniquely maximizes the total eccentricity index over $\mathfrak{H}_{n,0}$.

6.3 Graphs with fixed number of cut vertices

Since every tree with s cut vertices has $n-s$ pendant vertices, so the next result follows from Proposition 6.2.1.

Theorem 6.3.1. *Let $T \in \mathfrak{C}^{\mathfrak{t}}_{\mathfrak{n},\mathfrak{s}}$. Then*

$$\varepsilon(T) \leqslant \varepsilon(T(l, n-l-s, s)), \quad \textit{for any } 1 \leqslant l \leqslant n-s-1,$$

and

$$\varepsilon(T) \geqslant \begin{cases} \varepsilon(T_{n,n-s}) & \text{if } (n-s) \nmid n-2, \\ \varepsilon(T^t_{n,n-s}) & \text{if } (n-s) \mid n-2, \end{cases} \quad \text{for any } 1 \leqslant t \leqslant n-s-1.$$

We now study the problems of finding the graphs which minimize or maximize the total eccentricity index over $\mathfrak{C}_{\mathfrak{n},\mathfrak{s}}$. Let $K^n_m(l_1, l_2, \ldots, l_m)$ with $l_i \geqslant 1$, for $i = 1, 2, \ldots, m$ be the graph defined in Section 5.3.

Lemma 6.3.2. *Let $m \geqslant 2$ and $l_k = \max\{l_1, l_2, \ldots, l_m\}$. Suppose $l_j \leqslant l_k - 2$, for some $j \in \{1, \ldots, l_{k-1}, l_{k+1}, \ldots, l_m\}$. Then $\varepsilon(K^n_m(l_1, l_2, \ldots, l_j + 1, \ldots, l_k - 1, \ldots, l_m)) \leqslant \varepsilon(K^n_m(l_1, l_2, \ldots, l_m))$.*

Proof. Let $G = K^n_m(l_1, l_2, \ldots, l_m)$. Let $P_{l_j} : u_1u_2 \cdots u_{l_j}$ and $P_{l_k} : w_1w_2 \cdots w_{l_k}$ be the paths in G such that $\deg(u_1) = \deg(w_1) = 1, u_{l_j} = v_j$ and $w_{l_k} = v_k$. Delete the edge $\{w_1, w_2\}$ and add the edge $\{u_1, w_1\}$ in G to form a new graph G'. Clearly $G' \cong K^n_m(l_1, l_2, \ldots, l_j + 1, \ldots, l_k - 1, \ldots, l_m)$.

If $m = 2$ then $G \cong P_{l_k+l_j} \cong G'$ and so $\varepsilon(G') = \varepsilon(G)$. Therefore, assume $m \geqslant 3$. Let $S_1 = \{w_1, w_2, \ldots, w_{l_k} = v_k, u_1, \ldots, u_{l_j} = v_j\}$ and $S_2 = V(G) \setminus S_1 = V(G') \setminus S_1$. So, $S_1 \cap S_2 = \emptyset$ and $S_1 \cup S_2 = V(G) = V(G')$. We show that, while moving to G' from G, the eccentricity of every vertex decreases or remains the same. Suppose $v \in V(G) = V(G')$. Following are the two cases.

Case-I: $v \in S_2$

Since $l_k = \max\{l_1, l_2, \ldots, l_m\}$, for any $v \in S_2$, w_1 is an eccentric vertex of v in G. Then, $e_G(v) = d_G(v, w_1)$ and $e_{G'}(v)$ is either $d_{G'}(v, w_2) = d_G(v, w_2)$ or $d_{G'}(v, w_2) + 1$. So we get, $e_G(v) \geqslant e_{G'}(v)$ for $v \in S_2$.

Case-II: $v \in S_1$

Let $l_q = \max\{l_1, \ldots, l_{k-1}, l_{k+1}, \ldots, l_m\}$ and let z be the pendant vertex of G associated with P_{l_q}. Since $l_k \geqslant l_j + 2$ so $l_q \geqslant l_j$. First consider $l_q > l_j$. Then $e_G(v) = d_G(v, w_1)$ or $d_G(v, z)$.

<u>Subcase-I:</u> $e_G(v) = d_G(v, w_1)$

Then $v \neq w_1$ and $d_G(v, z) \leqslant d_G(v, w_1)$. Since $l_q > l_j$, so $e_{G'}(v) = d_{G'}(v, w_2)$ or $d_{G'}(v, z)$. But $d_{G'}(v, w_2) = d_G(v, w_2) < d_G(v, w_1) = e_G(v)$ and $d_{G'}(v, z) = d_G(v, z) \leqslant d_G(v, w_1) = e_G(v)$. So, $e_{G'}(v) \leqslant e_G(v)$.

<u>Subcase-II:</u> $e_G(v) = d_G(v, z)$

If $v = w_1$, then $d_{G'}(w_1, w_2) = d_G(w_1, u_1) < d_G(w_1, z)$. We have $e_{G'}(w_1) = d_{G'}(w_1, w_2) < d_G(w_1, z) = e_G(w_1)$ or $e_{G'}(w_1) = d_{G'}(w_1, z) = l_j + l_q < l_k - 1 + l_q = d_G(w_1, z) = e_G(w_1)$. If $v \neq w_1$ then a similar argument as in Subcase-I will give $e_{G'}(v) \leqslant e_G(v)$.

Now consider $l_q = l_j$. Then either w_1 or u_1 is an eccentric vertex of v in G. Also in G' either w_2 or w_1 is an eccentric vertex of v. Let A_1 be the $w_1 - u_1$ path in G and let A_2 be the $w_2 - w_1$ path in G'. Then $|V(A_1)| = |V(A_2)| = l_k + l_j$. So $\sum_{v \in S_1} e_G(v) = \varepsilon(P_{l_k + l_j}) = \sum_{v \in S_1} e_{G'}(v)$.

Hence from Case-I and Case-II, $\varepsilon(G') \leqslant \varepsilon(G)$ and this completes the proof. □

Corollary 6.3.3. *Let $G \cong K^n_{n-s}(l_1, l_2, \ldots, l_{n-s})$ for some $l_1, l_2, \ldots, l_{n-s}$. Then, $\varepsilon(K^n_{n-s}(l'_1, l'_2, \ldots, l'_{n-s})) \leqslant \varepsilon(G)$, where $|l'_i - l'_j| \leqslant 1$ for every $i, j \in \{1, 2, \ldots, n-s\}$.*

We now count $\varepsilon(K^n_{n-s}(l_1, l_2, \ldots, l_{n-s}))$ where $|l_i - l_j| \leqslant 1$ for every $i, j \in \{1, 2, \ldots, n-s\}$. Let $q = \lfloor \frac{n}{n-s} \rfloor$ and take $r = n-(n-s)q$. Then $0 \leqslant r < n-s$. Observe that K_{n-s} is a subgraph of $K^n_{n-s}(l_1, l_2, \ldots, l_{n-s})$ and $K^n_{n-s}(l_1, l_2, \ldots, l_{n-s}) \setminus E(K_{n-s}) \cong rP_{q+1} \cup (n-s-r)P_q$. We may consider P_q and P_{q+1} as $P_q : u_1 u_2 \cdots u_q$ and $P_{q+1} : w_1 w_2 \cdots w_{q+1}$, respectively, where u_1 and w_1 are pendant vertices in $K^n_{n-s}(l_1, l_2, \ldots, l_{n-s})$.

If $r = 0$, then $q = \frac{n}{n-s}$ and $K^n_{n-s}(l_1, l_2, \ldots, l_{n-s}) \setminus E(K_{n-s}) \cong (n-s)P_q$. So,

$$\begin{aligned}
\varepsilon(K_{n-s}^{n}(l_1,l_2,\ldots,l_{n-s})) &= (n-s)\sum_{i=1}^{q} e_{K_{n-s}^{n}(l_1,l_2,\ldots,l_{n-s})}(u_i)\\
&= (n-s)\sum_{i=1}^{q}(2q-i)\\
&= q(3q-1)\left(\frac{n-s}{2}\right)\\
&= \left(\frac{n}{n-s}\right)\left(\frac{3n}{n-s}-1\right)\left(\frac{n-s}{2}\right)\\
&= \frac{n(2n+s)}{2(n-s)}.
\end{aligned}$$

If $r=1$ then $K_{n-s}^{n}(l_1,l_2,\ldots,l_{n-s})\setminus E(K_{n-s})\cong P_{q+1}\cup(n-s-1)P_q$. So

$$\begin{aligned}
\varepsilon(K_{n-s}^{n}(l_1,l_2,\ldots,l_{n-s})) &= \sum_{j=1}^{q+1} e_{K_{n-s}^{n}(l_1,l_2,\ldots,l_{n-s})}(w_j)+(n-s-1)\sum_{i=1}^{q} e_{K_{n-s}^{n}(l_1,l_2,\ldots,l_{n-s})}(u_i)\\
&= \sum_{j=1}^{q+1}(2q+1-j)+(n-s-1)\sum_{i=1}^{q}(2q+1-i)\\
&= (n-s)\sum_{i=1}^{q}(2q+1-i)+q\\
&= \frac{q}{2}\left[3(n-s)q+(n-s+2)\right].
\end{aligned}$$

If $r\geqslant 2$ then $K_{n-s}^{n}(l_1,l_2,\ldots,l_{n-s})\setminus E(K_{n-s})\cong rP_{q+1}\cup(n-s-r)P_q$. So

$$\begin{aligned}
\varepsilon(K_{n-s}^{n}(l_1,l_2,\ldots,l_{n-s})) &= r\sum_{j=1}^{q+1} e_{K_{n-s}^{n}(l_1,l_2,\ldots,l_{n-s})}(w_j)+(n-s-r)\sum_{i=1}^{q} e_{K_{n-s}^{n}(l_1,l_2,\ldots,l_{n-s})}(u_i)\\
&= r\sum_{j=1}^{q+1}(2q+2-j)+(n-s-r)\sum_{i=1}^{q}(2q+1-i)\\
&= (n-s)\sum_{i=1}^{q}(2q+1-i)+2rq+r\\
&= \frac{1}{2}\left[2r(2q+1)+q(3q+1)(n-s)\right].
\end{aligned}$$

This leads to the following Lemma.

Lemma 6.3.4. *Let* $0 \leqslant s \leqslant n-2$. *Then*

$$\varepsilon(K^n_{n-s}(l_1, l_2, \ldots, l_{n-s})) = \begin{cases} \frac{n(2n+s)}{2(n-s)} & \text{if } r = 0 \\ \frac{q}{2}\left(3(n-s)q + (n-s+2)\right) & \text{if } r = 1 \\ \frac{1}{2}\left[2r(2q+1) + q(3q+1)(n-s)\right] & \text{if } r \geqslant 2, \end{cases}$$

where $q = \lfloor \frac{n}{n-s} \rfloor$ *and* $r = n - (n-s)q$.

We will now prove the main result of this section regarding minimization .

Theorem 6.3.5. *Let* $0 \leqslant s \leqslant n-2$ *and* $G \in \mathfrak{C}_{n,s}$. *Then* $\varepsilon(K^n_{n-s}(l'_1, l'_2, \ldots, l'_{n-s})) \leqslant \varepsilon(G)$, *where* $|l'_i - l'_j| \leqslant 1$ *for every* $i, j \in \{1, 2, \ldots, n-s\}$.

Proof. Let $G \in \mathfrak{C}_{n,s}$ and let H be the graph $K^n_{n-s}(l'_1, l'_2, \ldots, l'_{n-s})$ where $|l'_i - l'_j| \leqslant 1$ for every $i, j \in \{1, 2, \ldots, n-s\}$. If $G \cong K^n_{n-s}(l_1, l_2, \ldots, l_{n-s})$ for some $l_1, l_2, \ldots, l_{n-s}$ then by Corollary 6.3.3, $\varepsilon(H) \leqslant \varepsilon(G)$.

Suppose $G \ncong K^n_{n-s}(l_1, l_2, \ldots, l_{n-s})$ for any $l_1, l_2, \ldots, l_{n-s}$. If some blocks, say $B_1, B_2, \ldots, B_l$ of G are not complete, then form a new graph G_1 from G by joining the non-adjacent vertices of each B_i, $1 \leqslant i \leqslant l$ with edges such that each block of G_1 becomes complete, otherwise take G_1 as G. Observe that $G_1 \in \mathfrak{C}_{n,s}$ and by Lemma 6.1.1, $\varepsilon(G_1) \leqslant \varepsilon(G)$. If $s = 0$, then $G \cong K_n \cong K^n_n(1, 1, \ldots, 1)$ and the result follows.

Suppose $s \geqslant 1$. Then every cut vertex of G_1 is shared by at least two blocks. If w is a cut vertex of G_1 and $C_1, C_2, \ldots, C_k$ with $k \geqslant 3$ are the blocks sharing the vertex w, then join every pair of non adjacent vertices of $\bigcup_{i=2}^{k} V(C_i)$ by an edge. Repeat this for each cut vertex of G_1 which is shared by more than two blocks. This way we get a new graph G_2. If every cut vertex of G_1 is shared by exactly two blocks then take G_2 as G_1. Clearly $G_2 \in \mathfrak{C}_{n,s}$ and by Lemma 6.1.1, $\varepsilon(G_2) \leqslant \varepsilon(G_1)$. Note that G_2

is a graph in which, every block is complete and every cut vertex is shared by exactly two blocks. If $G_2 \cong K_{n-s}^n(l_1, l_2, \dots, l_{n-s})$, for some $l_1, l_2, \dots, l_{n-s}$ then by Corollary 6.3.3, $\varepsilon(H) \leqslant \varepsilon(G_2)$ and the result follows.

Suppose G_2 is not isomorphic to $K_{n-s}^n(l_1, l_2, \dots, l_{n-s})$ for any $l_1, l_2, \dots, l_{n-s}$. We further consider two cases depending on whether $s = 1$ or $s \geqslant 2$.

First suppose $s = 1$. Then G_2 has exactly two complete blocks with a common cut vertex w. Let B_1 and B_2 be the two blocks of G_2 with $V(B_1) = \{u_1, u_2, \dots, u_{m_1} = w\}$ and $V(B_2) = \{v_1, v_2, \dots, v_{m_2} = w\}$ with $m_1, m_2 \geqslant 3$. Construct a new graph G_2' from G_2 as follow: Delete the edges $\{u_1, u_i\}, i = 2, 3, \dots, m_1 - 1$ and add the edges $\{u_i, v_j\}, i = 2, 3, \dots, m_1 - 1; j = 1, 2, \dots, m_2 - 1$. Then $V(G_2') = V(G_2)$ and G_2' is isomorphic to $K_{n-1}^n(2, 1, \dots, 1)$. Note that $e_{G_2'}(w) = e_{G_2}(w) = 1$ and for $x \in V(G_2') \setminus w = V(G_2) \setminus w$, $e_{G_2'}(x) = e_{G_2}(x) = 2$. So $\varepsilon(G_2') = \varepsilon(G_2)$ and the result follows.

Now suppose $s \geqslant 2$. Then G_2 has $s + 1$ blocks and B_{G_2}, the block graph of G_2 is a tree. So G_2 has either one central block or two adjacent central blocks and at least one non central block. Let C be a central block in G_2. Suppose P is a longest path in G_2. Then P passes through exactly two vertices of C. Suppose B_1 is a non central block in G_2 which is not isomorphic to K_2. Then $|V(B_1)| \geqslant 3$. Let $b \in V(B_1)$ be a cut vertex of G_2 such that $d(B_1, C) = d(b, c)$, where $c \in V(C)$ is a cut vertex of G_2. Let B_2 be the block adjacent to B_1 sharing the cut vertex b with B_1 (B_2 may be same as C). Let $V(B_1) = \{b = v_1, v_2, \dots v_{m_1}\}$ and $V(B_2) = \{b = u_1, u_2, \dots, u_{m_2}\}$. If P passes through B_1, then P also passes through B_2. So, P must contain b and some other vertex of B_1, say v_2. Construct a new graph G_2' from G_2 by deleting the edges $\{v_2, v_i\}$ $i = 3, 4, \dots m_1$ and adding the edges $\{v_i, u_j\}$ $i = 3, 4, \dots, m_1, j = 2, 3, \dots, m_2$. If P does not pass through B_1, we can chose any vertex of B_1 in place of v_2. Clearly $G_2' \in \mathfrak{C}_{n,s}$ and the number of blocks in G_2' is same as the number of blocks in G_2.

Note that P is still a longest path in G_2'. So, the block corresponding to C in G_2' is still a central block in G_2'. We will now show that $\varepsilon(G_2') \leqslant \varepsilon(G_2)$.

Let $v \in V(G_2) = V(G_2')$ and let v' be an eccentric vertex of v in G_2 lies on the longest path P. Since P is a longest path in both G_2 and G_2', so v' is also an eccentric vertex of v in G_2'. Thus we have $d_{G_2'}(v,v') \leqslant d_{G_2}(v,v')$. So, $e_{G_2'}(v) = d_{G_2'}(v,v') \leqslant d_{G_2}(v,v') = e_{G_2}(v)$ and hence $\varepsilon(G_2') \leqslant \varepsilon(G_2)$.

If G_2' has some non central block which is not isomorphic to K_2, then repeat the same process until we get a graph in which all the non central blocks are K_2. Name the new graph as $\tilde{G}$. Note that (as we have shown while moving to G_2' from G_2) in each intermediate step between G_2 and $\tilde{G}$, the block corresponding to C is the central block in each step and the total eccentricity index decreases or remains the same. If all the non central blocks of G_2 are isomorphic to K_2 then take G_2 as $\tilde{G}$. So $\varepsilon(\tilde{G}) \leqslant \varepsilon(G_2)$.

If $\tilde{G}$ has exactly one central block then it is isomorphic to $K^n_{n-s}(l_1, l_2, \ldots, l_{n-s})$ for some positive integers $l_1, l_2, \ldots, l_{n-s}$ and the result follows from Corollary 6.3.3.

Suppose $\tilde{G}$ has two adjacent central blocks C and C' sharing the cut vertex z. Let $V(C) = \{x_1, x_2, \ldots, x_s = z\}$ and $V(C') = \{y_1, y_2, \ldots, y_t = z\}$. Since P is a longest path of $\tilde{G}$, it must contain a vertex , say x_1 of C different from z. Construct a new graph $\bar{G}$ from $\tilde{G}$ by deleting the edges $\{x_1, x_i\}$, $2 \leqslant i \leqslant s-1$ and adding the edges $\{x_i, y_j\}$ $2 \leqslant i \leqslant s-1; 1 \leqslant j \leqslant t-1$. For $v \in V(\tilde{G}) = V(\bar{G})$, the shortest path between v and its eccentric vertex (both for $\tilde{G}$ and $\bar{G}$) passes through z, so $e_{\tilde{G}}(v) = e_{\bar{G}}(v)$. Hence $\varepsilon(\bar{G}) = \varepsilon(\tilde{G}_2)$. Note that $\bar{G}$ is isomorphic to $K^n_{n-s}(l_1, l_2, \ldots, l_{n-s})$ for some $l_1, l_2, \ldots, l_{n-s}$. So the result follows from Corollary 6.3.3. $\square$

We will now study about the graphs which maximize the total eccentricity index over $\mathfrak{C}_{n,s}$. We have the following theorem for $s = 0$.

Theorem 6.3.6. *Let $n \geqslant 3$ and $G \in \mathfrak{C}_{n,0}$. Then $\varepsilon(G) \leqslant n\lfloor \frac{n}{2} \rfloor$ and equality happens if $G \cong C_n$.*

Proof. Since $s = 0$, so G has exactly one block and the result follows from Lemma 6.1.6. $\square$

We will now find a graph which maximizes the total eccentricity index over $\mathfrak{C}_{n,1}$. To obtain the graph, the following lemma is very useful.

Lemma 6.3.7. *Let H be a graph with at least two vertices and $w \in V(H)$. Let G be the graph obtained from H, C_{m_1} and C_{m_2} by identifying w, a vertex of C_{m_1} and a vertex of C_{m_2}. Let G' be the graph obtained from H and $C_{m_1+m_2-1}$ by identifying w with a vertex of $C_{m_1+m_2-1}$. Then $\varepsilon(G') \geqslant \varepsilon(G)$.*

Proof. Consider the following labelling of vertices of C_{m_1}, C_{m_2} and $C_{m_1+m_2-1}$:

$$C_{m_1} : wu_1 \cdots u_{\lfloor \frac{m_1}{2} \rfloor} u_{\lfloor \frac{m_1}{2} \rfloor + 1} \cdots u_{m_1-1}w,$$

$$C_{m_2} : wv_1 \cdots v_{\lfloor \frac{m_2}{2} \rfloor} v_{\lfloor \frac{m_2}{2} \rfloor + 1} \cdots v_{m_2-1}w$$

and

$$C_{m_1+m_2-1} : wu_1 \cdots u_{m_1-1}v_{m_2-1}v_{m_2-2} \cdots v_1w.$$

Let $v \in V(G) = V(G')$ and v' be an eccentric vertex of v in G. Let $h \in V(H)$ such that $d(h, w) = \max\{d(x, w) : x \in V(H)\}$. Without loss of generality, assume that $m_1 \geqslant m_2$. We now consider the following cases.

Case I: $d(w, h) > \lfloor \frac{m_1}{2} \rfloor$

Suppose $v \in V(G) \backslash V(H) = \{u_1, u_2, \ldots, u_{m_1-1}, v_1, v_2, \ldots, v_{m_2-1}\}$. Then we can take v' as h and so $d_{G'}(v, h) = d_{G'}(v, w) + d_{G'}(w, h) \geqslant d_G(v, w) + d_G(w, h) = d_G(v, h) = e_G(v)$. This implies $e_{G'}(v) \geqslant e_G(v)$.

Now suppose $v \in V(H)$. Then either $v' \in V(H)$ or $v' = u_{\lfloor \frac{m_1}{2} \rfloor}$. If $v' \in V(H)$, then $d_{G'}(v, v') = d_G(v, v') = e_G(v)$. This implies $e_{G'}(v) \geqslant e_G(v)$. If $v' = u_{\lfloor \frac{m_1}{2} \rfloor}$, then $d_{G'}(v, v') = d_{G'}(v, u_{\lfloor \frac{m_1}{2} \rfloor}) = d_{G'}(v, w) + d_{G'}(w, u_{\lfloor \frac{m_1}{2} \rfloor}) = d_G(v, w) + d_G(w, u_{\lfloor \frac{m_1}{2} \rfloor}) = d_G(v, v') = e_G(v)$. This implies $e_{G'}(v) \geqslant e_G(v)$. Thus $\varepsilon(G') \geqslant \varepsilon(G)$.

Case II: $d(w, h) \leqslant \lfloor \frac{m_1}{2} \rfloor$

Suppose $v \in V(H)$. For any $z \in V(H)$, $d_G(v, z) \leqslant d_G(v, w) + d_G(w, z) \leqslant d_G(v, w) + \lfloor \frac{m_1}{2} \rfloor = d_G(v, u_{\lfloor \frac{m_1}{2} \rfloor})$. Therefore, we can take v' as $u_{\lfloor \frac{m_1}{2} \rfloor}$ and so the eccentric vertices of v in G' are in $C_{m_1+m_2-1}$. Therefore, $e_{G'}(v) = d_{G'}(v, w) + \lfloor \frac{m_1+m_2-1}{2} \rfloor > d_G(v, w) + \lfloor \frac{m_1}{2} \rfloor = e_G(v)$. This implies $e_{G'}(v) \geqslant e_G(v) + 1$ for all $v \in V(H)$.

Now suppose $v \in V(G) \setminus V(H)$. If $v' \in V(H)$, we can choose $v' = h$ and in this case $d_{G'}(v, v') = d_{G'}(v, w) + d_{G'}(w, h) \geqslant d_G(v, w) + d_G(w, v') = d_G(v, v') = e_G(v)$. This implies $e_{G'}(v) \geqslant e_G(v)$. If $v' \in V(G) \setminus V(H)$ then we have two subcases.

<u>Subcase I:</u> At least one of m_1 or m_2 is odd

In this case, $e_G(v) \leqslant \lfloor \frac{m_1}{2} \rfloor + \lfloor \frac{m_2}{2} \rfloor \leqslant \lfloor \frac{m_1+m_2-1}{2} \rfloor \leqslant e_{G'}(v)$.

<u>Subcase II:</u> Both m_1 and m_2 are even

Suppose $v \in \{u_1, u_2, \ldots, u_{m_1-1}, v_1, v_2, \ldots, v_{m_2-1}\} \setminus \{u_{\frac{m_1}{2}}, v_{\frac{m_2}{2}}\}$. Then $d_G(v, v') \leqslant \frac{m_1}{2} + \frac{m_2}{2} - 1$ and $e_{G'}(v) \geqslant \lfloor \frac{m_1+m_2-1}{2} \rfloor = \frac{m_1+m_2-2}{2} = \frac{m_1}{2} + \frac{m_2}{2} - 1 \geqslant d_G(v, v') = e_G(v)$.

For $v \in \{u_{\frac{m_1}{2}}, v_{\frac{m_2}{2}}\}$, $e_G(v) = \frac{m_1+m_2}{2}$. We have

$$e_{G'}(u_{\frac{m_1}{2}}) \geqslant \left\lfloor \frac{m_1 + m_2 - 1}{2} \right\rfloor = \frac{m_1 + m_2}{2} - 1 = e_G(u_{\frac{m_1}{2}}) - 1$$

and

$$e_{G'}(v_{\frac{m_2}{2}}) \geqslant \left\lfloor \frac{m_1 + m_2 - 1}{2} \right\rfloor = \frac{m_1 + m_2}{2} - 1 = e_G(v_{\frac{m_2}{2}}) - 1.$$

As $|V(H)| \geqslant 2$, there exists $w' \in V(H)$ different from w such that

$$\begin{aligned} e_{G'}(u_{\frac{m_1}{2}}) + e_{G'}(v_{\frac{m_2}{2}}) + e_{G'}(w) + e_{G'}(w') &\geqslant e_G(u_{\frac{m_1}{2}}) - 1 + e_G(v_{\frac{m_2}{2}}) - 1 + e_G(w) + 1 \\ &\quad + e_G(w') + 1 \\ &= e_G(u_{\frac{m_1}{2}}) + e_G(v_{\frac{m_2}{2}}) + e_G(w) + e_G(w'). \end{aligned}$$

Therefore, $\varepsilon(G') \geqslant \varepsilon(G)$ and this completes the proof. $\square$

Now we count the total eccentricity index of the graph $C^n_{m_1,m_2}$, where $m_1 + m_2 - 1 = n$. There are four cases depending upon whether m_1 and m_2 are even or odd. Let us consider the case when m_1 and m_2 are both even. We label the vertices of C_{m_1} and C_{m_2} in $C^n_{m_1,m_2}$ as $C_{m_1} : wu_1 \cdots u_{\frac{m_1}{2}-1} u_{\frac{m_1}{2}} u_{\frac{m_1}{2}+1} \cdots u_{m_1-1} w$ and $C_{m_2} : wv_1 v_2 \cdots v_{\frac{m_2}{2}-1} v_{\frac{m_2}{2}} v_{\frac{m_2}{2}+1} \cdots v_{m_2-1} w$. Without loss of generality, assume that $m_1 \geqslant m_2$. Take $m_1 = m_2 + k$, so $k \geqslant 0$ is even. Then

- for $i = 1, 2, \dots \frac{m_2}{2}$, $e(v_i) = e(v_{m_2-i}) = i + \frac{m_1}{2}$;
- $e(w) = \frac{m_1}{2}$;
- for $j = 1, 2, \dots \frac{k}{2}$, $e(u_j) = e(m_1 - j) = \frac{m_1}{2}$;
- for $\frac{k}{2} + 1 \leqslant j \leqslant \frac{m_1}{2}$, $e(u_j) = e(u_{m_1-j}) = j + \frac{m_2}{2}$.

So,

$$\begin{aligned} \varepsilon(C^n_{m_1,m_2}) &= e(w) + \sum_{i=1}^{m_2-1} e(v_i) + \sum_{j=1}^{m_1-1} e(u_j) \\ &= e(w) + 2\sum_{i=1}^{\frac{m_2}{2}-1} e(v_i) + e(v_{\frac{m_2}{2}}) + 2\sum_{j=1}^{\frac{k}{2}} e(u_j) + 2\sum_{j=\frac{k}{2}+1}^{\frac{m_1}{2}-1} e(u_j) + e(u_{\frac{m_1}{2}}) \\ &= \frac{1}{2}(m_1^2 + m_2^2 + m_1 m_2 - m_1). \end{aligned}$$

For the other three cases the total eccentricity index of $C^n_{m_1,m_2}$ with $m_1+m_2-1=n$ can be counted similarly. Based on these calculations, we have

$$\varepsilon(C^n_{m_1,m_2}) = \begin{cases} \frac{1}{2}(m_1^2+m_2^2+m_1m_2-m_1) & \text{if both } m_1 \text{ and } m_2 \text{ are even,} \\ \frac{1}{2}(m_1^2+m_2^2+m_1m_2-m_1-m_2) & \text{if } m_1 \text{ is even and } m_2 \text{ is odd,} \\ \frac{1}{2}(m_1^2+m_2^2+m_1m_2-2m_1+1) & \text{if } m_1 \text{ is odd and } m_2 \text{ is even,} \\ \frac{1}{2}(m_1^2+m_2^2+m_1m_2-2m_1-m_2) & \text{if both } m_1 \text{ and } m_2 \text{ are odd.} \end{cases}$$

Next we count the total eccentricity index of $U^p_{n,g}$ where $3 \leqslant g \leqslant n-1$. Suppose g is even. Let $w_1, w_2, \ldots, w_{n-g}$ be the pendant vertices of $U^p_{n,g}$ and $C_g : v_0v_1\cdots v_{g-1}v_0$ such that $deg(v_0) = n-g+2$. Then we have

- for $j = 1, \cdots, n-g$, $e(w_j) = 1 + \frac{g}{2}$
- for $i \in \{0, 1, \ldots, g-1\} \setminus \{\frac{g}{2}\}$, $e(v_i) = \frac{g}{2}$
- $e(v_{\frac{g}{2}}) = \frac{g}{2} + 1$.

So, $\varepsilon(U^p_{n,g}) = (n-g)(1+\frac{g}{2}) + (g-1)(\frac{g}{2}) + (\frac{g}{2}+1) = \frac{ng}{2} + n - g + 1$. Similarly $\varepsilon(U^p_{n,g})$ can be counted when g is odd and we get

$$\varepsilon(U^p_{n,g}) = \begin{cases} \frac{ng}{2} + n - g + 1 & \text{if } g \text{ is even,} \\ \frac{n(g-1)}{2} + n - g + 2 & \text{if } g \text{ is odd.} \end{cases}$$

In particular for $g = n-1$, $U^p_{n,n-1} \cong U^l_{n,n-1}$ and

$$\varepsilon(U^l_{n,n-1}) = \begin{cases} \frac{n(n-2)}{2} + 3 & \text{if } n \text{ is even,} \\ \frac{n(n-1)}{2} + 2 & \text{if } n \text{ is odd.} \end{cases} \tag{6.3.1}$$

Based on these calculations we have the following lemma.

Lemma 6.3.8. *Let $m_1 \geqslant m_2 \geqslant 3$ and $n \geqslant 5$.*

(i) If $m_1 + m_2 - 1 = n$ then $\varepsilon(C^n_{m_1,m_2}) \leqslant \varepsilon(U^l_{n,n-1})$. Furthermore the equality happens if and only if m_1 is even and $m_2 = 3$.

(ii) For $3 \leqslant g \leqslant n-2$, $\varepsilon(U^p_{n,g}) \leqslant \varepsilon(U^p_{n,g+1})$ and equality holds if and only if g is even.

For $n = 3$, the path P_3 is the only graph with one cut vertex. For $n = 4$, the star $K_{1,3}$ and $U^l_{4,3}$ are the only two graphs with one cut vertex and $\varepsilon(K_{1,3}) = \varepsilon(U^l_{4,3}) = 7$. So we consider $n \geqslant 5$.

Theorem 6.3.9. *Let $n \geqslant 5$ and $G \in \mathfrak{C}_{n,1}$. Then $\varepsilon(G) \leqslant \varepsilon(U^l_{n,n-1})$.*

Proof. Suppose G is not isomorphic to $U^l_{n,n-1}$. If G has no cycle then $G \cong K_{1,n-1}$ and $\varepsilon(G) = \varepsilon(K_{1,n-1}) = 2n - 1 < \varepsilon(U^l_{n,n-1})$, by (6.3.1). Suppose G has some cycles. Since G has a unique cut vertex, so all the blocks of G are pendant blocks. Let w be the cut vertex in G and let $B_1, B_2, \ldots, B_k$ be the blocks of G with atleast three vertices. Construct a new graph G' from G by replacing each B_i, $1 \leqslant i \leqslant k$ with a cycle on same number of vertices. Then $G' \in \mathfrak{C}_{n,1}$ and by Lemma 6.1.6, $\varepsilon(G) \leqslant \varepsilon(G')$. If G' has exactly one cycle, then G' is isomorphic to $U^p_{n,g}$ for some $g \geqslant 3$. The result follows from Lemma 6.3.8 (ii).

Suppose G' has at least two cycles. Let C_{m_1} and C_{m_2} be two cycles in G'. If $m_1 + m_2 - 1 = n$, then $G' \cong C^n_{m_1,m_2}$. So, by Lemma 6.3.8 (i), $\varepsilon(G') \leqslant \varepsilon(U^l_{n,n-1})$ and the result follows. If $n > m_1 + m_2 - 1$, then there are at least three blocks sharing the common vertex w in G'. Replace the blocks C_{m_1} and C_{m_2} by the cycle $C_{m_1+m_2-1}$ in G' to get a new graph G''. Note that $G'' \in \mathfrak{C}_{n,1}$ and by Lemma 6.3.7, $\varepsilon(G') \leqslant \varepsilon(G'')$.

If all the blocks of G'' are cycles, then repeat this process(if necessary) until we get a graph $\tilde{G}$ on exactly two blocks. By Lemma 6.3.7, $\varepsilon(G'') \leqslant \varepsilon(\tilde{G})$ and $\tilde{G} \cong C^n_{m,m'}$ where $m + m' - 1 = n$. Now the result follows from Lemma 6.3.8 (i).

If G'' contains K_2 as block then repeat the above process (if necessary) until we get a graph $\bar{G}$ having exactly one cyclic block. Note that $\bar{G} \in \mathfrak{C}_{n,1}$ and $\bar{G} \cong U^p_{n,g}$ for some $g \geqslant 3$. By Lemma 6.3.8 (ii), $\varepsilon(\bar{G}) \leqslant \varepsilon(U^l_{n,n-1})$ and this completes the proof. $\square$

The path P_n is the only graph in $\mathfrak{C}_{n,n-2}$. We will now obtain a graph which maximizes the total eccentricity index over $\mathfrak{C}_{n,n-3}$.

Theorem 6.3.10. *Let $n \geqslant 5$ and $G \in \mathfrak{C}_{n,n-3}$. Then $\varepsilon(G) \leqslant \varepsilon(U^l_{n,3})$.*

Proof. Suppose G is not isomorphic to $U^l_{n,3}$. If G is a tree then it has exactly one vertex of degree 3. Using grafting of edges operation sequentially (if necessary), we get the tree $T(2,1,n-3)$ from G and by Lemma 6.1.2, $\varepsilon(G) \leqslant \varepsilon(T(2,1,n-3))$. Let v_1 and v_2 be the two pendant vertices of $T(2,1,n-3)$ such that $d(v_1, v_2) = 2$. Form a new graph G' from $T(2,1,n-3)$ by joining v_1 and v_2 with an edge. Then $G' \cong U^l_{n,3}$. Since $\varepsilon(T(2,1,n-3)) = \varepsilon(U^l_{n,3})$ so the result follows. If G is not a tree then it must be a unicyclic graph with girth 3 and the result follow from Proposition 6.2.2. $\square$

6.4 Future works

We have obtained the graphs which maximize the total eccentricity index over $\mathfrak{C}_{n,s}$ for $s = 0, 1, n-3$ and $n-2$. Also the total eccentricity index of these graphs are known. Based on our observation, we conjecture the following for $2 \leqslant s \leqslant n-4$.

Conjecture 6.4.1. *Let $n \geqslant 6$ and $2 \leqslant s \leqslant n-4$. If $G \in \mathfrak{C}_{n,s}$ then $\varepsilon(G) \leqslant \varepsilon(U^l_{n,n-s})$.*

In many classes of graphs, the extremal graphs for the total eccentricity index and the Wiener index are same. For example, over trees on n vertices, the path P_n

maximizes both the total eccentricity index and the Wiener index, and the star K_n minimizes both these indices. But it is not necessary that for two graphs G_1 and G_2, if $W(G_1) < W(G_2)$ then $\varepsilon(G_1) < \varepsilon(G_2)$. For that, we have the following example.

Example 6.4.1. $W(G_1) = 13, W(G_2) = 14, \varepsilon(G_1) = 10, \varepsilon(G_2) = 9$

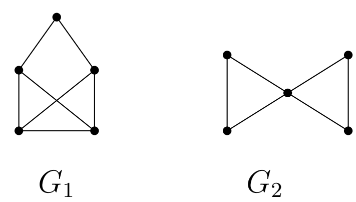


Figure 6.3: Two graphs G_1 and G_2 with $W(G_1) < W(G_2)$ but $\varepsilon(G_1) > \varepsilon(G_2)$

A detailed study may be required to understand the relation between the Wiener index and the total eccentricity index. In [10], the authors have studied some relations between total eccentricity index and Wiener index in graphs. In particular, they have given some bounds on Wiener index in terms of total eccentricity index and also studied the difference $W(G) - \varepsilon(G)$. It will be interesting to study such relations between the total eccentricity index and the Wiener index over $\mathfrak{H}_{n,k}$ and $\mathfrak{C}_{n,s}$.

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