Some Extremal Trees and Unicyclic Graphs w.r.t. Non-self-centrality Number

By

Faryal Karim

Supervised by

Dr. Rashid Farooq

Department of Mathematics

School of Natural Sciences
National University of Sciences and Technology
H-12, Islamabad, Pakistan
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National University of Sciences & Technology

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Examination Committee Members

1. Name: DR. MATLOOB ANWAR Signature: ____________

2. Name: DR. MUHAMMAD ISHAQ Signature: ____________

External Examiner: DR. NASIR REHMAN Signature: ____________

Supervisor's Name: PROF. RASHID FAROOQ Signature: ____________

Head of Department

16/08/2021
Date

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Dean/Principal

Dedication

I dedicate this thesis to my parents for their endless support and encouragement. Thanks to them for giving me this opportunity and being my strength to chase my dreams.

Acknowledgement

First and foremost praise is to Allah Almighty, on whom ultimately we depend for sustenance and guidance. Allhamdulillah, all praises to Him for the strength and His blessing in successful completion of this thesis.

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Abstract

The concept of centrality of a graph is introduced by Camille Jorden in 19th century for the analysis of different network models which is widely used in facility location problems. To measure the non-self-centrality extent of a graph Xu et al. introduced an eccentricity based graph invariant called Non-self-centrality number (NSC number). The centrality concept and eccentricity measures of a graph is used in network sciences, opimization theory, facility location problem, chemical graph theory and many more.

In this thesis we have considered some problems of extremal graph theory with respect to this distance based graph invariant NSC number. We have considered the class $\mathcal{T}(n,p)$ of all non-self centered tree graphs of order n with p pendant vertices. We found out the unique maximal graph $D_{n,p}$ with respect to NSC number among all the graphs in $\mathcal{T}(n,p)$ and also formulated the mathematical expressions for it and hence gave the upper bound. Further we extended our study to find the maximal graph among a class of unicyclic graphs $\mathcal{U}_n(3,\Delta)$ with some fixed parameters, that is, fixed degree Δ and atmost three central vertices. We found the unique graph $\widetilde{U}_{n,3}$ which attains the maximum value of NSC number in this class.

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Chapter 1

Introduction to Graph Theory

In recent years, graph theory has grown in importance as a branch of mathematics, as it is an important mathematical tool with applications in a wide variety of subjects like operations research, mathematical chemistry, biochemistry, architecture, geography, networking, electrical engineering, physics, social sciences, computer sciences and many more. Basically graph theory is concerned with the study of mathematical structures or network of points, that are said to be vertices of graph which are connected by lines, called edges that shows the pairwise relation between those points.

The origin of graph theory is specifically dated back to 1735, when a Swiss mathematician Leonard Euler was asked to find a possible path over the seven bridges of Königsberg city which was divided into four regions by river Pregel, to walk around the city and return back to the starting point (if possible) after crossing each of the seven bridges only once. The problem was called Königsberg bridge problem. Königsberg bridge problem could be stated in the terminology of the modern graph theory as follows;

If there exist a path along the edges of a multigraph, that transverses each of the edge once and only once, then there exist atmost two vertices that have odd degree. Moreover, if that path starts and ends at a same vertex in that graph, then no vertex will have odd degrees[1].

Euler sketched this problem by a graph in which the four regions were represented by points and the bridges connecting them were considered as edges. He stated that the desired path doesn't exist in this problem and proved the first theorem in graph theory.

1.1 Graphs and basic definitions

A graph G, is an ordered pair $G = (V_G, E_G)$ of vertex set denoted by V_G and edge set denoted by E_G. If there is an edge between two vertices v_i and v_j then the edge is denoted by v_iv_j or v_jv_i, where v_i, v_j are called the end points of the edge. In a graph, the cardinality of the vertex set V_G is called order of that graph, where cardinality of the egde set E_G is called size of that graph. Two vertices $v_i, v_j \in V_G$ in a graph are called adjacent in G if there exist an edge between v_i and v_j in graph G; that is, for some $u, v \in V_G$, we have $uv \in E_G$; otherwise, they are non-adjacent. Any two vertices in G are neighbors of each other if they are adjacent in G. For any vertex $v \in V_G$, the set of neighbours of v is denoted by

$$\Gamma_G(v) := \{u \in V_G \mid uv \in E_G\}.$$

An edge that connects a vertex to itself is said to be a loop. When two or more edges share the same ends then these edges are said to be multiple or parallel edges. A graph without a loop and a parallel edge is called a simple graph. By allowing loops and parallel edges we can generalize simple graphs to multigraphs. In the Figure 1.1, two edges are placed parallel that connects the common ends v_4 and v_5. Their is also a loop at vertex v_4.

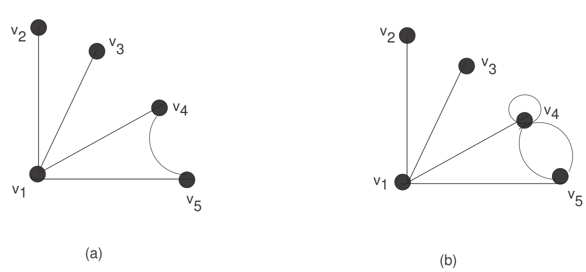


Figure 1.1: Simple and multi graphs

Definition 1.1.1. For some $v_i \in V_G$, the set $\Gamma_G(v_i) = \{v_j \in G \mid v_iv_j \in G\}$ is called neighbor of v_i in G. Degree of $v_i \in G$, denoted by $d_G(v_i)$, is defined as

$$d_G(v_i) = |\Gamma_G(v_j)|.$$

A vertex of degree 0 is called an isolated vertex. If $d_G(v_i) = 1$ then v is said to be a leaf or a pendant vertex. For a graph G, the minimum and maximum degree is defined as:

$$\delta(G) = \min\{d_G(v_i) \mid v_i \in G\}.$$

$$\Delta(G) = \max\{d_G(v_i) \mid v_i \in G\},$$

A very famous lemma of graph theory is given below.

Theorem 1.1.1 ([2])**.** *For any graph G*

$$\sum_{v \in V_G} d_G(v) = 2|E_G|.$$

Moreover, G has even number of vertices with odd degree.

Above theorem is also known as degree sum formula that shows that the number of odd degree vertices in a graph is always even.

Definition 1.1.2. A vertex $v \in V_G$ of a graph G of order n is called universal vertex or dominating vertex if v is adjacent to all other vertices in G. And $n_{n-1}(G)$ denotes the number of universal vertices in a graph G.

Definition 1.1.3. Let $G = (V_G, E_G)$ be a given graph with $u, v \in V_G$. A path from u to v is defined as a finite sequence of edges $\{v_iv_{i+1} \mid i = 1, 2, ..., m-1\}$ such that $v_i \neq v_j$ for all $i \neq j$.

A path P_n has $(n-1)$ edges, that is, $|V_{P_n}| = |E_{P_n}| + 1$.
If their exists a path between any two arbitrary vertices of a graph G, then G is said to be a connected graph otherwise disconnected.

Definition 1.1.4. A trail in a graph is defined as a finite sequence of edges, such that all edges are distinct.

Definition 1.1.5. A cycle C_l is a closed trail $\{v_1, v_2, ..., v_{l-1}, v_l\}$ with $l \geq 3$, in which $v_1 = v_l$ and all other vertices are different.

Definition 1.1.6. A graph G is called acyclic if it contains no cycle. A connected, acyclic graph is called a tree graph. Acyclic graph is also called a forest.

Theorem 1.1.1 ([2]). *For any graph T, the following statements are equivalent:*
i) T is a tree.
ii) For some $u, v \in E_T$ there is a unique path connecting u and v.
iii) T is acyclic with $|E_T| = |V_T| - 1$.

A graph G is a rooted graph if a single vertex $v \in V_G$ can be distinguished as its root.

Definition 1.1.7. The length of a shortest path between two vertices $v_i, v_j \in V_G$ is the distance between v_i and v_j which is denoted by $d_G(v_i, v_j)$. Eccentricity of a vertex $v_i \in V_G$ is defined as:

$$\epsilon(v_i) = \max_{v_j \in V_G} d_G(v_i, v_j).$$

Definition 1.1.8. Diameter of a graph G is the maximum eccentricity of a vertex among all eccentricities of vertices in G. It is denoted by $d(G)$. If $\epsilon_G(v_i) = d(G)$ then v_i is called peripheral vertex in G.

Definition 1.1.9. The minimum eccentricity among all the vertices in G is the radius of the graph G, denoted by $r(G)$. The vertices with eccentricity $\epsilon(v_i) = r(G)$ are the central vertices. In general, we have $d(G) \leq 2r(G)$.

Definition 1.1.10. The center of a graph G, denoted by $\mathbf{C}(G)$ is a subgraph of G induced by central vertices of G.

Center of a complete graph K_n is the graph itself since for all $v_i \in K_n$, $\epsilon(v_i) = 1 = r(K_n) = d(K_n)$. Similarly center of a path P_n is either K_1 or K_2

If for all $v_i \in V_G, \epsilon(v_i) = r(G) = d(G)$ then the graph G is self-centered, that is, all vertices are central. If $r(G) \neq d(G)$ then graph is non-self-centered. Xu.et al. [3] introduced an efficient graph invariant that indicates the non-self centrality of a graph that is named as non-self centrality number.

Definition 1.1.11. The non-self centrality number of a graph G (henceforth NSC number) is defined as:

$$N(G) = \sum_{1 \leq i < j \leq k} l_i l_j (\epsilon_i - \epsilon_j), \tag{1.1}$$

where ϵ_i, $1 \leq i \leq k$, are the distinct eccentricities of G such that $\epsilon_1 > \epsilon_2 > \cdots > \epsilon_k$ with $l_1, l_2, \ldots, l_k$ as their respective multiplicities. NSC number of a graph can also be defined as

$$N(G) = \sum_{v_i \neq v_j} |\epsilon_i - \epsilon_j|,$$

where the summation is over all the unordered pairs of vertices of graph G.

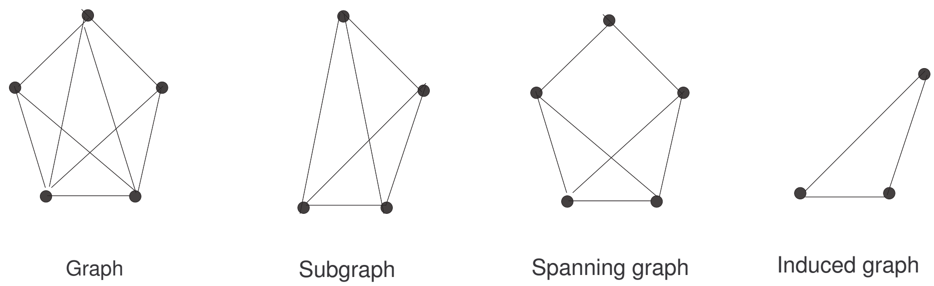
1.2 Subgraphs and Isomorphic Graphs

Sometimes we need to deal with a smaller part of a graph to determine its properties in order to determine a solution. The solution can be found out by determining the properties of those parts of graph and combining them. For instance any property that can be found out by the degree of a vertex v_i (that is, number of neighbors of the vertex v_i) or a property that can be determined by set of independent sets in that graph. In such circumstances we need to study subgraphs.

1.2.1 Subgraphs

A graph $H = (V_H, E_H)$ is said to be a subgraph of the graph $G = (V_G, E_G)$, if $V_H \subseteq V_G$ and $E_H \subseteq E_G$.

Definition 1.2.1. If $G = (V_G, E_G)$ is a graph with $H = (V_H, E_H)$ its subgraph then H is called a spanning graph if $V_G = V_H$.



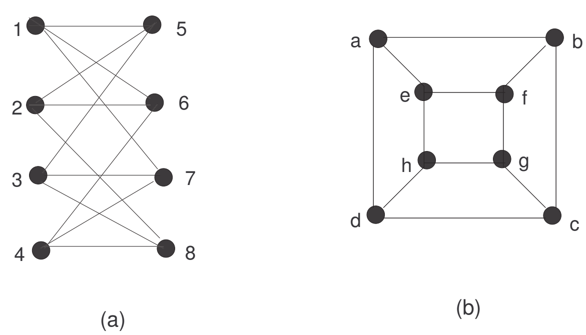
(a) Subgraph

Figure 1.2: Subgraphs

For some $E_H \subseteq E_G$, $H = (V_H, E_H)$ is called edge induced subgraph by E_H where $v \in V_H$ if and only if v appears in an edge in E_H.
Similarly, if $S \subset V_G$ and $V_G - S = V_H$ then, $H = (V_H, E_H)$ is a vertex induced subgraph by vertices V_H obtained by deleting all vertices of S and $uv \in E_H$ if $\{u, v\} \in V_H$.

1.2.2 Isomorphic Graphs

Any two simple graphs G_1 and G_2 are said to be isomorphic graphs if there exist a bijection $\psi : V_{G_1} \to V_{G_2}$ such that for all $u, v \in V_{G_1}$, $uv \in E_{G_1}$ iff $\psi(u)\psi(v) \in E_{G_2}$. All isomorphic graphs have same physical and chemical properties. Infact for any arbitrary graph there may exist infinitely many isomorphic graphs. In Figure 1.3, the graphs G and G' are isomorphic.



(a) Isomorphic

Figure 1.3: Isomorphic graphs

1.3 Some Special Graphs

In this section, we define some classes of graphs.

A graph $G = (V_G, E_G)$ with only one vertex is trivial graph; otherwise, it is non-trivial.

Definition 1.3.1. A complete graph K_n on n-vertices, is a graph such that every two vertices in G are adjacent, that is, a vertex v in K_n is adjacent to all other $(n-1)$ vertices. Hence we have $d_G(v) = (n-1)$ for all $v \in V_{K_n}$, K_n is self centered graph.

Definition 1.3.2. A graph G with every vertex of same degree is called a regular graph. If for all vertices $v \in V(G), d_G(v) = r$ then G is a r-regular graph. A very well-known Petersen graph of order 10 is a 3-regular graph.

Definition 1.3.3. A tree T of order n with p pendant vertices is a double broom with diameter $d(T) = n - p + 1$ such that $\lceil \frac{p-2}{2} \rceil$ pendant vertices are adjacent with a single vertex of eccentricity $d(T) - 1$ and $\lfloor \frac{p-2}{2} \rfloor$ pendant vertices are adjacent with a single central vertex in T. An n-vertex double broom with p pendant vertices has the eccentricity sequence of the form

$$\xi(T) = \{e_1^{\lceil \frac{p+2}{2} \rceil}, e_2^2, \ldots, e_{k-2}^2, e_{k-1}^{\lfloor \frac{p+2}{2} \rfloor}, e_k^{l_k}\}, \tag{1.2}$$

and is denoted by $D_{n,p}$. Since center of $D_{n,p}$ is K_1 or K_2, we have $l_k = 1$ when $d(D_{n,p})$ is even and $l_k = 2$ when $d(D_{n,p})$ is odd.

Definition 1.3.4. A graph G of order n and $p+1$ pendant vertices is called a p-broom if G has diameter $n-p$ and the eccentricity sequence of the form

$$\xi(G) = \{e_1^{\lceil \frac{p+2}{2} \rceil}, e_2^2, \ldots, e_{s-1}^2, e_s^3, e_{s+1}^2, \ldots, e_{k-2}^2, e_{k-1}^{\lfloor \frac{p+2}{2} \rfloor}, e_k^{l_k}\}, \tag{1.3}$$

where $2 \leq s \leq (k-1)$ for $k \geq 4$. If $k < 4$ then, the graph will be a double broom. We denote the class of n-vertex p-brooms by $\mathcal{P}_n^p$.

Definition 1.3.5. The complement of a graph $G = (V_G, E_G)$, denoted by $\overline{G} = (V_{\overline{G}}, E_{\overline{G}})$, is defined as a graph with $V_G = V_{\overline{G}}$ and $e \in E_{\overline{G}}$ if and only if $e \notin E_G$

The complement of a complete graph is a 0-regular graph.

Definition 1.3.6. If the vertex set V_G of a graph $G = (V_G, E_G)$ can be partitioned into two sets say A and B such that every edge $v_iv_j \in E_G$ connects some $v_i \in A$ and some $v_j \in B$, then we say G is a bipartite graph with bipartition A and B.
A bipartite graph G with the bipartition A, B is called a complete (p, q)-bipartite if $|A|= p$, $|B|= q$ and for all $u \in A$ and $v \in B$, we have an edge $uv \in E_G$.

Theorem 1.3.1 ([2]). *A graph G is bipartite graph if and only if G contain no odd cycles as its subgraph.*

1.4 Adjacency Matrix

Let $G = (V_G, E_G)$ be a finite simple graph. The adjacency matrix, $A = [a_{uv}]$ of G is a $\{0, 1\}$-matrix indexed by vertices of G in which $a_{uv} = 1$ when $uv \in E_G$ and $a_{uv} = 0$ otherwise.
The eigenvalues of an adjacency matrix A of the graph G are the eigenvalues of G. If $\lambda_1, \lambda_2, ..., \lambda_s$ are the distinct eigenvalues of A, then $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_s$, where all the eigenvalues of A are real.

Definition 1.4.1. For any graph G, the graph energy is defined as;

$$E(G) = \sum_{i=1}^{s} |\lambda_i|,$$

that is, energy of the graph G is the sum of the absolute values of all eigenvalues. In any two graphs say G_1 and G_2 if the equality $E(G_1) = E(G_2)$ holds then G_1 and G_2 are said to be equi-energetic.

1.5 Networks and Connectivity

Networking or network science is also a part of graph theory in which we study the symmetric and asymmetric relation between nodes which are the representation of discrete objects. Network science has applications in wide variety of disciplines like computer sciences, statistical sciences, operations research, finance, engineering, economics, social networking and many more. The most important terminology that we

use in networking is connectivity.
The pattern in which the vertices are connected with each other in a graph defines different properties of that graph. If we can disconnect a graph by removing a single vertex $v_i \in G$ then we say that G has connectivity 1 and the vertex v is a cut point. If removing two such vertices the graph becomes disconnected then G has connectivity 2.

Definition 1.5.1. A vertex $v \in V_G$ is a cut-vertex of G if $(G-v)$ has more components than that of G. Deletion of a vertex $v \in V_G$ results in deletion of all edges which are incident on v in G.
Let $M \subseteq V_G$. The set M is called a separating set if $(G - M)$ has more components than G. In other words, if G is a connected graph then, $(G - M)$ is disconnected.

Definition 1.5.2. If $M \subset V_G$ then, the vertex connectivity number of a graph G, which is denoted by $\kappa(G)$ is defined as;

$$\kappa(G) = |M|,$$

such that $(V_G - M)$ is disconnected or trivial, where M is the smallest set for which $(V_G - M)$ is disconnected.

If $\kappa(G) \geq k$ in graph G, then G is called a k-connected graph. The graph K_n (complete graph) is the only graph that have connectivity $(n - 1)$. A disconnected graph has 0 connectivity. There may exist graphs without a separating set.

Definition 1.5.3. If G is a connected graph and $S \subseteq E_G$ then S is said to be an edge cut, if $(G-S)$ is disconnected. Edge cut is denoted by $\lambda(G)$. The graph is k-connected if $\lambda(G) \geq k$.

Edge connectivity is undefined for a trivial graph (one vertex graph). Any two vertices in G can be disconnected by removing all the edges incident to a single vertex. Thus we have the relation

$$\lambda(G) \leq \delta(G).$$

Also

$$\delta(G) \leq (n-1).$$

This implies $\delta(G) \leq (n-1)$.
Since deletion of a vertex also deletes all edges incident to it, therefore we have

$$\kappa(G) \leq \lambda(G).$$

Definition 1.5.1. A graph G is called maximal connected if it is connected with respect to the property of connectedness. In other word, G is maximally connected if connectivity of G is equal to the minimum degree of G.

Definition 1.5.2. A subgraph of a graph G that is connected and also not contained in some other connected sub-graph of G is called a maximal connected subgraph. Block is a maximal connected subgraph that contains no cut-vertex.

Definition 1.5.3. An edge $e \in E_G$ in graph G is a bridge of G if deletion of e increases the number of components in G.

If G is a connected graph and e is a bridge then, $(G-e)$ is disconnected. If G has m connected components then, $(G-e)$ has $(m+1)$ connected components. In Figure 1.4, $e = uu^{'}$ and $e = vv^{'}$ are bridges in G where $u, u^{'}$ and $v, v^{'}$ are in different components.

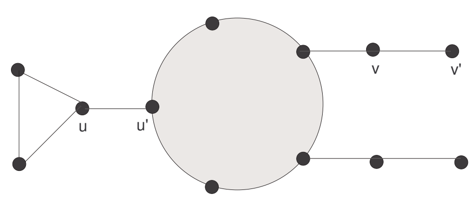


Figure 1.4: A connected graph

In tree graph $T = (V_T, E_T)$, every edge $e \in E_T$ is a bridge.

Theorem 1.5.4 ([2])**.** *Any edge $e \in E_G$ is a bridge of G iff e is not in a cycle of G.*

1.6 Extremal Graphs

It's a branch of mathematics that study how a graph's global feature affect its local substructure. It includes a large number of results that explain how certain graph features like; size, egde, density, chromatic number, girth, guarantee the existence of particular local substructures, such as weather they contain or do not contain one. In the area of graph theory, extremal graph is one of the main study. Extremal graphs are minimal or maximal with respect to some parameters such as edge coloring, degree or clique number such that, they contain or do not contain a local substructure. A basic theorem in extremal graph theory given by Mantel in 1907 khown as Mental theorem which is stated below;

Theorem 1.6.1 ([4]). *Any graph $G = (V_G, E_G)$ with $|V_G|= n$, $|E_G|= m$, if G is a graph with girth ≥ 4 or no induces 3-cycle, then $m \leq \lfloor \frac{n^2}{4} \rfloor$. Furthermore the equality holds if $G \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ with $m = \lfloor \frac{n^2}{2} \rfloor$.*

The generalization of Mantels's theorem is given by Paul in 1941 by considering the clique size of graph equal to q.

Theorem 1.6.2 ([5]). *An n-vertex complete balanced k-partite graph doesn't contain K_{q+1} but every n-vertex graph with more edges must contain K_{q+1}, where K_{q+1} is a complete graph on $(q + 1)$ vertices.*

Throughout this dissertation we only consider finite, simple un-directed graphs that are non-self centered. Our main focus in this thesis is to find the extremal graphs among all the n vertex trees with fixed pendant vertices with respect to the graph invariant NSC number and the extremal unicyclic graphs with fixed paremeter w.r.t. the same graph invariant i.e NSC number.

Chapter 2

Literature Review

2.1 Background and motivation

Finding the non-self-centrality number of a non-self-centered graph is of great importance, as it is used in a wide number of fields like in theory of networks, optimization theory , facility location problems, chemical graph theory and many more. To measure the non-self-centrality extent of the non-self-centered graphs Xu et al. [3] introduced two eccentricity based graph invariants named the third Zegreb eccentricity index $E^3(G)$ defined as;

$$E^3(G) = \sum_{e=v_iv_j \in E_G} |\epsilon_j - \epsilon_i| \tag{2.1}$$

and the Non-self-centrality number (NSC number) defined as;

$$N(G) = \sum_{1 \le i < j \le k} l_i l_j |\epsilon_i - \epsilon_j| \tag{2.2}$$

where ϵ_i, $1 \le i \le k$, are the distinct eccentricities of G such that $\epsilon_1 > \epsilon_2 > \cdots > \epsilon_k$ with $l_1, l_2, \ldots, l_k$ as their respective multiplicities [3], where, the summation is applied to all pairs of vertices in graph G that are unordered [1]. If G has k distinct eccentricities $\epsilon_1, \epsilon_2, \ldots, \epsilon_k$ with $l_1, l_2, ..., l_k$ their respective multiplicities, then, the eccentric sequence of G is the set

$$\xi(G) = \{\epsilon_1^{l_1}, \epsilon_2^{l_2}, ..., \epsilon_k^{l_k}\}.$$

Since Xu et al. [3] recently introduced this eccentricity based graph invariant and a few mathematical results on NSC number have been obtained yet. Xu et al. [3] determined the unique extremal graphs in the family of tree graphs that are $\mathcal{P}_n$ path and $\mathcal{S}_n$ star graph which attains the maximum and minimum value among all n-vertex trees and thus determined the upper and lower bounds on NSC number of tree graphs. For a graph G to be non-self-centered, the following conditions must hold;
(i) NSC$(G) = 0$, if G is self-centered.
(ii) For any two graphs G and G' which are isomorphic, we have NSC$(G) =$ NSC(G').
The third zegreb eccentricity index also appears to be a very reliable indicator of non-self-centrality but, $E^3(G)$ doesn't satisfies the conditions (i)$-$(ii). And for any tree graph $T \in \mathcal{T}_n$ we have $N(S_n) \leq N(T) \leq N(P_n)$ but $E^3(S_n) = E^3(P_n) = (n-1)$ for all odd order graphs on $n \geq 5$. Thus NSC number is a better approach to measure the non-self-centrality of any graph.

2.2 Some known results on NSC number

In this section, the literature on NSC number of graphs is reviewed.

2.2.1 Extremal tree graphs with respect to NSC number

Let $T \in \mathcal{T}_n$ be an n^{th} order tree graph and $G \in \mathcal{G}_n$ be any arbitrary graph of order n, then we have following known results.

Theorem 2.2.1 ([3]). *Let G be any non-trivial connected graph of order n, then, $N(G) \geq \mathrm{E}^3(G)$. The equality holds iff $d(G) \leq 2$.*

Theorem 2.2.1 ([3]).

(i) If $G \in \mathcal{G}_n$ of order n with $4 \leq n \leq m \leq (2n-4)$, where $|E_G| = m$, then we have $N(G) \geq (n-1)$. The equality holds iff $G \cong S_n$, where $|E_{S_n}| = |E_G| = m$.

(ii)The NSC number of an almost peripheral graph G of order $n \geq 3$ is equal to $(n-1)$.

A *doublestar* denoted by $DS_{n',n''}$ is defined as a tree obtained by adding an edge e between the centers of two star graphs $S_{n'+1}$ and $S_{n''+1}$ such that, order of $DS_{n',n''}$ is $n = n^{'} + n^{''}$.

Theorem 2.2.2 ([3]). *Let G be an n^{th} order graph on $(n \geq 4)$, then we have;*

(i) $N(G) \geq 2.(n-2)$, if G is not an almost peripheral (AP) graph. The equality holds if and only if almost self centered (ASC) or weak almost peripheral (WAP) graph.

(ii) If $T \in \mathcal{T}_n$ and $T \ncong S_n$, then, $N(T) \geq 2(n-2)$ and the equality holds if $T \cong DS_{n_1,n_2}$ with $n_1 + n_2 = n$.

A *caterpiller* ζ_n of order n is defined as a graph obtained from a path $P_{s+1} = v_1 v_2, \ldots, v_{s+1}$ by attaching $a_m \geq 0$ pendant vertices to vertex $v_m \in P_{s+1}$ for $m = 2, 3, \ldots, s$, where, $\mathbf{C}(\zeta_n) = K_1$ or K_2 for even and odd s respectively. It is denoted by $P^n_{s+1}(a_1, a_2, \ldots, a_s)$ with $\sum_{m=2}^{s} a_m = n - s - 1$.

Let $v_{\frac{s}{2}+1} \in V_{\mathbf{C}(\zeta_n)}$ for even s and $v_{\frac{s+1}{2}}$ and $v_{\frac{s+3}{2}} \in V_{\mathbf{C}(\zeta_n)}$ for odd s respectively with $a_2 + a_s > 0$, then, ζ_n is called a *balancedcaterpiller* if
$|a_2 + a_s - a_{\frac{s}{2}+1}| \leq 2$ for even s and $|a_2 + a_s - a_{\frac{s+1}{2}} - a_{\frac{s+3}{2}}| \leq 2$ for odd s.
A *balancedcaterpiller* of order n and diameter d is denoted by $B\zeta_{n,d}$.

Theorem 2.2.3 ([3]).

(i) For any n order tree $T \in \mathcal{T}_{n,d}$ with $4 \leq d \leq (n-2)$ and $d = 2s$, we have

$$N(T) \leq ns^2 - \frac{4}{3}s^3 + \frac{s}{3} + (s-1)\left\lfloor \frac{n-2s-2}{2} \right\rfloor \left\lceil \frac{n-2s-2}{2} \right\rceil$$

and equality holds if $T \in B\zeta_{n,2s}$ with $a_2 + a_{2s} = a_{s+1}$ or $a_{s+1} + 1$.

(ii) For any n order tree $T \in \mathcal{T}_{n,d}$ with $5 \leq d \leq (n-2)$ and $d = 2s+1$ we have

$$N(T) = n(s^2 - s + 2) - \frac{2}{3}(2s^2 - 5s + 6) + (s-1)\left\lfloor \frac{n-2s}{2} \right\rfloor \left\lceil \frac{n-2s}{2} \right\rceil$$

and equality holds if $T \in B\zeta_{n,2s+1}$ with $a_2 + a_{2s+1} \leq a_{s+1} + a_{s+2} + 2$.

Theorem 2.2.4 ([3])**.** *Let $T \in T_n$ and $n \geq 4$, then, we have*

$$N(T) = \begin{cases} \dfrac{n(n-2)(n+2)}{12}, & \text{if } n \geq 6 \text{ is even} \\ \dfrac{(n-1)n(n+1)}{12}, & \text{if } n \geq 5 \text{ is odd} \end{cases} \tag{2.3}$$

and the equality holds iff $T \cong P_n$.

A *starliketree* is a graph G of order n, obtained by attaching p paths of length $m_1, m_2, \ldots, m_p$ to a single vertex such that $\sum_{i=1}^{p} m_i = (n-1)$. Such a graph is denoted by $T_n(m_1, m_2, \ldots, m_p)$. If m_i appears l_i times, then, we will write $T_n(m_1^{l_1}, m_2^{l_2}, \ldots, m_p^{l_p})$.

Theorem 2.2.5 ([3])**.** *Let $T \in \mathcal{T}_n$ be a graph of order n. Then,*

(i) The NSC number of T is given by

$$N(T) \leq \begin{cases} \dfrac{(n-2)[(n+4)(n-2)+2]}{12}, & \text{if } n \geq 6 \text{ is even} \\ \dfrac{(n-3)(n-1)(n+4)}{12}, & \text{if } n \geq 5 \text{ is odd} \end{cases} \tag{2.4}$$

and the equality holds if $T \cong \mathcal{T}_n(1^2, n-3)$.

(ii) If $T \cong \mathcal{T}_n(1^2, n-3)$ then we have

$$N(T) \leq \begin{cases} \dfrac{(n-2)(n^2+2n-12)}{12} + 1, & \text{if } n \geq 6 \text{ is even} \\ \dfrac{(n-3)(n^2+3n-16)}{12} + 2, & \text{if } n \geq 7 \text{ is odd} \end{cases} \tag{2.5}$$

and the equality holds if $T \cong (1, \lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil)$.

Let G be an n^{th} order graph and G_1, G_2 be the two copies of G. If $v_{1_i}, v_{1_j} \in V_{G_1}$ and $v_{2_i}, v_{2_j} \in V_{G_2}$ then the *doublegraph* [6] of G denoted by DG is formed by adding edges between every vertex v_{1_i}, v_{2_j} and every vertex $v_{1_j} v_{2_i}$ in DG when their exist an edge $e = v_i v_j \in E_G$.

Theorem 2.2.6 ([3])**.** *Let DG be a double graph of a connected graph G on $n \geq 3$. Then, $N(DG) = 0$ if $\delta(G) = \max\{d_G(v) \mid v \in V_G\} = (n-1)$ and $N(DG) = 4.N(G)$ otherwise.*

2.2.2 Comparison of NSC number and irregularity of graphs

The non-self-centrality number (NSC number) of a graph G is defined in terms of eccentricities of vertices whereas the irregularity measure of G is based on the vertices' degrees in G. We denote irregularity of a graph G as G_{irrt} which is defined by

$$G_{irrt} = \sum_{v_i \neq v_j} |d_G(v_i) - d_G(v_j)|. \tag{2.6}$$

In general the irregularity of a graph and its non-self-centrality is incomparable. Here we present some results on the non-self-centrality and irregularity of graphs.

Theorem 2.2.7 ([7]).

(i) For any non-self-centered graph G on $n \geq 6$ vertices and diameter $d(G) \geq 2$, their exists a graph with $G_{irrt} > N(G)$.

(ii) Let $T \in \mathcal{T}_n$ and $n \geq 10$. If T has diameter $d(T) \geq \frac{2+\sqrt{26}}{11}n$ and $\delta(T) = \max\{d_T(v) \mid v \in V_T\} = 4$ avoiding degree 3. Then, $N(T) > T_{irrt}$.

(iii) Let $T \in \mathcal{T}_n$ and $T \ncong P_n$ be a tree graph of diameter 3 then, $T_{irrt} > N(T)$.

(iv) Let $T \in \mathcal{T}_n$ on $n \geq 8$ vertices and $d(T) = 4$. If $c \in V_{\mathbf{C}(T)}$ having m non-pendant neighbors and $3 \leq m < d_T(c)$ then, $T_{irrt} > N(T)$.

(v) Let $U \in \mathcal{U}_n$ and $U \ncong C_6$. If $d(U) = 3$ then $U_{irrt} > N(U)$.

Further results on the irregularity of a graph is given in (ref 2,5).

2.2.3 Results on some graph products

This section is a review of the literature on NSC number of some graph products.
(i) Join: Let $G = (V_G, E_G)$, $H = (V_H, E_H)$ be two connected graphs with $V_G \cap V_H = \phi$, then join of graph G and H also known as their sum, is the union $G \cup H$, such that $G \cup H$ contains all the edges that join V_G and V_H.

Theorem 2.2.8 ([8])**.** *The* NSC number of join of m graphs $G_1, G_2, \ldots, G_m$ of order $n_1, n_2, \ldots, n_m$, respectively, is given by

$$N(G_1 \cup G_2 \cup \ldots \cup G_m) = \left(\sum_{i=1}^{m} n_{n_i-1}(G_i)\right)\left(n - \sum_{i=1}^{m} n_{n_i-1}(G_i)\right),$$

where $n = \sum_{i=1}^{m} n_i$.

(ii) Disjunction: The disjunction of two graphs G and H of order n_1 and n_2, respectively, denoted by $G \vee H$ is a graph with the vertex set $V_G \times V_H$ and we have $(u_i, u_j)(v_i, v_j) \in E_{G \vee H}$ if and only if $u_i v_i \in E_G$ and $u_j v_j \in E_H$.

Theorem 2.2.9 ([8])**.** *The* NSC *number of disjunction of two graphs* G *and* H *of order* n_1, n_2 *respectively, is given by*

$$N(G \vee H) = n_{n_1-1}(G).n_{n_2-1}(H)\{n_1 n_2 - n_{n_1-1}(G).n_{n_2-1}(H)\}.$$

(iii) Symmetric difference: The symmetric difference $(G \oplus H)$ of graph G and graph H is a graph with the vertex set $V_{G \oplus H} = V_G \times V_H$ and

$$E_{(G \oplus H)} = \{(u_i, u_j)(v_i, v_j) : u_i v_i \in E_G \text{ or } u_j v_j \in E_H \text{ but not both}\}.$$

Theorem 2.2.10 ([8])**.** *The graph* $G \oplus H$ *of two connected graphs* G *and* H *is a self centered graph, that is,* $N(G \oplus H) = 0$.

(iv) Lexicographic product: The lexicographic product of the graphs G and H of order n_1 and n_2, respectively, denoted by $G[H]$ also known as their composition is a graph with the vertex set $V_{G[H]} = V_G \times V_H$ and edge set

$$E_{G[H]} = \{(u_i, u_j)(v_i, v_j) \text{ iff } u_i v_i \in E_G \text{ or}(u_i = v_i \in V_G \text{ and } u_j v_j \in E_H)\}$$

Theorem 2.2.11 ([8])**.** *The lexicographic product of graph* G *and* H *of order* n_1 *and* n_2 *respectively is given by*

$$N(G[H]) = n_{n_1-1}(G).n_{n_2-1}(H)\{n_1 n_2 - n_{n_1-1}(G).n_{n_2-1}(H)\}$$

if G *has universal vertices and* $N(G[H]) = n_2^2.N(G)$ *otherwise.*

(v) Strong product: Let G and H be any two graphs of order n_1 and n_2 respectively, then the strong product $(G \boxtimes H)$ of G and H is a graph with vertex set $V_{(G\boxtimes H)} = V_G \times V_H$ and the edge set $E_{(G\boxtimes H)}$, where $(u_i, u_j)(v_i, v_j) \in E_{G\boxtimes H}$ if and only if $\{u_i = v_i \in V_G$ and $u_j v_j \in E_H\}$ or $\{u_j = v_j \in V_H$ and $u_i v_i \in E_G\}$ or $\{u_i v_i \in E_G$ and $u_j v_j \in E_H\}$.

Theorem 2.2.12 ([8])**.** *Let G and H be two graphs respectively, of order n_1 and n_2, with $r(H) \geq d(G)$, then the* NSC number of $(G \boxtimes H)$ is given by

$$N(G \boxtimes H) = n_1^2.\mathrm{NSC}(H).$$

(vi) Cartesian product: The cartesian product $G\Box H$ of the graphs G and H is a graph with vertex set $V_G \times V_H$ and $(u_i, u_j)(v_i, v_j) \in E_{G\Box H}$ if $\{u_i = v_i \in V_G$ and $u_j v_j \in E_H\}$ or $\{u_j = v_j \in V_H$ and $u_i v_i \in E_G\}$.

Theorem 2.2.13 ([8])**.** *The* NSC number of the cartessian product $(G\Box H)$ of graphs G with $|V_G|= n_1$ and H with $|V_H|= n_2$ is given by

$$N(G\Box H) = n_1^2.\mathrm{NSC}(H) + n_2^2.\mathrm{NSC}(G).$$

(vii) Rooted product: The rooted product $G\{H\}$ of graph G of order n_1 and a rooted graph H of order n_2 is obtained by taking a copy of G with n_1 copies of H and identifying thr root vertex of to the i^{th} vertex of G, where $1 \leq i \leq n_1$.

Theorem 2.2.14 ([8])**.** *Let H be a rooted graph with rooted vertex v_r and $|V_H|= n_2$ and G be a graph of order n_1, then the* NSC number of the rooted product $G\{H\}$ is given by

$$N(G\{H\}) = n_2^2 N(G) + \frac{n_1^2}{2} \sum_{u,v \in V_H} |d_H(u, v_r) - d_H(v, v_r)|.$$

2.3 Applications of eccentricity and centrality measures

In this section we present some applications of eccentricity measures and the centrality concept of graphs in some graph theory problems.

2.3.1 Networking and facility location problem

The concept of centrality of a graph is introduced by Camille Jorden [9] for the analysis of different network models which is widely used in facility location problems [10, 11, 12]. For instance, where should we situate a facility in a network that span a large region. When establishing the location of an emergency institute such as a hospital or a fire station, we want to reduce the time it takes for that facility to respond to an emergency. Similarly in selecting location for some service center such as a power station or post office we would reduce the aggregate of travel time distance, needed to reach everyone in the region. Same for other general service facilities like railway lines, superhighways or irrigation pipelines etc. Logically the appropriate allocation of a facility in a system or a network is at a central vertex. The maximum eccentricities of vertices $v_i's$ in a graph of network is the smallest possible for a most efficient facility. Thus, all these problems can be modeled graphically. Centrality concept and eccentricity measures could give us the best model for locating facilities.

2.3.2 Chemical graph theory

The topology of a chemical structure can be represented by a molecular graph [13]. The chemical graph theory's main aim is to use some algebraic invariants to reduce the topology of a molecular structure to a single numerical value that characterizes either the energy of that molecule as a whole or its molecular branching, its structural fragments or its orbitals and its electronic structure among others.

The topological index (TI) of a chemical structure or molecular graph is the final outcome of the logical and the mathematical operations that convert the facts stored in the chemical molecule into a numerical value or a beneficial number which is a graph invariant that characterizes the molecular properties (both physical and chemical) like boiling point, melting point, surface tension, molar fraction, molar volume, heat of vaporization and many more [14] and the structural features like bonding pattern, branching, symmetry, the neighboring pattern of atoms in that molecule [15, 16, 17]. It also describes the biological behavior of the compound such as lipophilicity, stimu-

lation of cell growth, toxicity, pH regulation and nutritives[18, 19, 20].
The quantitative relationship between the properties (or activities) of a molecule with its molecular structure is actually the basis of so called "quantitative structure versus property (activity) relationship (QSPR, QSAR)" studies. Here the term "property" refer to physico-chemical properties, whereas "activity" means the biological and pharmaceutical activities of that compound [21], where the environmental hazard assessment of a chemical is termed as quantitative structure versus toxicity relationship (QSTR) [22].
The QSTR focuses on identifying the properties directly from the molecular structure, where the trail and error method and the random screening for activity in pharmaceutical research is both time consuming and uneconomical. By using QSAR/QSPR the most promising compound is selected for the characteristic or property that is desirable, and thus reduces the number of compounds which needs to be manufactured during the designing process of new drugs [23, 24, 25]. The QSAR/QSPR studies are not only the powerful tool for environmental toxicology assessment, but they are also being used in chemical documentation, virtual screening lead optimization, combinatorial library design and isomer discrimination [26]. Wiener Herold [27] laid a good foundation for determining the correlation between molecular structure and its properties by considering the distances between atoms or more specifically the electron clouds by introducing the first eccentricity based topological index.
Here we list some of the results on a few eccentricity based topological indices.
Wiener Index. The first index proposed by Herold Wiener [27] in 1947 known as Wiener Index (WI) was used to analyze the chemical properties specificaly the boiling point of paraffins (alkanes). Weiner index in a chemical graph is defined as, the sum of the distances between all pairs of vertices and is given by;

$$WI(G) = \sum_{\{v_i,v_j\}\subset V_G} d_G(v_i, v_j).$$

This index can be used to determine the density of a chemical graph as well as the interaction between the atoms in it.
A similiar index to WI proposed by Klavazar and Gutman [28] in 1996 called Szeged

index denoted by Sz(G) is given as;

$$Sz(G) = \sum_{v_1 \in V(G)} n_{v_2}(v_1) n_{v_1}(v_2),$$

where $N_{v_2}(v_1) = \{v_3 \in V(G) \mid d(v_2, v_3) > d(v_1, v_3)\}$, and $n_{v_2}(v_1) = |N_{v_2}(v_1)|$. Some results on Wiener index and Szeged index are give in [29, 30]. In 2000, based of the considerable research on WI, and SzI, Khadikar [31] proposed edge Padmakar Ivan (PI_e) defined as;

$$PI_e = \sum_{e=v_1v_2 \in E(G)} \{n'_{v_2}(v_1) + n'_{v_1}(v_2)\},$$

where $n'_{v_2}(v_1) = \{e \in E(G) \mid d'(v_2, e) > d'(v_1, e)\}$, $n'_{v_2}(v_1) = |N'_{v_2}(v_1)|$. This index is used in the field of nanotechnology. Further application of PI_e index is investigated in [31, 32].

Eccentric connetivity index. Eccentric connectivity index of a graph G was introduced by Sharma et al. in 1997 [33] which is defined by;

$$\xi^c(G) = \sum_{v_i \in V_G} d_G(v_i) \epsilon(v_i).$$

This molecular descriptor is used to model pharmaceutical, chemical and other properties of a molecular graph. Since this index is applied to characterize the pharmaceutical compound and is mainly used in formation of anti-HIV compounds.

Kirchhoff Index. In an electrical network the resistance between any two arbitrary vertices can be obtained by studying the Laplacian matrix associated to that network in terms of the eigen values and eigen vectors associated to that matrix. The concept of resistance distance is widely used in chemical studies [34]. A novel distance function on graph named Kifchhoff index was proposed by Klein and Randic [34] which is defined as, the sum of the resistance distances between all the pairs of vertices. mathematically it is defined as

$$Kf(G) = \sum_{i<j} r_{ij},$$

where r_{ij} is the resistance between i^{th} and j^{th} vertex. Kirchhoff index can also defined as;

$$Kf(G) = n\sum_{i=1}^{n-1}\frac{1}{\mu_i},$$

where $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_{n-1} = 0$ are the eigen values of Laplacian matrix associated to that graph. As a molecular structure descriptor, the noteworthy applications of Kirchhoff index in chemistry is given in [35, 36].

Schultz index. Another molecular structure descriptor was introduced by Harry P. Schultz in 1989 [37] to characterize alkanes by an integer. Schultz named it "Molecular topological index" (MTI), which later became better known as "Schutlz index" is defined as;

$$Sc(G) = \frac{1}{2}\sum_{v_i,v_j \in V(G)}[d_G(v_i) + d_G(v_j)]d(v_i, v_j).$$

These molecular descriptors are found to be useful in design of molecules with desired properties. In [38] Dankelmann et al. established the relashionship betwen Wiener index and Gutman index or modified Schultz index and also found the upper bound on it. For more detailed study about this molecular descriptor readers can see the artile series [39, 40, 41, 42].

Total-Eccentricity Index. The total-eccentricity index of a graph introduced by Farooq et al. [43] is defined as;

$$\xi^t(G) = \sum_{v_i \in V_G}\epsilon(v_i).$$

Some results on total eccentricity index are found in literature [44, 45]. The average eccentricity index is defined as;

$$Ave(G) = \frac{1}{n}\sum_{(v_i \in V_G)}\epsilon(v_i).$$

The relationship between total eccentricity index and average eccentricity index is $Avg(G) = \frac{1}{|V_G|}\zeta(G)$. Eccentricity based topological indices are widely used in QSPR/QSAR studies. For further details on applications of eccentricity based indices readers are refered to [46, 47].

Detour index. In Graph theory, the concept of detour matrix was introduced by F Harary [48]. The (i, j) entry of the detour matrix records the length of longest distance between two pair of vertives v_i and v_j. This matrix attained some attention in the chemical literature [49]. Arnic and Trinajstic were the first to introduce Detour index defined as the sum of all entries above main diagonal of a detour matrix. Mathematically given as:

$$DI = \frac{1}{2} \sum_{v_i, v_j \in V_G} l_G(v_i, v_j).$$

Lukovits investigated the application of detour index in QSPR studies [50]. Followed by Lukovits works, Trinajstic et al. investigated the application of detour index in comparison with Wiener index in analyzing physical properties of molecular structures A multiple regression analysis has shown that the selected molecular properties which are size dependent (such as the boiling points of alkanes) has a correlation with both Wiener and detour index, and thus it is found to be efficient in structure-property relation modeling of cyclic and acyclic hydrocarbons.

Chapter 3

Maximal Trees with Fixed Pendant vertices w.r.t. NSC Number

In this chapter, we determine a tree with largest NSC number in the class of all n-vertex trees with fixed pendant vertices denoted by $\mathcal{T}(n,p)$. Let us denote the set of pendant vertices of a tree T by $P(T)$. Consider an n-vertex double broom with p pendant vertices $D_{n,p}$ defined in definition 1.3.3 and the class of n-vertex p-brooms $\mathcal{P}_n^p$ defined in definition 1.3.4. Here we present some results on graphs $D_{n,p}$ and $\mathcal{P}_n^p$.

3.1 NSC number of $D_{n,p}$ and $B \in \mathcal{P}_n^p$

Firstly, we will derive general formulas for the NSC number of $D_{n,p}$ and $B \in \mathcal{P}_n^p$ and then compare the results to prove that $N(B) < N(D_{n,p})$.

Lemma 3.1.1. Let $r = r(D_{n,p})$ and $d = d(D_{n,p})$. Then the NSC number of $D_{n,p}$ is given by

$$N(D_{n,p}) = \begin{cases} (r-1)(p+2)(r-2) + \dfrac{(r-2)(2r^2-5r+9)}{3} + \\ \left\lfloor \dfrac{p+2}{2} \right\rfloor \left(\left\lceil \dfrac{p+2}{2} \right\rceil (r-1) + 1 \right) + \left\lceil \dfrac{p+2}{2} \right\rceil (r) & \text{if } d \text{ is even} \\ (p+2)(r-3)(r-2) + \dfrac{2(r-3)(r^2-3r+8)}{3} + \\ \left\lceil \dfrac{p+2}{2} \right\rceil \left(\left\lfloor \dfrac{p+2}{2} \right\rfloor (r-2) + 2(r-1) \right) + 2\left\lfloor \dfrac{p+2}{2} \right\rfloor & \text{if } d \text{ is odd.} \end{cases} \tag{3.1}$$

Proof. We consider the two cases:

Case 1. When $d(D_{n,p})$ is even

In this case, the eccentricity sequence of $D_{n,p}$ is given by

$$\xi(D_{n,p}) = \{\epsilon_1^{\lceil \frac{p+2}{2} \rceil}, \epsilon_2^2, \ldots, \epsilon_{k-2}^2, \epsilon_{k-1}^{\lfloor \frac{p+2}{2} \rfloor}, \epsilon_k^1\}. \tag{3.2}$$

Using formula (2.2), we obtain

$$\begin{aligned} N(D_{n,p}) &= 2\left\lceil \frac{p+2}{2} \right\rceil \frac{(k-3)(k-2)}{2} + \left\lceil \frac{p+2}{2} \right\rceil \left\lfloor \frac{p+2}{2} \right\rfloor (k-2) + \left\lceil \frac{p+2}{2} \right\rceil (k-1) \\ &+ 2.2\sum_{m=1}^{k-4} \frac{m(m+1)}{2} + 2\left\lfloor \frac{p+2}{2} \right\rfloor \frac{(k-3)(k-2)}{2} + (k-1)(k-2) \\ &- 2 + \left\lfloor \frac{p+2}{2} \right\rfloor \\ &= \left\lceil \frac{p+2}{2} \right\rceil \left\lfloor \frac{p+2}{2} \right\rfloor (k-2) + \left\lceil \frac{p+2}{2} \right\rceil (k-3)(k-2) + \left\lceil \frac{p+2}{2} \right\rceil (k-1) \\ &+ \left\lfloor \frac{p+2}{2} \right\rfloor (k-3)(k-2) + \left\lfloor \frac{p+2}{2} \right\rfloor + \frac{2(k-4)(k-3)(k-2)}{3} \\ &+ (k-2)(k-1) - 2 \end{aligned}$$

Since $d(D_{n,p})$ is even therefore $k = r + 1$. Thus equation (3.3) can be written as

$$\begin{aligned} N(D_{n,p}) &= \left\lceil \frac{p+2}{2} \right\rceil \left\lfloor \frac{p+2}{2} \right\rfloor (r-1) + (r-1)(r-2)(p+2) + \left\lceil \frac{p+2}{2} \right\rceil (r) \\ &+ \left\lfloor \frac{p+2}{2} \right\rfloor + \frac{2(r-3)(r-2)(r-1) + 3(r-1)r - 6}{3} \\ &= \frac{(r-2)(2r^2 - 5r + 9)}{3} + (p+2)(r-2)(r-1) + \left\lceil \frac{p+2}{2} \right\rceil (r) \\ &+ \left\lfloor \frac{p+2}{2} \right\rfloor \left(\left\lceil \frac{p+2}{2} \right\rceil (r-1) + 1 \right). \end{aligned} \tag{3.3}$$

Case 2. When $d(D_{n,p})$ is odd

In this case, the eccentricity sequence of $D_{n,p}$ is given by

$$\xi(D_{n,p}) = \{\epsilon_1^{\lceil \frac{p+2}{2} \rceil}, \epsilon_2^2, \ldots, \epsilon_{k-2}^2, \epsilon_{k-1}^{\lfloor \frac{p+2}{2} \rfloor}, \epsilon_k^2\}. \tag{3.4}$$

Again using the formula (2.2), we obtain

$$\begin{aligned} N(D_{n,p}) &= \left\lceil \frac{p+2}{2} \right\rceil (k-3)(k-2) + \left\lceil \frac{p+2}{2} \right\rceil \left\lfloor \frac{p+2}{2} \right\rfloor (k-2) + 2\left\lceil \frac{p+2}{2} \right\rceil (k-1) \\ &\quad + 4\sum_{m=1}^{k-4} \frac{m(m+1)}{2} + \left\lfloor \frac{p+2}{2} \right\rfloor (k-2)(k-3) + 2(k-2)(k-1) - 4 \\ &\quad + 2\left\lceil \frac{p+2}{2} \right\rceil \\ &= \left(\left\lceil \frac{p+2}{2} \right\rceil + \left\lfloor \frac{p+2}{2} \right\rfloor \right)(k-3)(k-2) + \left\lceil \frac{p+2}{2} \right\rceil \left\lfloor \frac{p+2}{2} \right\rfloor (k-2) \\ &\quad + 2\left\lceil \frac{p+2}{2} \right\rceil (k-1) + \frac{2(k-2)\{(k-3)(k-4)+3(k-1)\}-12}{3} \\ &\quad + 2\left\lfloor \frac{p+2}{2} \right\rfloor \\ &= (p+2)(k-3)(k-2) + \left\lceil \frac{p+2}{2} \right\rceil \left\lfloor \frac{p+2}{2} \right\rfloor (k-2) + 2\left\lceil \frac{p+2}{2} \right\rceil (k-1) \\ &\quad + 2\left\lfloor \frac{p+2}{2} \right\rfloor + \frac{2(k-3)(k^2-3k+8)}{3} \end{aligned}$$

Since $d(D_{n,p})$ is odd therefore $k=r$. Now above can be written as

$$\begin{aligned} N(D_{n,p}) &= \frac{2(r-3)(r^2-3r+8)}{3} + (p+2)(r-3)(r-2) + 2\left\lfloor \frac{p+2}{2} \right\rfloor \\ &\quad + \left\lceil \frac{p+2}{2} \right\rceil \left(\left\lfloor \frac{p+2}{2} \right\rfloor (r-2) + 2r - 2 \right). \end{aligned} \tag{3.5}$$

The proof is complete. □

In next lemma, we give NSC number of p-broom in $\mathcal{P}_n^p$

Lemma 3.1.2. Let $B \in \mathcal{P}_n^p$ be a p-broom with radius r and eccentricity sequence given by (1.3). Then NSC number of B is given by

$$N(B) = \begin{cases} (p+2)(r-2)(r-1) + l_1 l_{k-1}(r-1) + l_1(r+s-1) + l_{k-1}(r-s+1) & \\ \quad + (s-2)(s-1) + \dfrac{(r-1)(2r^2-7r+12)}{3} + (r-s)^2 & \text{if } d \text{ is even,} \\ (p+2)(r-3)(r-2) + l_1 l_{r-1}(r-2) + l_1(2r+s-3) + l_{k-1}(r-s+1) & \\ (s-2)(s-1) + \dfrac{2(r-2)(r^2)-4r+9}{3} + (r-s-2)(r-s) - 2 & \text{if } d \text{ is odd.} \end{cases} \tag{3.6}$$

Proof. We have following two cases for p-broom.

Case 1. When $d(B)$ is even

Then the eccentricity sequence is given by

$$\xi(B) = \{\epsilon_1^{\lceil \frac{p+2}{2} \rceil}, \epsilon_2^2, \ldots, \epsilon_s^3, \ldots, \epsilon_{k-2}^2, \epsilon_{k-1}^{\lfloor \frac{p+2}{2} \rfloor}, \epsilon_k^1\}. \tag{3.7}$$

Using formula (2.2), we obtain

$$\begin{aligned} N(B) &= l_1(k-2)(k-3) + l_1 l_{k-1}(k-2) + l_1(k+s-2) + l_{k-1}(k-2)(k-3) \\ &+ \frac{2(k-2)(k-3)(k-4)}{3} + (k-2)(k-1) - 1 + (s-2)(s-1) \\ &+ (k-s-2)(k-s-1) + l_{k-1}(k-s) + (k-s) \\ &= (l_1 + l_{k-1})(k-3)(k-2) + l_1 l_{k-1}(k-2) + l_1(k+s-2) + l_{k-1}(k-s) \\ &+ \frac{(k-2)(2k^2-11k+21)}{3} + (k-s-1)^2 + (s-2)(s-1). \end{aligned} \tag{3.8}$$

Since $d(B)$ is even therefore we have $k = r+1$. Also substituting $l_1 + l_{k-1} = p+2$ we obtain

$$\begin{aligned} N(B) &= (p+2)(r-1)(r-2) + l_1 l_{k-1}(r-1) + l_1(r+s-1) + l_{k-1}(r-s+1) \\ &+ (s-2)(s-1) + \frac{(r-1)(2r^2-7r+12)}{3} + (r-s)^2. \end{aligned}$$

Case 2. When $d(B)$ is odd

Then we have the following eccentricity sequence

$$\xi(B) = \{\epsilon_1^{\lceil \frac{p+2}{2} \rceil}, \epsilon_2^2, \ldots, \epsilon_s^3, \ldots, \epsilon_{k-2}^2, \epsilon_{k-1}^{\lfloor \frac{p+2}{2} \rfloor}, \epsilon_k^2\}. \tag{3.9}$$

By equation (2.2) we have

$$\begin{aligned} N(B) &= l_1(k-3)(k-2) + l_1 l_{k-1}(k-2) + l_1(2k+s-3) + l_{k-1}(k-3)(k-2) \\ &+ \frac{2(k-4)(k-3)(k-2)}{3} + (k-2)(k-1) - 4 + (s-2)(s-1) + (k-s) \\ &+ (k-s-2)(k-s-1) + l_{k-1}(k-s+1) \\ &= (l_1 + l_{k-1})(k-2)(k-3) + l_1 l_{k-1}(k-2) + l_1(2k+s-3) +_{k-1} (k-s+1) \\ &+ (s-2)(s-1) + \frac{2(k-2)(k^2) - 4k + 9}{3} + (k-s-2)(k-s) - 2 \end{aligned}$$

When $d(B)$ is odd we have $k = r$, this implies

$$\begin{aligned} N(B) &= (p+2)(r-3)(r-2) + l_1 l_{r-1}(r-2) + l_1(2r+s-3) + l_{k-1}(r-s+1) \\ &+ (s-2)(s-1) + \frac{2(r-2)(r^2) - 4r + 9}{3} + (r-s-2)(r-s) - 2. \end{aligned}$$

□

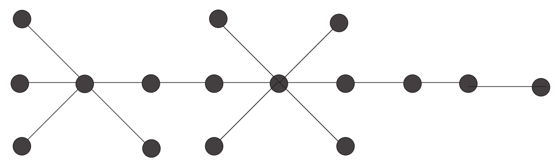


Figure 3.1: Double broom $D_{16,9}$

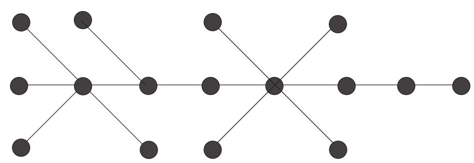


Figure 3.2: p-double broom $B \in \mathcal{P}_{16}^{10}$

3.2 Some results on graphs in $\mathcal{T}(n, p)$

We have generalized the formula for NSC number of a double broom $D_{n,p}$ and a p-broom $B \in \mathcal{P}_n^p$ in Lemma 3.1.1 and Lemma 3.1.2. Now we use those results to prove $N(D_{n,p}) > N(B)$.

Theorem 3.2.1. For $n \geq 4$, we have $N(D_{n,p}) > N(B)$ for any $B \in \mathcal{P}_n^p$.

Proof. Consider an n-vertex p-broom $B \in \mathcal{P}_n^p$. We divide the proof into two cases:

Case 1 When $d(B)$ is odd.

In this case, the eccentricity sequence of B is given by equation (3.9). We know that the $d(B) = n - p$ and $d(D_{n,p}) = n - p + 1$. Hence $d(D_{n,p})$ is even with the eccentricity sequence

$$\xi(D_{n,p}) = \{(e_1 + 1)^{\lceil \frac{p+2}{2} \rceil}, e_1^2, e_2^2, \ldots, e_{k-2}^2, e_{k-1}^{\lfloor \frac{p+2}{2} \rfloor}, e_k^1\}. \tag{3.10}$$

Now using equations (3.7) and (3.10) and formula (2.2), we have

$$\begin{aligned} N(D_{n,p}) - N(B) &= 2(s-2)(k-s-1) + \left\lceil \frac{p+2}{2} \right\rceil (k-s) + \left\lfloor \frac{p+2}{2} \right\rfloor (k+s-4) \\ &\quad + \left\lceil \frac{p+2}{2} \right\rceil \left(\left\lfloor \frac{p+2}{2} \right\rfloor - 1 \right) + 2 > 0. \end{aligned}$$

Therefore, $N(D_{n,p}) > N(B)$.

Case 2 When $d(B)$ is even.

The eccentricity sequence of B with even diameter is given by equation (3.7), and eccentric sequence of $D_{n,p}$ is given in equation (3.4) with $\xi(D_{n,p}) = \xi(B)$. Thus, we can easily prove that

$$\begin{aligned} N(D_{n,p}) - N(B) &= \left\lceil \frac{p+2}{2} \right\rceil (k-s) + 2(s-2)(k-s) + (k-s+1)(k-s-2) \\ &+ 2(k-s). \end{aligned}$$

This implies, $N(D_{n,p}) > N(B)$.

The proof is complete. □

It is obvious that corresponding to any n-vertex tree T with p number of pendant vertices, there is a caterpillar H satisfying $\xi(T) = \xi(H)$ and vice versa. We can see that $P(T) \leq P(H)$. Let $q = p+a$, where $a \geq 0$, denote the number of pendant vertices in H that are not pendant vertices in T. Our aim is to construct a tree $T_1 \in \mathcal{T}(n,p)$ such that $N(T) < N(T_1)$. By using next lemmas, we will construct a sequence of trees $H_1, H_2, \ldots, H_m$ in $\mathcal{T}(n,p)$ such that $N(T) < N(T_1) < N(T_2) < \cdots < N(T_m)$.

Lemma 3.2.1. Let $T \in \mathcal{T}(n,p)$ such that $T \ncong D_{n,p}$, $T \notin \mathcal{P}_n^p$ and

$$\xi(T) = \{\epsilon_1^{l_1}, \epsilon_2^{l_2}, \ldots, \epsilon_s^{l_s}, \ldots, \epsilon_k^{l_k}\},$$

where $2 \leq s \leq k-1$ and $l_s > 3$. Then there exists $T_1 \in \mathcal{T}(n,p)$ such that $d(T_1) = d(T) + 2$ and $N(T_1) > N(T)$.

Proof. Let H be an n-vertex caterpillar such that $\xi(T) = \xi(H)$. Also let P be a diametrical u,v-path in H and uwz be a path of length 2 on P, where w is the neighbor of u on P. Since $T \ncong D_{n,p}$ and $T \notin \mathcal{P}_n^p$ therefore there exist two pendant vertices x_1, x_2 other than u and v such that $\epsilon(x_1) = \epsilon_s$ and $\epsilon(x_2) = \epsilon_t$, where $1 \leq s, t \leq (k-1)$ and s and t are the least integers for which $l_s + l_t \geq 6$. Also let y_1 and y_2 be the neighbors of x_1 and x_2, respectively, on P. Now construct a caterpillar H_1 such that

$$H_1 \cong \{H - \{x_1y_1, x_2y_2\}\} \cup \{wx_1, x_1z, vx_2\}. \tag{3.11}$$

Here we have two different cases for l_s:

Case 1 When $l_s = 3$.

In this case $\epsilon_s \neq \epsilon_t$. We will prove the result when $s - t = 1$ and when $s - t \neq 1$. Firstly, assume that $s - t \neq 1$. We have two possibilities, that is, either $s = 1$ or $s > 1$. For $s = 1$ the eccentricity sequence for H_1 is given by

$$\xi(H_1) = \{(\epsilon_1 + 2)^{l_1 - 1}, (\epsilon_1 + 1)^2, (\epsilon_2 + 1)^2, \ldots, (\epsilon_t + 1)^{l_t - 1}, \ldots, (\epsilon_k + 1)^{l_k}\}.$$

Hence by using formula (2.2) we have,

$$N(H_1) \;\; = \;\; N(H) + (l_1 - 1)(t - 2) + \sum_{i=t}^{k} l_i(l_1 + t - 2) > 0.$$

Now for $s > 1$, H_1 has the eccentricity sequence of the form

$$\begin{aligned}\xi(H_1) \;\; = \;\; & \{(\epsilon_1 + 2)^2, (\epsilon_1 + 1)^2, (\epsilon_2 + 1)^2, \ldots, (\epsilon_s + 1)^{l_s - 1}, (\epsilon_{s+1} + 1)^2, \ldots, \\ & (\epsilon_t + 1)^{l_t - 1}, \ldots, (\epsilon_k + 1)^{l_k}\}.\end{aligned}$$

Therefore by using formula (2.2) we have

$$N(H_1) \;\; = \;\; N(H) + \sum_{i=t}^{k} l_i(s + t) + 2s(t - s) + 2s > 0.$$

This implies $N(H_1) > N(H)$.

Now, if $s - t = 1$ then for $s = 1$ the eccentricity sequence for H_1 is given by

$$\xi(H_1) \;\; = \;\; \{(\epsilon_1 + 2)^{l_1 - 1}, (\epsilon_1 + 1)^2, (\epsilon_2 + 1)^{l_2 - 1}, \ldots, (\epsilon_k + 1)^{l_k}\}. \tag{3.12}$$

When $s > 1$, we have

$$\xi(H_1) = \{(\epsilon_1 + 2)^2, (\epsilon_1 + 1)^2, (\epsilon_2 + 1)^2, \ldots, (\epsilon_s + 1)^{l_s - 1}, (\epsilon_t + 1)^{l_t - 1}, \ldots, (\epsilon_k + 1)^{l_k}\}. \tag{3.13}$$

Hence by equations (3.12) and (3.13) and formula (2.2) we can easily prove that $N(H_1) > N(H)$.

Case 2 When $l_s > 3$.

In this case $\epsilon_s = \epsilon_t$. We have two possibilities, that is, $s = 1$ and $s > 1$. Firstly, assume that $s = 1$. Here the eccentricity sequence of H_1 is given by

$$\xi(H_1) = \{(\epsilon_1 + 2)^{l_2-2}, (\epsilon_1 + 1)^2, (\epsilon_2 + 1)^{l_2}, \ldots, (\epsilon_k + 1)^{l_k}\}. \tag{3.14}$$

Hence by using formula (2.2) we have

$$N(H_1) \quad = \quad N(H) + 2(l_1 - 2) + \sum_{i=2}^{k} l_1(l_1 - 2) > 0.$$

Now for $s > 1$ we have

$$\xi(H_1) = \{(\epsilon_1 + 2)^2, (\epsilon_1 + 1)^2, (\epsilon_2 + 1)^2, \ldots, (\epsilon_s + 1)^{l_s-2}, \ldots, (\epsilon_k + 1)^{l_k}\}. \tag{3.15}$$

Hence by using formula (2.2) we can easily prove that $N(H_1) > N(H)$.

The proof is complete. □

Lemma 3.2.1 is applicable if $a \geq 2$. By the iterative application of Lemma 3.2.1 we get a caterpillar H_m having diameter $(n - p + 1)$ or $(n - p)$ for even and odd a, respectively.

In Lemma 3.2.2 we will transform caterpillar F, obtained after applying Lemma 3.2.1, into a new caterpillar by choosing the pendant vertices with greatest possible eccentricities. The application of Lemma 3.2.2 will give a caterpillar with $l_1 = \lceil \frac{p+2}{2} \rceil$.

Lemma 3.2.2. Let $T \in \mathcal{T}(n, p)$ such that $T \ncong D_{n,p}$, $T \notin \mathcal{P}_n^p$ and

$$\xi(T) = \{\epsilon_1^{l_1}, \epsilon_2^{l_2}, \ldots, \epsilon_s^{l_s}, \ldots, \epsilon_k^{l_k}\},$$

where $2 \leq s \leq k - 1$, $l_1(T) < \lceil \frac{p+2}{2} \rceil$ and $l_s > 3$. Then there exist a tree $T_1 \in \mathcal{T}(n, p)$ such that $l_1(T_1) = l_1(T) + 1$ and $N(T_1) > N(T)$.

Proof. Let F be a caterpillar such that $\xi(T) = \xi(F)$ and either $P(F) = P(T)$ or $P(F) = P(T) + 1$.

Consider a diametrical u, v-path P in F and w be the neighbor of u on P. Let x be a pendant vertex other than u and v such that $\epsilon_1 \neq \epsilon(x) = \epsilon_s$, where $2 \leq s \leq (k-1)$. Also let y be the neighbor of x on P. Now construct a caterpillar F_1 such that

$$F_1 \cong \{F - \{xy\}\} \cup \{wx\}. \tag{3.16}$$

Hence the eccentricity sequence for F_1 is given by

$$\xi(F_1) = \{\epsilon_1^{l_1+1}, \epsilon_2^2, \ldots, \epsilon_s^{l_s-1} \ldots, \epsilon_k^{l_k}\}.$$

Therefore by using formula (2.2) and simplifying we obtain

$$N(F_1) = N(F) + \sum_{i=s}^{k} l_i(s-1) - (l_1+1)(s-1). \tag{3.17}$$

We know that each l_i can be written as

$$l_i = l'_i + 2, \tag{3.18}$$

where l'_i is the number of pendant vertices in F. Also, $l_1(F) < \lceil \frac{p+2}{2} \rceil$ and $l_i = 2$ for each $2 \leq i \leq (s-1)$. Therefore by (3.18) we have

$$\begin{aligned}\sum_{i=s}^{k} l_i(s-1) &= \sum_{i=s}^{k-1}(l'_i + 2)(s-1) + l_k(s-1)\\ &= \sum_{i=s}^{k-1} l'_i(s-1) + \sum_{i=s}^{k-1} 2(s-1) + l_k(s-1).\end{aligned}$$

As $l_1(F) < \lceil \frac{p+2}{2} \rceil$, which gives

$$\sum_{i=s}^{k} l'_i \geq \left\lceil \frac{p+2}{2} \right\rceil.$$

Hence

$$\sum_{i=s}^{k} l'_i(s-1) - (l_1+1)(s-1) \geq 0.$$

So, equation (3.17) can be written as

$$N(F_1) = N(F) + \sum_{i=s}^{k} l'_i(s-1) - (l_1+1)(s-1) + \sum_{s}^{k} 2(s-1) > 0.$$

Therefore, $N(F_1) > N(F)$.

This completes the proof. $\square$

In Lemma 3.2.3 we will transform the caterpillar W, obtained by the application of Lemma 3.2.2, into a new caterpillar by choosing the pendant vertices with smallest possible eccentricities. The application of Lemma 3.2.3 will give a caterpillar with $l_{k-1} = \lceil \frac{p+2}{2} \rceil$.

Lemma 3.2.3. Let $T \in \mathcal{T}(n,p)$ such that $T \ncong D_{n,p}$, $T \notin \mathcal{P}_n^p$ and

$$\xi(T) = \{\epsilon_1^{l_1}, \epsilon_2^{l_2}, \ldots, \epsilon_s^{l_s}, \ldots, \epsilon_k^{l_k}\},$$

where $2 \le s \le k-1$, $l_1(T) = \lceil \frac{p+2}{2} \rceil$ and $l_s > 3$. Then there exist a tree $T_1 \in \mathcal{T}(n,p)$ such that $l_{k-1}(T_1) = l_{k-1}(T) + 1$ and $N(T_1) > N(T)$.

Proof. Let W be a caterpillar such that $\xi(T) = \xi(W)$ and either $P(W) = P(T)$ or $P(W) = P(T) + 1$.

Consider a diametrical u,v-path P in W and w be the neighbor of u on P. Let x be a pendant vertex other than u and v such that $\epsilon_1 \ne \epsilon(x) = \epsilon_s$, where $2 \le s \le k-2$. Also let y be the neighbor of x on P. Now construct a caterpillar W_1 such that

$$W_1 \cong \{W - \{xy\}\} \cup \{wx\}. \tag{3.19}$$

Hence the eccentricity sequence for W_1 is given by

$$\xi(W_1) = \{\epsilon_1^{l_1}, \epsilon_2^{l_2}, \ldots, \epsilon_s^{l_s-1}, \epsilon_{s+1}^2 \ldots, \epsilon_{k-1}^{l_{k-1}+1}, \epsilon_k^{l_k}\}.$$

Therefore by using formula (2.2) and simplifying we obtain

$$\begin{aligned} N(W_1) = N(W) &+ [l_1 - l_{k-1} - 1][k-s-1] + \sum_{i=2}^{s-1} l_i(k-s-1) \\ &+ [l_s - l_k][k-s-1]. \end{aligned}$$

Since $l_1 = \lceil \frac{p+2}{2} \rceil$, therefore $l_{k-1} < \lfloor \frac{p+2}{2} \rfloor$. Hence $l_1 - l_k > 1$. Also $l_s > 3$ and $l_k \le 2$. Therefore, $l_s - l_k > 0$. This implies $N(W_1) > N(W)$.
This finishes the proof. $\square$

3.3 Maximal graph in $\mathcal{T}(n,p)$

Theorem 3.3.1. *Among all n vertex tree graphs $T \in \mathcal{T}(n,p)$ the graph $D_{n,p}$ has the maximum* NSC number.

Proof. For any arbitrary graph $T \in \mathcal{T}(n,p)$ their exist a corresponding caterpiller H with $\xi(H) = \xi(T)$ such that $P(H) \geq P(T)$ say $P(H) = q = p + a$, where $a \geq 0$. If $a \geq 2$, then, Lemma 3.2.1 can be applied $\lfloor \frac{a}{2} \rfloor$ times to get a caterpiller, say $H^{'}$ with $P(H^{'}) \leq p + 1$. Now applying Lemma 3.2.2 and Lemma 3.2.3, $H^{'}$ can be transformed to $H^{''}$ such that either $H^{''} \cong D_{n,p}$ if $P(H^{''}) = p$ or $H^{''} \in \mathcal{P}_n^p$ if $P(H^{''}) = p + 1$ satisfying $N(H) < N(H^{'}) < N(H^{''})$. Thus, Theorem 3.2.1 implies $H^{''} \cong D_{n,p}$ attains the maximum value w.r.t NSC number in the class $\mathcal{T}(n,p)$. The proof is complete. □

3.4 Conclusion

We considered the problem of finding maximal graphs with respect to NSC number in the class $\mathcal{T}(n,p)$ of all n order tree graphs on $n \geq 4$ with p pendant vertice. We found the unique graph $D_{n,p}$ which attains the maximum value of NSC number in class $\mathcal{T}(n,p)$. We formulated the general mathematical formula for the maximum NSC number for $T \in \mathcal{T}(n,p)$ given by

$$N(T) \leq \begin{cases} (p+2)(r-2)(r-1) + \dfrac{(r-2)(2r^2-5r+9)}{3} + \\ \left\lfloor \dfrac{p+2}{2} \right\rfloor \left(\left\lceil \dfrac{p+2}{2} \right\rceil (r-1) + 1 \right) + \left\lceil \dfrac{p+2}{2} \right\rceil (r) & \text{if } d(T) \text{ is even,} \\ (p+2)(r-3)(r-2) + \dfrac{2(r-3)(r^2-3r+8)}{3} + \\ \left\lceil \dfrac{p+2}{2} \right\rceil \left(\left\lfloor \dfrac{p+2}{2} \right\rfloor (r-2) + 2(r-1) \right) + 2\left\lfloor \dfrac{p+2}{2} \right\rfloor & \text{if } d(T) \text{ is odd.} \end{cases} \tag{3.20}$$

Chapter 4

Maximal graph w.r.t. NSC number in the class of unicyclic graphs with some fixed parameters

In this chapter, we determine a unicyclic graph with largest NSC number in a class of n-vertex unicyclic graphs with some fixed parameters, that is, fixed degree Δ and atmost three central vertices. We denote this class by $\mathcal{U}_n(3, \Delta)$.

4.1 Preliminaries

We use the notation $\mathcal{U}_n$ for the class of n-vertex unicyclic graphs and the notation $\mathcal{U}_{n,l}$ for n-vertex graphs containing cycle C_l.

Theorem 4.1.1 ([51]). *Center of a unicyclic graph U is contained in a block of U. This implies, for any unicyclic graph $U \in \mathcal{U}_n$ containing unique cycle C_l, either $\mathbf{C}(U) = K_1$ or K_2 or $\mathbf{C}(U) \subset C_l$.*

We are considering the class $\mathcal{U}_n(3, \Delta)$ that contains the graphs with atmost three central vertices. It is obvious to see that corresponding to any n-vertex unicyclic graph $U \in \mathcal{U}_n$ with center either K_1 or K_2, we can find a caterpiller $T \in \mathcal{T}_n$ with center K_1 or K_2 and all pendant vertices on a unique diametrical path, such that, $d(U) = d(T) = d$, $\xi(U) = \xi(T)$ and hence $N(U) = N(T)$. When U is a graph with eccentricity sequence given by

$$\xi(U) = \{\epsilon_1^{l_1}, \epsilon_2^{l_2}, \ldots, \epsilon_{k-1}^{l_{k-1}}, \epsilon_k^{l_k}\}, \tag{4.1}$$

where $l_k = 1$ or 2 and diameter $d(U) = d$, we can obtain the corresponding caterpiller by taking a diametrical path , say u, v-path of length d and adding pendant vertices on u, v-path for $l_m \geq 3$ in (4.1) for all $m \in \{1, 2, \ldots, k-1\}$. In a similar way, for any graph $U \in \mathcal{U}_{n,l}$ with 3 central vertices we can find a uicyclic graph $U_1 \in \mathcal{U}_{n,3}$ with center $\mathbf{C}(U_1) = K_3 = C_3$ and all pendant vertices on a unique diametrical path in U_1 such that, $\xi(U) = \xi(U_1)$. Hence $N(U) = N(U_1)$. Thus we consider the corresponding caterpiller T for graphs in $U \in \mathcal{U}_n(3, \Delta)$ with 1 or 2 central vertices and consider the corresponding graph U_1 for $U \in \mathcal{U}_n(3, \Delta)$ with 3 central vertices for our convenience in proving the results.
Now, we define some special graphs in $\mathcal{U}_n(3, \Delta)$.

A *cyclic broom* denoted by $\widetilde{U}_{n,3}$, is a unicyclic graph of order n with maximum degree Δ and diameter $d = n - \Delta + 1$ such that, $\Delta - 3$ pendant vertices are adjacent to a single vertex ,say v, of eccentricity $d - 1$. Also $\widetilde{U}_{n,3}$ has a cycle C_3 at vertex v, such that, $deg(v) = \Delta$. The eccentricity sequence of cyclic broom is of the form

$$\xi(\widetilde{U}_{n,3}) = \{\epsilon_1^{\Delta}, \epsilon_2^{2}, \epsilon_3^{2} \ldots, \epsilon_{k-1}^{2}, \epsilon_k^{l_k}\}, \tag{4.2}$$

where $l_k = 1$ or 2 respectively for cyclic broom with even and odd diameter.

Replacing the cycle C_3 in $\widetilde{U}_{n,3}$ with 2 pendant vertices, we get a tree graph called *broom* [52], denoted by $\mathcal{B}_{n,0}^{\Delta}$ with the same eccentricity sequence given in (4.2), where *1-broom* [52], denoted by $\mathcal{B}_{n,1}^{\Delta}$ is again a tree of order n with $\Delta + 1$ pendant vertices and eccentricity sequence of the form

$$\xi(\mathcal{B}_{n,1}^{\Delta}) = \{\epsilon_1^{\Delta}, \epsilon_2^{2}, .., \epsilon_{i-1}^{2}, \epsilon_i^{3}, \epsilon_{i+1}^{2}, \ldots, \epsilon_{k-1}^{2}, \epsilon_k^{l_k}\},$$

where, $2 \leq i \leq k-1$.
Firstly, we give the general expression for the NSC number of n-vertex cyclic broom, then present some lemmas on unicyclic graphs $U \in \mathcal{U}_n(3, \Delta)$.

Theorem 4.1.2. *Let $\widetilde{U}_{n,3} \in \mathcal{U}_n(3,\Delta)$ be a graph of diameter d. Then the* NSC *number of $\widetilde{U}_{n,3}$ is given by;*

$$N(\widetilde{U}_{n,3}) = \begin{cases} \left(\dfrac{2\Delta^2(\Delta-n-3)+2\Delta(3n+2)+n(n^2-1)}{12}\right) & \text{if } d \text{ is even,} \\ \left(\dfrac{\Delta^2(2\Delta-3n-6)+2\Delta(3n+2)+n^2(n-4)}{12}\right) & \text{if } d \text{ is odd.} \end{cases} \tag{4.3}$$

Proof. We have following two cases:

Case 1: When $d(\widetilde{U}_{n,3})$ is even

In this case the eccentricity sequence of $\widetilde{U}_{n,3}$ is given by (4.2) with $l_k = 1$ Using definition (2.2) and simplifying, we obtain

$$N(\widetilde{U}_{n,3}) = \Delta(k-1)^2 + (k-2)(k-1)\left(\frac{2k-3}{3}\right). \tag{4.4}$$

For $l_k = 1$ equation (4.2) implies $n = 2(k-2)+\Delta+1$. It holds that $k = \left(\frac{n+3-\Delta}{2}\right)$. So equation (4.4) becomes,

$$N(\widetilde{U}_{n,3}) = \frac{2\Delta^2(\Delta-n-3)+2\Delta(3n+2)+n(n^2-1)}{12}.$$

Case 2: When $d(\widetilde{U}_{n,3})$ is odd

Then the eccentricity sequence of $\widetilde{U}_{n,3}$ is given by (4.2) with $l_k = 2$. Using definition (2.2) and simplifying, we obtain

$$N(\widetilde{U}_{n,3}) = \left((k-1)k\Delta + \frac{2(k-2)(k-1)k}{3}\right). \tag{4.5}$$

Since $n = 2(k-1)+\Delta$, it holds that $k = \left(\frac{n+2-\Delta}{2}\right)$. So equation (4.5) becomes

$$N(\widetilde{U}_{n,3}) = \frac{\Delta^2(2\Delta-3n-6)+2\Delta(3n+2)+n^2(n-4)}{12}.$$

This completes the proof. $\square$

Remark. *The n-vertex graphs $B^{\Delta}_{n,0}$ and $\widetilde{U}_{n,3}$ have same* NSC number. Since $\xi(B^{\Delta}_{n,0}) = \xi(\widetilde{U}_{n,3})$, it holds that $N(B^{\Delta}_{n,0}) = N(\widetilde{U}_{n,3})$.

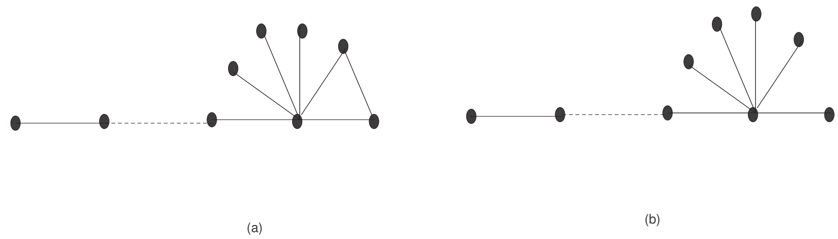


Figure 4.1: Graphs with same NSC number

4.2 Some graph transformations

Lemma 4.2.1. *Let $U \in \mathcal{U}_n$ be a unicyclic graph with atmost 3 central vertices and the eccentricity sequence of U given by*

$$\xi(U) \quad = \quad \{\epsilon_1^{l_1}, \epsilon_2^{l_2}, \ldots, \epsilon_k^{l_k}\}. \tag{4.6}$$

If $n \geq 2(k-1)+l_k+2$ (or equivalently $n \geq 2k+l_k$), then, there exists a unicyclic graph $U^{'} \in \mathcal{U}_n$ with either $d(U^{'}) = d(U)+2$ or $r(U^{'}) = r(U)+1$ such that $N(U^{'}) > N(U)$.

Proof. For our convenience, we consider the corresponding graph say U_1, where $U_1 \cong T$ (caterpiller) when $|V_{\mathbf{C}(U)}|= 1$ or 2 and $U_1 \cong U_{n,3}$ (unicyclic graph) when $|V_{\mathbf{C}(U)}|= 3$ discussed in Section 4.1 satisfying $N(U) = N(U_1)$. Let P be a diametrical u, v-path in U. If $n < 2k + l_k$. then U may have atmost one pendant vertex other than u, v. So we consider all graphs of order $n \geq 2k + l_k$. Also, let x_1, x_2 be two pendant vertices other than u, v with y_1, y_2 be the neighbors of x_1 and x_2 respectively on P with $\epsilon(x_1) = \epsilon_i$ and $\epsilon(x_2) = \epsilon_j$. Here we choose x_1 with $\epsilon(x_1) = \epsilon_i$ and x_2 with $\epsilon(x_2) = \epsilon_j$ such that, i, j are the least integers for which $l_i + l_j \geq 6$ and $j > i$. Now construct $U^{'}$ defined as

$$U^{'} \quad \cong \quad \{U_1 - \{x_1, x_2\}\} \cup \{ux_1, vx_2\}. \tag{4.7}$$

Then, the eccentricity sequence for $U^{'}$ is given by

$$\xi(U^{'}) \quad = \quad \{(\epsilon_1+2)^2, (\epsilon_1+1)^{l_1}, \epsilon_1^{l_2}, \ldots, \epsilon_{i-1}^{l_i-1}, \ldots, \epsilon_{j-1}^{l_j-1}, \ldots, \epsilon_{k-1}^{l_k}\}, \tag{4.8}$$

where $l_m = 2$ for $m \in \{1, \ldots, (j-1)\}\backslash\{i\}$. Using (2.2) the NSC of $U^{'}$ is given by

$$\begin{aligned} N(U^{'}) &= N(U_1) - 2(i+j) - \sum_{m=i+1}^{j-1} l_m(j-m) - \sum_{m=i+1}^{k} l_m(m-i) \\ &+ 2\sum_{m=1}^{k} ml_m + (1-l_i)(j-i) - \sum_{m=1}^{i-1} l_m(i+j-2m) - \sum_{m=j+1}^{k} l_m(m-j) \\ &= N(U_1) + \sum_{m=1}^{i-1} l_m(4m-i-j) + \sum_{m=i+1}^{j-1} l_m(2m+i-j) + \sum_{m=j+1}^{k} l_m(i+j) \\ &+ \{(2il_i - 2i) + (2jl_j - 2j)\} + (j-i)(1-l_i-l_j). \end{aligned}$$

We have following two possibilities:

(i) If $\epsilon_i \neq \epsilon_j$, then $l_i = 3$. Thus substituting $l_m = 2$ for $m \in \{1, \ldots, (j-1)\}\backslash\{i\}$ and after simplification we get

$$\begin{aligned} N(U^{'}) = N(U_1) + \sum_{m=j+1}^{k} l_m(i+j) + 2i\{(l_i-2) + (j-i)\} \\ + (i+j)(l_j-2). \end{aligned} \tag{4.9}$$

(ii) If $l_i > 3$, then $i = j$. Hence the eccentricity sequence in equation (4.8) reduces to

$$\xi(U^{'}) = \{(\epsilon_1+2)^2, (\epsilon_1+1)^{l_1}, \epsilon_1^{l_2}, \ldots, \epsilon_{i-1}^{l_i-2}, \ldots, \epsilon_{k-1}^{l_k}\}, \tag{4.10}$$

where $l_m = 2$ for all $m \in \{1, 2, ..., (i-1)\}$ in equation (4.10). Therefore, using formula (2.2) and simplifying, we obtain

$$N(U^{'}) = N(U_1) + \sum_{m=1}^{i-1} l_m(4m-2i) + i(2l_i-4) + 2i\sum_{m=i+1}^{k} l_m.$$

Here, note that

$$\sum_{m=1}^{i-1} l_m(4m-2i) = 0.$$

Thus

$$N(U^{'}) = N(U_1) + i(2l_i-4) + 2i\sum_{m=i+1}^{k} l_m. \tag{4.11}$$

Since

$$\sum_{m=j+1}^{k} l_m(i+j) + 2i\{(l_i - 2) + (j-i)\} + (i+j)(l_j - 2) > 0$$

and

$$i(2l_i - 4) + 2i \sum_{m=i+1}^{k} l_m > 0.$$

Thus from equations (4.9) and (4.11) we have

$$N(U^{'}) > N(U_1) = N(U).$$

The proof is complete. □

Lemma 4.2.2. *Let $U \in \mathcal{U}_n(3,\Delta)$ with diameter $d(U)$. Let Λ be the set of all pendant vertices in U. If $|\Lambda| \geq \Delta + 2$, then there exists $U^{'} \in \mathcal{U}_n(3,\Delta)$ such that $N(U^{'}) > N(U)$ and $d(U^{'}) > d(U)$.*

Proof. Consider an arbitrary unicyclic graph $U \in U_n(3,\Delta)$ with eccentricity sequence

$$\xi(U) = \{\epsilon_1^{l_1}, \epsilon_2^{l_2}, \epsilon_3^{l_3}, ..., \epsilon_k^{l_k}\} \tag{4.12}$$

and a diametrical u,v-path in U. We consider respectively the corresponding caterpiller when $|V_{\mathbf{C}(U)}| = 1$ or 2 and the corresponding unicyclic graph with center C_3 when $|V_{\mathbf{C}(U)}| = 3$ discussed in Section 4.1, for convenience in proving the result. We have following two possibilities; either $l_1 \geq \Delta$ or $l_1 < \Delta$.

Case 1: When $l_1 \geq \Delta$

Then we have further two possibilities.

Subcase I: When $\mathbf{C}(U) = K_2$ or K_3.

Consider x_i the central vertex with y_i its neighbor in U_1. Construct a graph $U^{'}$ defined as

$$U^{'} \quad = \quad \{U_1 - \{v_1, v_2\}\} \cup \{x_1v_1y_1, x_2v_2y_2\} \tag{4.13}$$

where $\{v_1, v_2\} \in \Lambda_{U_1}$.

(i) If $\epsilon(v_1) = \epsilon(v_2) = \epsilon_i$ (say), we choose v_i such that $1 \leq i \leq (k-1)$ and i is the largest positive integer for which for which $l_i > 3$ and $l_m = 2$ for all $m \in \{i+1, i+2, ..., k-1\}$. Then the eccentricity sequence of $U^{'}$ will be;

$$\xi(U^{'}) = \{(\epsilon_1 + 2)^{l_1}, (\epsilon_1 + 1)^{l_2}, \epsilon_1^{l_3}, ..., \epsilon_{i-1}^{l_i - 2}, ..., \epsilon_{k-3}^{l_{k-1}}, \epsilon_{k-2}^{2}, \epsilon_{k-1}^{l_k}\} \quad (4.14)$$

where $d(U_1) + 2 = d(U^{'})$ and $r(U_1) + 1 = r(U^{'})$. Now using definition of NSC we have:

$$\begin{aligned} N(U^{'}) &= N(U_1) + \left[\sum_{m=1}^{i-1} 2l_m(k-i) - 2l_k(k-i)\right] + \sum_{m=1}^{k-1} l_m l_k \\ &+ 2(k-i)(l_i - 2) + l_k l_i. \end{aligned}$$

Thus $N(U^{'}) > N(U_1) = N(U)$.

(b) If $\epsilon(v_1) \neq \epsilon(v_2)$. Consider $\epsilon(v_1) = \epsilon_i$ and $\epsilon(v_2) = \epsilon_j$, where $i < j$ for some $i + 1 \leq j \leq k - 1$, $l_i \geq l_j$ and i, j are the largest positive integers for which $l_i + l_j \geq 6$. In this case, we have $l_j = 3$ and $l_m = 2$ for all $m \in \{i+1, i+2, \ldots, k-1\} \setminus j$. Thus eccentricity sequence of $U^{'}$ will be

$$\xi(U^{'}) = \{(\epsilon_1 + 2)^{l_1}, (\epsilon_1 + 1)^{l_2}, \epsilon_1^{l_3}, ..., \epsilon_{i-2}^{l_i - 1}, ..., \epsilon_{j-2}^{l_j - 1}, ..., \epsilon_{k-2}^{2}, \epsilon_{k-1}^{l_k}\}. \quad (4.15)$$

Again we have

$$\begin{aligned} N(U^{'}) &= \mathrm{N}(U) + \sum_{m=1}^{i} l_m\{(k-j) + (k-i) + l_k\} + 2j(k-j) + 2i\{(k-i) - 2\} \\ &+ 2i(j-i) + 2(k-i-1)(l_k - 1) + l_k(j-i+2) + (j-i). \end{aligned}$$

This implies

$$N(U^{'}) > N(U).$$

Subcase II: When $\mathbf{C}(U) = K_1$

Let U_1 be the corresponding caterpiller with Λ_{U_1} the set of all pendant vertices in U_1,where, $\Lambda_{U_1} \geq (\Delta + 2)$, $\mathbf{C}(U_1) = K_1$ and $x \in V_{U_1} \cap \mathbf{C}(U_1)$, satisfying $\xi(U) = \xi(U_1)$. Then construct $U^{'}$ defined by;

$$U^{'} = \{U_1 - \{v_1, v_2\}\} \cup \{xv_1y_1, xv_2y_2\},$$

where $v_1, v_2 \in \Lambda$.

(i) If $\epsilon(v_1) = \epsilon(v_2) = \epsilon_i$ such that i is the largest positive integer for which $l_i \geq 4$ and $i = k-1$, then eccentricity sequence of $U^{'}$ becomes;

$$\xi(U^{'}) = \{(\epsilon_1+2)^{l_1}, (\epsilon_1+1)^{l_2}, \epsilon_1^{l_3}, ..., (\epsilon_{k-4})^{l_k-2}, (\epsilon_{k-3})^2, \epsilon_{k-2}^{(l_{k-1})-2}, \epsilon_{k-1}^{l_k}\}. \quad (4.16)$$

Substituting $\xi(U^{'})$ in (2.2) we have;

$$N(U^{'}) = N(U_1) + \sum_{m=1}^{k-2} l_m\{l_{k-1} + l_k - 2\} + 2(l_{k-1} - 2) + 2l_k.$$

If $\epsilon(v_1) = \epsilon(v_2) = \epsilon_i$ with $i < (k-1)$, where i is the largest positive integer for which $l_m > 4$, then, the eccentricity sequence of $U^{'}$ is again of the form (4.14). Thus it holds that $N(U^{'}) > N(U_1) > N(U)$. The result is true in this case.

(ii) If $\epsilon(v_1) \neq \epsilon(v_2)$, say, $\epsilon(v_1) = \epsilon_i$ and $\epsilon(v_2) = \epsilon_j$ with either $i < j$, $j < (k-1)$ or $i < (k-1)$, $j \leq (k-1)$ where i, j are the largest positive integers for which $l_i + l_j \geq 8$. The eccentric sequence of $U^{'}$ is again of the form (4.15). Again we get $N(U^{'}) > N(U_1) = N(U)$.

Thus the result holds in above all cases.

Case 2: When $l_1 < \Delta$

Since $U \in \mathcal{U}_n(3, \Delta)$ thus there exist atleast one l_m in equation (4.12) such that $l_m = \Delta$. Let $l_q = \Delta$ and $l_m \geq 2$ for $m \in \{1, 2, 3, ..., (q-1)\}$. By applying Lemma 4.2.1, such graphs can be transformed to a graph say $U^{'}$ with eccentricity sequence of the form

$$\xi(U^{'}) = \begin{cases} \{\epsilon_1^2, \epsilon_2^2, ..., \epsilon_{q-1}^2, \epsilon_q^{\Delta}, ..., \epsilon_k^{l_k}\}, & \text{if } \sum_{m=1}^{q-1} l_m \text{ is even,} \\ \{\epsilon_1^2, \epsilon_2^2, ..., \epsilon_p^3, ..., \epsilon_{q-1}^2, \epsilon_q^{\Delta}, ..., \epsilon_k^{l_k}\}, & \text{if } \sum_{m=1}^{q-1} l_m \text{ is odd.} \end{cases} \quad (4.17)$$

Now we can get a graph say, $U^{''}$ discussed below in subcase (1) equation (4.18), subcase (2) equation (4.21) from $U^{'}$, with $l_1 = \Delta$ such that $N(U^{''}) > N(U^{'})$.

Subcase I: When $\sum_{m=1}^{q-1} l_m$ is even.

Let u, v-diametrical path in $U^{'}$ with w be the unique neighbor of u in $U^{'}$. Define $S \subset V_{U'}$ such that, $S = \{v_i \in S \text{ and } \epsilon(v_i) = \epsilon_q\}$. Now, construct $U^{''}$ defined by

$$U^{''} = \{U^{'} - \{v_1, v_2, \ldots, v_{(\Delta-2)}\}\} \cup \{wv_1, wv_2, ..., wv_{(\Delta-2)}\} \quad (4.18)$$

So the eccentricity sequence of $U^{''}$ will be

$$\xi(U^{''}) = \{\epsilon_1^{l_1+(\Delta-2)}, \epsilon_2^{l_2}, ..., \epsilon_q^{l_q-(\Delta-2)}, ..., \epsilon_k^{l_k}\} \tag{4.19}$$

Using definition of NSC we have

$$N(U^{''}) = N(U^{'}) + (\Delta - 2)\sum_{m=q+1}^{k} l_m(2m - q - 1) > 0. \tag{4.20}$$

Subcase II: When $\sum_{m=1}^{q-1} l_m$ is odd.
Let $p \in V_{U'}$ with $\epsilon(p) = \epsilon_p$,$l_p = 3$ and $v_i \in V_{U'}$ for $i \in \{1, 2, \ldots, (\Delta - 3)\}$ with $\epsilon(v_i) = \epsilon_q$, $l_q = \Delta$. Then define $U^{''}$ by

$$U^{''} = \{U^{'} - \{p, q_1, q_2, ..., q_{(\Delta-3)}\}\} \cup \{wp, wq_1, wq_2, ..., wq_{(\Delta-3)}\}, \tag{4.21}$$

where w is the unique neighbor of u in $U^{'}$. Then, the eccentricity sequence of $U^{''}$ becomes

$$\xi(U^{''}) = \{\epsilon_1^{l_1+\Delta-2}, \epsilon_2^{2}, ..., \epsilon_p^{l_p-1}, ..., \epsilon_q^{l_q-(\Delta-3)}, ..., \epsilon_k^{l_k}\} \tag{4.22}$$

Again using definition of NSC we obtain

$$\begin{aligned} N(U^{''}) &= N(U^{'}) + \Big[\Delta\{-p + 1 - \Delta(q-1) + 3q - 3\} + \Delta\{3(p-1) \\ &+ l_q(q-1)\} - 2\{3(p-1) + l_q(q-1)\}\Big] + \sum_{m=2}^{p-1} l_m\{\Delta(2m - q - 1) \\ &- 4m + 3q - p + 2\} + \sum_{m=p+1}^{q-1} l_m\{\Delta(2m - q - 1) - 6m + 3q + p + 2\} \\ &+ \sum_{m=q+1}^{k} l_m\{\Delta(q-1) - 3(q-1) + (p-1)\} \\ &= N(U^{'}) + \Delta(p-1) + 2p(q-p) + 2 + \Big[\sum_{m=q+1}^{k} l_m\{(\Delta-3)(q-1) + (p-1)\} \\ &- 2q\Big] > 0 \end{aligned}$$

Thus the result holds in all cases. We have $N(U^{''}) > N(U^{'}) > N(U_1) = N(U)$. Since $l_1 = \Delta$ in $U^{''}$ so Case I of Lemma 4.2.2 can be applied to get the desired graph. This completes the proof. □

Lemma 4.2.3. *Let $U \in \mathcal{U}_n(3, \Delta)$ and diameter $d(U)$. Let Λ be the set of all pendant vertices in U. If $U \ncong \widetilde{U}_{n,3}$ and $|\Lambda|< \Delta + 2$, then there exists $U^{'} \in \mathcal{U}_n(3, \Delta)$ such that $N(U^{'}) > N(U)$.*

Proof. Consider $U \in U_n(3, \Delta)$. Then, either $|\Lambda|= \Delta$ or $|\Lambda|= (\Delta + 1)$. We have further two cases:

Case 1: When $l_k = 1$ or 2

In this case either $l_1 = \Delta$ or $l_1 \neq \Delta$.

i) When $l_1 = \Delta$ and $|\Lambda|= \Delta$, then, $U \cong B^{\Delta}_{n,0}$ with $d(U) = (n - \Delta + 1)$ and $U \cong B^{\Delta}_{n,1}$ with $d(U) = (n-\Delta)$ when $|\Lambda|= (\Delta+1)$. Thus $N(B^{\Delta}_{n,0}) > N(B^{\Delta}_{n,1})$ result holds directly from Lemma (3) [52].

ii) When $l_1 \neq \Delta$, let $l_j = \Delta$ for some $j \in \{2, 3, \ldots, (k - 1)\}$. Since $U \in U_n(3, \Delta)$. Also $l_m = 2$ for all $m \in \{1, 2, .., (k - 1)\} \setminus \{j\}$ when $|\Lambda|= \Delta$ and $l_m = 2$ for all $m \in \{1, 2, ..., (k - 1)\} \mid \{i, j\}$ when $|\Lambda|= (\Delta + 1)$, where $l_i = 3$ for $2 \leq i < j \leq (k - 1)$ or $2 \leq j < i \leq (k - 1)$.

Now,

If $i > j$ with $|\Lambda|= \Delta$ or $|\Lambda|= (\Delta+1)$, apply transformation (4.18) to get $U^{'}$ with $l_1 = \Delta$ such that $U^{'} \cong B^{\Delta}_{n,0}$ or $B^{\Delta}_{n,1}$ satisfying $N(U^{'}) > N(U)$.

If $i < j$, then we apply equation (4.21) to get $U^{'}$ with $l_1 = \Delta$, such that $U^{'} \cong B^{\Delta}_{n,0}$ or $B^{\Delta}_{n,1}$ for $|\Lambda|= \Delta$ and $|\Lambda|= (\Delta + 1)$ respectively, satisfying $N(U^{'}) > N(U)$.

Case 2: When $l_k = 3$

i) When $l_1 = \Delta$, we have the following eccentricity sequence for U;

$$\xi(U) = \begin{cases} \{\epsilon_1^{\Delta}, \epsilon_2^{2}, ..., \epsilon_{i-1}^{2}, \epsilon_i^{3}, \epsilon_{i+1}^{2}, ..., \epsilon_k^{l_k}\}, & \text{if } |\Lambda|= (\Delta + 1) \\ \{\epsilon_1^{\Delta}, \epsilon_2^{2}, ..., \epsilon_{i-1}^{2}, \epsilon_i^{2}, \epsilon_{i+1}^{2}, ..., \epsilon_k^{l_k}\}. & \text{if } |\Lambda|= (\Delta) \end{cases} \tag{4.23}$$

For $|\Lambda|= \Delta + 1$. Let $p \in V_U$ with $\epsilon(p) = \epsilon_i < \epsilon_1$ and $x \in \mathbf{C}(U)$ but $x \notin uv$-diametrical path. We have $l_1 = \Delta$, $l_k = 3$ and $l_m = 2$ for all $m \in \{2, 3, , , , (k - 1)\} \setminus \{i\}$. Define

$U' \cong B^{\Delta}_{n,0}$ given by;

$$U' \quad \cong \quad B^{\Delta}_{n,0} = \{U - \{p, x\}\} \cup \{vx, xp\} \tag{4.24}$$

This implies

$$\xi(U') = \{\epsilon_1^{\Delta}, \epsilon_2^{2} ..., \epsilon_i^{l_i - 1}, ..., \epsilon_k^{l_k - 1}, \epsilon_{k+1}^{2}\}.$$

Using 2.2 and simplifying we get

$$N(U') \quad = \quad N(U) + \Delta(k - i + 2) + \sum_{m=1}^{i-1}(k - i + 2) + 2(2k - 2i + 3).$$

For $|\Lambda| = \Delta$ and $x \in \mathbf{C}(U)$ but x does not lie on uv-diametrical path. We have $l_1 = \Delta$, $l_k = 3$ and $l_m = 2$ for all $m \in \{2, 3, , , , (k-1)\}$. Define $U' \cong B^{\Delta}_{n,0}$ given by;

$$U' \quad = \quad \{U - \{x\}\} \cup \{vx\}. \tag{4.25}$$

Then, the eccentricity sequence of U' will be

$$\xi(U') = \{\epsilon_1^{\Delta}, \epsilon_2^{2} ..., \epsilon_i^{2}, ..., \epsilon_k^{l_k - 1}, \epsilon_{k+1}^{1}\}.$$

This gives

$$N(U') \quad = \quad N(U) + \sum_{m=1}^{k} l_m + (l_k - 2),$$

where

$$l_k = \begin{cases} 2, & \text{if d(U) is odd,} \\ 1, & \text{if d(U) is even.} \end{cases} \tag{4.26}$$

Hence

$$N(U') > N(U).$$

ii) When $l_1 \neq \Delta$ let $l_j = \Delta$. We have again subcase (2) of case (II), lemma 4.2.2. Thus the result holds in all cases.

This completes the proof □

4.3 Maximal graph in $\mathcal{U}_n(3, \Delta)$

Theorem 4.3.1. *Among all n-vertex unicyclic graphs $U \in U_n(3, \Delta)$ (on $n \geq 4$), the graph $\widetilde{U}_{n,3}$ has the maximum* NSC number.

Proof. Consider an arbitrary graph $U \in \mathcal{U}_n(3, \Delta)$. It is obvious to see that there exist a corresponding caterpiller $T \in \mathcal{T}_n$ or respectively a unicyclic graph $U_{n,3} \in \mathcal{U}_n$ such that either $\xi(T) = \xi(U)$ or $\xi(U_{n,3}) = \xi(U)$. When $U \cong T$, applying Lemma 4.2.2 and Lemma 4.2.3, T can be transformed to a graph T' such that $T' \cong B^{\Delta}_{n,0}$ or $T' \cong B^{\Delta}_{n,1}$ satisfying $N(U) = N(T) < N(T')$. When $U \cong U_{n,3}$, applying Lemma 4.2.2 and Lemma 4.2.3, again we can get a graph $U' \cong \widetilde{U}_{n,3}$ or $U' \ncong \widetilde{U}_{n,3}$ but with eccentricity sequence of the form (4.3), such that $N(U') = N(B^{\Delta}_{n,0})$ or $N(U') = N(B^{\Delta}_{n,1})$. Thus from Remmark 4.1 and Lemma (3) [52], it holds that $\widetilde{U}_{n,3}$ attains the maximum NSC number among all graphs in $\mathcal{U}_n(3, \Delta)$. This completes the proof. □

4.4 Conclusion

In this chapter, we defined a class $\mathcal{U}_n(3, \Delta)$ of n-vertex unicyclic graphs on $n \geq 4$. We find the unicyclic graph in $\mathcal{U}_n(3, \Delta)$ with maximum non-self-centrality number, that is the unique graph $\widetilde{U}_{n,3}$. We also formulated the general mathematical expression for NSC number of graph $\widetilde{U}_{n,3}$ given by

$$N(U) \leq \begin{cases} \left(\dfrac{2\Delta^2(\Delta - n - 3) + 2\Delta(3n+2) + n(n^2-1)}{12}\right) & \text{if } d \text{ is even,} \\ \left(\dfrac{\Delta^2(2\Delta - 3n - 6) + 2\Delta(3n+2) + n^2(n-4)}{12}\right) & \text{if } d \text{ is odd.} \end{cases} \tag{4.27}$$

It will be an interesting problem to find the maximal graph in general class of unicyclic graphs $\mathcal{U}_n$ with no fixed parameters.

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