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On Topological Indices And Domination Numbers Of Graphs

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ON TOPOLOGICAL INDICES AND DOMINATION NUMBERS OF GRAPHS

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ABSTRACT

Topological indices and dominating problems are popular topics in Graph Theory. There are various topological indices such as degree-based topological indices, distance-based topological indices and counting related topological indices et al. These topological indices correlate certain physicochemical properties such as boiling point, stability of chemical compounds. The concepts of domination number and independent domination number, introduced from the mid-1860s, are very fundamental in Graph Theory.

In this dissertation, we provide new theoretical results on these two topics. We study k-trees and cactus graphs with the sharp upper and lower bounds of the degree-based topological indices(Multiplicative Zagreb indices). The extremal cacti with a distance-based topological index(PI index) are explored. Furthermore, we provide the extremal graphs with these corresponding topological indices.

We establish and verify a proposed conjecture for the relationship between the domination number and independent domination number. The corresponding counterexamples and the graphs achieving the extremal bounds are given as well.

DEDICATION

This dissertation is dedicated to my parents Xiliang Wang and Yinquan Yang, and my wife Yongli Sang. They have supported me throughout my entire educational career. Without their love and encouragement, this would not have been possible.

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TABLE OF CONTENTS

ABSTRACT ii

DEDICATION iii

ACKNOWLEDGEMENTS iv

List of Figures vii

1 INTRODUCTION 1

1.1 NOTATIONS 1

1.2 THE CONCEPT OF K-TREES 2

1.3 THE CONCEPT OF CACTUS GRAPHS 3

1.4 DEGREE-BASED TOPOLOGICAL INDICES 4

1.5 DISTANCE-BASED TOPOLOGICAL INDICES 10

1.6 DOMINATION AND INDEPENDENT DOMINATION 15

1.7 DISSERTATION STRUCTURE 17

2 MULTIPLICATIVE ZAGREB INDICES 19

2.1 K-TREES 19

2.2 CACTUS GRAPHS 30

3 PADMAKAR-IVAN(PI) INDEX 45

3.1 K-TREES 45

3.2 CACTUS GRAPHS 56

4 THE RATIO OF DOMINATION AND INDEPENDENT DOMINATION 63

4.1 THE RATIO 63

4.2 EXTENDED RESULTS 65

5 FUTURE RESEARCH 67

5.1 TOPOLOGICAL INDICES 67

5.2 DOMINATION NUMBERS 67

5.3 LONG CYCLE 68

6 CONCLUSION 69

6.1 SUMMARY AND CONCLUSIONS 69

BIBLIOGRAPHY 70

VITA 80

LIST OF FIGURES

1.5.1 The cacti with extremal PI indices 14

1.6.1 One of the counterexamples of Furuya et al. 17

3.2.1 The cacti with extremal PI indices 56

4.2.1 One of the counterexamples for $\delta = 2$ 66

1 INTRODUCTION

1.1 NOTATIONS

Throughout this dissertation, $G = (V, E)$ is a connected finite simple undirected graph with vertex set $V = V(G)$ and edge set $E = E(G)$. Let $|G|$ or $|V|$ denote the cardinality of V. For a vertex $v \in V(G)$, the neighborhood of v is the set $N(v) = N_G(v) = \{w \in V(G), vw \in E(G)\}$. $d_G(v)$ or $d(v)$ is the degree of v with $d_G(v) = |N(v)|$. We use $d(u, v)$ to denote the distance between the vertices u and v in G, which is the number of edges of the shortest path connecting u and v.

For $S \subseteq V(G)$ and $F \subseteq E(G)$, we use $G[S]$ for the subgraph of G induced by S, and $G - S$ for the subgraph induced by $V(G) - S$ and $G - F$ for the subgraph of G obtained by deleting F. Let $w(G)$ be the number of components of G. We say that S is a cut set if $w(G - S) > w(G)$. We use $G \cong H$ to denote that G is isomorphic to H and $G \ncong H$ to denote that G is not isomorphic to H.

A pendant vertex is a vertex of degree one. An edge is called a pendant edge if one of its vertices is a pendant vertex. A tree T is called a pendant tree of G, if T has at most one vertex shared with some cycles in G. A block is a K_2 or a maximal 2-connected subgraph of a graph. In particular, the end block of a graph G contains at most one cut vertex of G.

For $r \geq 1$, let $P_1 = u_1u_2...u_pv_1, P_2 = u_1u_2...u_pv_2, ..., P_r = u_1u_2...u_pv_r$ be the paths of a graph G such that there exists at most one cycle C with $V(P_i) \cap V(C) = \{u_1\}$ and $d(v_i) = 1$, $i \geq 1$, then the induced subgraph $G[\{v_i, u_j, i \in [1, r], j \in [1, p]\}]$ is called a dense path. In particular, when $r = 1$, the dense path is a pendant path. The length of a dense path is the length of its pendant path. Let K_n, P_n and S_n denote the clique, the path and the star on n vertices, respectively. In particular, we say K_n is a k-clique for $n = k$.

Let $\lfloor x \rfloor$ be the largest integer that is less than or equal to x and $\lceil x \rceil$ be the smallest integer that is greater than or equal to x. Let $[a, b]$ be the set of all integers between a and b with $a \leq b$ including a, b, where a, b are integers. Also, let $(a, b] = [a, b] - \{a\}$ and $[a, b) = [a, b] - \{b\}$. In particular, $[a, b] = \phi$ for $a > b$. For any integer p, if $p \geq 0$, we denote $x_{max\{0,p\}} = x_p$; If $p < 0$, we say $x_{max\{0,p\}}$ does not exist.

1.2 THE CONCEPT OF K-TREES

Tree is a fundamental concept in Graph Theory and Combinatorics of Mathematics, and it has many applications in Computer Science, Chemistry, Biology, and so on. A tree is an undirected graph in which any pair of two vertices are connected by exactly one path. In other words, any acyclic connected graph is a tree. Based on the interests of trees, researchers are continuing to study some complicate extentions of trees. One of the branches is the k-tree for $k \geq 1$. In particular, a k-tree is a tree for $k = 1$.

It is commonly known that the class of k-trees is an important subclass of trangular graphs. Harry and Plamer [41] first introduced the 2-tree in 1968, which is showed to be maximal outerplanar graphs [23, 45]. Beineke and Pippert [9] gave the definition of k-trees in 1969. Relating to k-trees, there are many interesting applications to the study of computational complexity and the intersection between Graph Theory and Chemistry [19, 72]. We give the definitions below.

Definition 1.2.1. *The k-tree, denoted by T_n^k, for positive integers n, k with $n \geq k$, is defined recursively as follows: The smallest k-tree is the k-clique K_k. If G is a k-tree with $n \geq k$ vertices and a new vertex v of degree k is added and joined to the vertices of a k-clique in G, then the graph is a k-tree with $n + 1$ vertices.*

Definition 1.2.2. *The k-path, denoted by* P_n^k*, for positive integers* n, k *with* $n \geq k$*, is defined as follows: Starting with a k-clique* $G[\{v_1, v_2, ..., v_k\}]$*, for* $i \in [k+1, n]$*, the vertex* v_i *is adjacent to vertices* $\{v_{i-1}, v_{i-2}, ..., v_{i-k}\}$ *only.*

Definition 1.2.3. *The k-star, denoted by* $S_{k,n-k}$*, for positive integers* n, k *with* $n \geq k$*, is defined as follows: Starting with a k-clique* $G[\{v_1, v_2, ..., v_k\}]$ *and an independent set* S *with* $|S| = n - k$*, for* $i \in [k+1, n]$*, the vertex* v_i *is adjacent to vertices* $\{v_1, v_2, ..., v_k\}$ *only.*

Definition 1.2.4. *The k-spiral, denoted by* $T_{n,c}^{k*}$ *with* $c \in [1, k-1]$*, is defined as* $P_{n-c}^{k-c} + K_c$*, that is,* $V(T_{n,c}^{k*}) = \{v_1, v_2, ..., v_n\}$ *and* $E(T_{n,c}^{k*}) = E(P_{n-c}^{k-c}) \cup E(K_c) \cup \{v_1v_l, v_2v_l, ..., v_{n-c}v_l\}$*, for* $l \in [n-c+1, n]$*.*

Definition 1.2.5. *A vertex* $v \in V(T_n^k)$ *is called a k-simplicial vertex if* v *is a vertex of degree* k *of* T_n^k*. Let* $S_1(T_n^k)$ *be the set of all k-simplicial vertices of* T_n^k*, for* $n \geq k+2$*, and set* $S_1(K_k) = \phi, S_1(K_{k+1}) = \{v\}$*, where* v *is any vetex of* K_{k+1}*. If* $G = G_0, G_i = G_{i-1} - v_i$*, where* v_i *is a k-simplicial vertex of* G_{i-1}*, then* $\{v_1, v_2, ..., v_n\}$ *is called a simplicial elimination ordering of the n-vertex graph* G*.*

Definition 1.2.6. *If* $w(G-S) \leq 2$ *for any k-clique* $G[S]$ *of* T_n^k*, we say* T_n^k *is a hyper pendent edge; If there exists a k-clique* $G[S]$ *with* $w(G-S) \geq 3$*, let* C *be a component of* $T_n^k - S$ *and contain a unique vertex belonging to* $S_1(G)$*, then we say that* $G[V(S) \cup V(C)]$ *is a hyper pendent edge of* T_n^k*, denoted by* $\mathcal{P}$*. In particular, a k-path is a hyper pendent edge.*

1.3 THE CONCEPT OF CACTUS GRAPHS

Cactus graphs were first studied under the name of Husimi trees. Husimi tree used to refer to graphs in which every block is a complete graph (equivalently, the intersection graphs of the blocks in some other graphs). The regular definition of the cactus graph is as follows.

Definition 1.3.1. *A graph is a cactus if it is connected and all of its blocks are either edges or cycles, i.e., any two of its cycles have at most one common vertex.*

Since every cactus graph may have some pendant vertices which connect to one vertex only, set $\mathcal{C}_n^k$ to denote a set of cactus graphs with n vertices including k pendant vertices, where $n \geq k \geq 0$.

It is not hard to see that if we replaced each block by a vertex for the cactus graph, then the obtained graph is a tree. In other words, the cactus graphs are interesting extentions of trees. A cactus graph is used to be called a cactus tree, a mixed Husimi tree, or a polygonal cactus with bridges.

1.4 DEGREE-BASED TOPOLOGICAL INDICES

Chemical Graph Theory is a branch of Graph Theory whose focus of interest is finding topological indices of chemical graphs which correlate well with chemical properties of the chemical molecules. A topological index is a numerical parameter mathematically derived from the graph structure.

One of the topological indices used in mathematical chemistry is that of the so-called degree-based topological index, which is defined in terms of the degrees of the vertices of a graph. The first and second Zagreb indices of G are respectively defined as

$$\begin{aligned} M_1(G) &= \textstyle\sum_{u \in V(G)} d(u)^2, \\ M_2(G) &= \textstyle\sum_{uv \in E(G)} d(u)d(v). \end{aligned}$$

The background and applications of Zagreb indices can be found in [33, 35]. In the 1980s, Narumi and Katayama [63] characterized the structural isomers of saturated hydrocarbons and considered the product

$$NK(G) = \prod_{v \in V(G)} d(v),$$

which is called the NK index. Two fairly new indices with higher prediction ability [74], named the first and second multiplicative Zagreb indices, are respectively defined as

$$\Pi_1(G) = \prod_{v \in V(G)} d(v)^2, \ \Pi_2(G) = \prod_{uv \in E(G)} d(u)d(v).$$

Obviously, the first multiplicative Zagreb index is the power of the NK index. Moreover, the second multiplicative Zagreb index can be rewritten as $\prod_2(G) = \prod_{u \in V(G)} d(u)^{d(u)}$. The properties of $\prod_1(G), \prod_2(G)$ for some chemical structures have been studied extensively in [24, 34, 69, 81]

Due to this motivation, we consider the first generalized multiplicative Zagreb index defined in (1) below and the second multiplicative Zagreb index: for any real number $c > 0$,

$$\begin{aligned} &(1) \quad \textstyle\prod_{1,c}(G) = \prod_{v \in V(G)} d(v)^c, \\ &(2) \quad \textstyle\prod_2(G) = \prod_{uv \in E(G)} d(u)d(v). \end{aligned}$$

Eventually, for $c = 1, 2$, (1) is just the NK index and the first multuplicative Zagreb, respectively. For (2), it is easy to see that $\prod_2(G) = \prod_{v \in V(G)} d(v)^{d(v)}$.

1.4.1 Motivation on k-trees

There are many significant recent results about chemical indices and computational complexity, that lie in the intersection between graph theory and chemistry. We just list some interesting results about the chemical indices. In 2004, Das and Gutman provided sharp bounds of Zagreb indices of trees. Estes and Wei extended the result to k-trees in 2014. Theorem 1.4.2 is a result that extended Theorem 1.4.1 from trees to generalized trees, the k-trees below.

Theorem 1.4.1 (Das and Gutman [14]). *Let T_n be any tree with n vertices, then*

$$(i)M_1(P_n) \leq M_1(T_n) \leq M_1(S_n),$$
$$(ii)M_2(P_n) \leq M_2(T_n) \leq M_2(S_n).$$

Moreover, the left-side and the right-side equalities of (i),(ii) are reached if and only if $T_n \cong P_n$ and $T_n \cong S_n$, respectively.

Theorem 1.4.2 (Estes and Wei [23]). *Let T_n^k be any k-tree with n vertices, then*

$$(i)M_1(P_n^k) \leq M_1(T_n^k) \leq M_1(S_n^k),$$
$$(ii)M_2(P_n^k) \leq M_2(T_n^k) \leq M_2(S_n^k).$$

Moreover, the left-side and the right-side equalities of (i),(ii) are reached if and only if $T_n \cong P_n^k$ and $T_n \cong S_n^k$, respectively.

In 2011, Gutman [38] characterized the multipilicative Zagreb indices for trees and determined the unique trees that obtained maximum and minimun values for $\prod_1(G)$ and $\prod_2(G)$, respectively.

Theorem 1.4.3 (Gutman [38]). *If $n \geq 5$ and T_n is any tree with n vertices, then*

$$(i)\prod_1(S_n) \leq \prod_1(T_n) \leq \prod_1(P_n);$$
$$(ii)\prod_2(P_n) \leq \prod_2(T_n) \leq \prod_2(S_n).$$

Moreover, the left-side and the right-side equalities of (i) are reached if and only if $T_n \cong S_n$ and $T_n \cong P_n$, respectively. The left-side and the right-side equalities of (ii) are reached if and only if $T_n \cong P_n$ and $T_n \cong S_n$, respectively.

These topological indices have been found to be useful for establishing correlations between the structure of a molecular compound and its physicochemical properties or biological activity [13, 49, 58]. For other work on topological indices, the readers are referred to [11, 27, 28, 29, 32, 48, 56, 57, 59, 63, 73, 85, 86].

Motivated by the above results, we consider the multipilicative Zagreb indices for k-trees. In this work, we extend Gutman's result and find the bounds of the values of $\prod_{1,c}(G)$, $\prod_2(G)$ for k-trees, respectively, and determine the extremal graphs which attain the bounds.

Theorem 1.4.4 presents the upper and lower bounds of the first generalized multiplicative Zagreb index of k-trees and states the corresponding extremal graphs.

Theorem 1.4.4 (Wang and Wei [76]). *If T_n^k is a k-tree on $n \geq k$ vertices, then*

$$\prod\nolimits_{1,c}(S_{k,n-k}) \leq \prod\nolimits_{1,c}(T_n^k) \leq \prod\nolimits_{1,c}(P_n^k),$$

the left-side and the right-side equalities are reached if and only if $T_n^k \cong S_{k,n-k}$ and $T_n^k \cong P_n^k$, respectively.

Theorem 1.4.5 provides upper and lower bounds of the second multiplicative Zagreb index of k-trees and gives the corresponding extremal graphs.

Theorem 1.4.5 (Wang and Wei [76]). *If T_n^k is a k-tree on $n \geq k$ vertices, then*

$$\prod\nolimits_2(P_n^k) \leq \prod\nolimits_2(T_n^k) \leq \prod\nolimits_2(S_{k,n-k}),$$

the left-side and the right-side equalities are reached if and only if $T_n^k \cong P_n^k$ and $T_n^k \cong S_{k,n-k}$, respectively.

1.4.2 Motivation on Cactus graphs

In 1979, Cornuéjols and Pulleyblank[18] used the structure of a triangular cactus to find equivalent conditions for the existence of $\{K_2, C_n, n \geq 4\}$-factor. In 2012, Li et al. [60] gave upper bounds on Zagreb indices of cactus graphs and lower bounds of cactus graph with at least one cycle. Chen [12] gave the first three smallest Gutman indices among the cacti.

Based on these results, we investigate the bounds of multiplicative Zagreb indices of cactus graphs and try to characterize the extremal graphs. We obtain the following results. Theorem 1.4.6 gives the lower bounds of the first generalized Zagreb index of cactus graphs and states the corresponding extremal graphs.

Theorem 1.4.6 (Wang and Wei [77])**.** *For any graph G in $\mathcal{C}_n^k$,*

$$\prod_{1,c}(G) \geq \begin{cases} 3^{kc}2^{(n-2k)c}, & \text{if} \quad k = 0, 1, \\ 2^{(n-k-1)c}k^c, & \text{if} \quad k \geq 2, \end{cases}$$

the equalities hold if and only if their degree sequences are $\underbrace{3, 3, ..., 3}_{k}, \underbrace{2, 2, ..., 2}_{n-2k}, \underbrace{1, 1, ..., 1}_{k}$ *and* $k, \underbrace{2, 2, ..., 2}_{n-k-1}, \underbrace{1, 1, ..., 1}_{k}$*, respectively.*

Theorems 1.4.7 and 1.4.8 provide sharp upper bounds on the first generalized multiplicative Zagreb indices of cactus graphs and characterize the extremal graphs.

Theorem 1.4.7 (Wang and Wei [77])**.** *For a graph G in $\mathcal{C}_n^k$ with $n \leq k + 3$,*

$$\prod_{1,c}(G) \leq \begin{cases} k^c, & \text{if} \quad n = k + 1, \\ (\lceil \frac{k}{2} \rceil + 1)^c(\lfloor \frac{k}{2} \rfloor + 1)^c, & \text{if} \quad n = k + 2, \\ (\lceil \frac{k}{3} \rceil + 2)^c(\lfloor \frac{k}{3} \rfloor + 2)^c(k - \lceil \frac{k}{3} \rceil - \lfloor \frac{k}{3} \rfloor + 2)^c, & \text{if} \quad n = k + 3, \end{cases}$$

the equalities hold if and only if corresponding degree sequences are $k, \underbrace{1, 1, ..., 1}_{k}$*;* $\lceil \frac{k}{2} \rceil + 1, \lfloor \frac{k}{2} \rfloor + 1, \underbrace{1, 1, ..., 1}_{k}$ *and* $\lceil \frac{k}{3} \rceil + 2, \lfloor \frac{k}{3} \rfloor + 2, k - \lceil \frac{k}{3} \rceil - \lfloor \frac{k}{3} \rfloor + 2, \underbrace{1, 1, ..., 1}_{k}$*, respectively.*

Theorem 1.4.8 (Wang and Wei [77])**.** *For a graph G in $\mathcal{C}_n^k$ with $n \geq k + 4$ and $t \geq 0$,*

$$\prod_{1,c}(G) \leq \begin{cases} 16^c, & \text{if} \quad k = 0, n = 4, \\ 2^{(3t+6)c}, & \text{if} \quad k = 0, n = 2t + 5, \\ 2^{(3t+4)c}9^c, & \text{if} \quad k = 0, n = 2(t + 3), \end{cases}$$

the equalities hold if and only if corresponding degree sequences are $2, 2, 2, 2$; $\underbrace{4, 4, ..., 4}_{t+1}, \underbrace{2, 2, ..., 2}_{t+4}$ *and*

$\underbrace{4, 4, ..., 4}_{t}, 3, 3, \underbrace{2, 2, ..., 2}_{t+4}$, *respectively;*

For $k \neq 0$, *if* $\prod_{1,c}(G)$ *attains the maximal value, then one of the following statements holds: For any nonpendant vertices* u, v, *either (i)* $|d(u) - d(v)| \leq 1$ *or (ii)* $d(u) \in \{2, 3, 4\}$ *and* G *contains no cycles of length greater than 3, no dense paths of length greater than 1 except for at most one of them with length 2, and no paths of length greater 0 that connects only two cycles except for at most one of them with length 1.*

Theorem 1.4.9 gives sharp lower bounds on the second multiplicative Zagreb indices of cactus graphs and characterizes the extremal graphs.

Theorem 1.4.9 (Wang and Wei [77]). *For any graph* G *in* $\mathcal{C}_n^k$ *with* $\gamma = \frac{k-2}{n-k}$,

$$\prod_2(G) \geq \begin{cases} 3^{3k} 2^{2(n-2k)}, & \text{if} \quad k = 0, 1, \\ (2 + \lceil \gamma \rceil)^{(2+\lceil \gamma \rceil)[k-2-\lfloor \gamma \rfloor (n-k)]} (2 + \lfloor \gamma \rfloor)^{(2+\lfloor \gamma \rfloor)[n-2k+2+\lfloor \gamma \rfloor (n-k)]}, & \text{if} \quad k \geq 2, \end{cases}$$

the equalities hold if and only if corresponding degree sequences are $\underbrace{3, 3, ..., 3}_{k}, \underbrace{2, 2, ..., 2}_{n-2k}, \underbrace{1, 1, ..., 1}_{k}$ *and* $\underbrace{2 + \lceil \gamma \rceil, 2 + \lceil \gamma \rceil, ..., 2 + \lceil \gamma \rceil}_{k-2-\lfloor \gamma \rfloor (n-k)}, \underbrace{2 + \lfloor \gamma \rfloor, 2 + \lfloor \gamma \rfloor, ..., 2 + \lfloor \gamma \rfloor}_{n-2k+2+\lfloor \gamma \rfloor (n-k)}, \underbrace{1, 1, ..., 1}_{k}$, *respectively.*

Theorem 1.4.10 states sharp upper bounds on the second multiplicative Zagreb indices of cactus graphs and characterizes the extremal graphs.

Theorem 1.4.10 (Wang and Wei [77]). *For any graph* G *in* $\mathcal{C}_n^k$,

$$\prod_2(G) \leq \begin{cases} (n-2)^{n-2} 2^{2(n-k-1)}, & \text{if} \quad n - k \equiv 0 (mod\, 2), \\ (n-1)^{n-1} 2^{2(n-k-1)}, & \text{if} \quad n - k \equiv 1 (mod\, 2), \end{cases}$$

the equalities hold if and only if corresponding degree sequences are $n-2, \underbrace{2, 2, ..., 2}_{n-k-1}, \underbrace{1, 1, ..., 1}_{k}$ *and* $n-1$,

$\underbrace{2, 2, ..., 2}_{n-k-1}, \underbrace{1, 1, ..., 1}_{k}$, *respectively.*

1.5 DISTANCE-BASED TOPOLOGICAL INDICES

One of most important topological indices used in mathematical chemistry is called the distance-based topological index, which is proposed in terms of the distances of any pair of vertices of a graph.

The Wiener index is the oldest and most thoroughly examined topological index used in chemistry. In 1947, Harold Wiener[84] applied Wiener index to determine physical properties of types of Alkanes known as Paraffins and defined as

$$W(G) = \sum_{\{x,y\} \subset V(G)} d(x, y).$$

Similar to the Wiener index, Szeged index was given by Klavžar and Gutman[47] in 1996 as follows:

$$Sz(G) = \sum_{xy \in E(G)} n_{xy}(x) n_{xy}(y),$$

where $n_{xy}(x)$ is the number of vertices $w \in V(G)$ such that $d(x, w) < d(y, w)$, $n_{xy}(y)$ is the number of vertices $w \in V(G)$ such that $d(x, w) > d(y, w)$ and $w \neq x, y$. Currently, various work relating the Wiener index, the Sz index and their chemical meaning have been studied (see the surveys [2, 20, 21, 39]). Based on the considerable research of the Wiener index and the Sz index, Khadikar[49] proposed edge Padmakar-Ivan(PI_e) index in 2000, which is used in the field of nano-technology, as follows:

$$PI_e(G) = \sum_{e=xy \in E(G)} [n_{ex}(e|G) + n_{ey}(e|G)],$$

where $n_{ex}(e|G)$ denotes the number of edges which are closer to the vertex x than to the vertex y, and $n_{ey}(e|G)$ denotes the number of edges which are closer to the vertex y than to the vertex x, respectively. The detailed applications of PI_e indices between chemistry and graph theory are investigated in [4, 5, 6, 7, 8, 49, 50, 51]. As this definition does not count edges equidistant from both ends of the edge $e = xy$, Khalifeh et al.[52] continued to introduce a new PI index of vertex version below:

$$PI(G) = PI_v(G) = \sum_{xy \in E(G)} [n_{xy}(x) + n_{xy}(y)],$$

where $n_{xy}(x)$ denotes the number of vertices which are closer to the vertex x than to the vertex y.

1.5.1 Motivation on k-trees

Padmakar-Ivan indices are widely used in QSPR/QSAR/QSTR [65, 72]. In addition, there are nice results regarding vertex PI index in the study of computational complexity and the intersection between graph theory and chemistry. In [22], Das and Gutman obtained a lower bound on the vertex PI index of a connected graph in terms of numbers of vertices, edges, pendent vertices, and clique number. Hoji et al. [44] provided exact formulas for the vertex PI indices of Kronecker product of a connected graph G and a complete graph. Ili ć and Milosavljević[46] established basic properties of weighted vertex PI index and proved some lower and upper bounds. Pattabiraman and Paulraja [66] presented the expressions for vertex PI indices of the strong product of a graph and the complete multipartite graph.

Since the PI index is a distance-based index and not very easy to calculate, we first consider the bipartite graph G with n vertices. Then G has no odd cycle. By the definition of $PI(G)$, one can obtain that every edge of G has the PI-value as $n-2$. Thus, we can get the following proposition.

Proposition 1.5.1. *For any bipartite graph G with n vertices and m edges, $PI(G) = (n-2)m$. In particular, if G is a tree, then $PI(G) = (n-1)(n-2)$.*

Since a bipartite graph has no odd cycles, we will consider some graphs with odd cycles. For example, k-tree contains many odd cycles. Recently, we investigated the question of whether or not a k-star or a k-path attains the maximal or minimal bound for PI-indices of k-trees. The related results are listed below: Theorems 1.5.2 and 1.5.3 give the exact PI-values of k-stars, k-paths and k-spirals.

Theorem 1.5.2 (Wang and Wei, [78]). *For any k-star S_n^k and k-path P_n^k with $n = kp + s$ vertices, where $p \geq 0$ is an integer and $s \in [2, k+1]$,*

$$(i) PI(S_n^k) = k(n-k)(n-k-1),$$
$$(ii) PI(P_n^k) = \tfrac{k(k+1)(p-1)(3kp+6s-2k-4)}{6} + \tfrac{(s-1)s(3k-s+2)}{3}.$$

Theorem 1.5.3 (Wang and Wei, [78]). *For any k-spiral $T_{n,c}^{k*}$ with $n \geq k$ vertices, where $c \in [1, k-1]$,*

$$PI(T_{n,c}^{k*}) = \begin{cases} \frac{(n-k)(n-k-1)(4k-n+2)}{3}, & \text{if } \ n \in [k, 2k-c], \\ \frac{3c(n-2k+c-1)(n-2k+c)+(k-c)(2c^2+3nc-4kc+3kn-4k^2-6k+3n-2)}{3}, & \text{if } \ n \geq 2k-c+1. \end{cases}$$

Theorem 1.5.4 proves that k-stars achieve the maximal values of PI-values for k-trees.

Theorem 1.5.4 (Wang and Wei, [78]). *For any k-tree T_n^k with $n \geq k \geq 1$, $PI(T_n^k) \leq PI(S_n^k)$.*

Theorem 1.5.5 shows that k-paths do not attain the minimal values and certain PI-values of k-spirals are less than that of the PI-values of k-paths.

Theorem 1.5.5 (Wang and Wei, [78]). *For any k-spiral $T_{n,c}^{k*}$ with $n \geq k \geq 1$, then*

$$(i) \quad PI(P_n^k) \geq PI(T_{n,c}^{k*}) \ \text{ if } \ c \in [1, \tfrac{k+1}{2}),$$
$$(ii) \quad PI(P_n^k) \leq PI(T_{n,c}^{k*}) \ \text{ if } \ c \in [\tfrac{k+1}{2}, k-1].$$

1.5.2 Motivation on Cactus graphs

Many results were obtained by Lin, et al. on the cacti in both Chemistry and Graph Theory. Lin et al.(2007) [61], and Liu and Lu (2008) [62] obtained some sharp bounds of several chemical indices of cactus graphs, such as the Wiener index, the Merrifield-Simmons index, the Hosoya index and the Randić index. Wang and Kang (2015) [82] found the extremal bounds of another chemical index, the Harary index, for the cactus graphs as well. Feng and Yu [26] found the cacti in $\mathcal{C}_{n,k}$ with the smallest hyper-Wiener indices, which is a renovated version of Wiener index. Wang and Tan [83] characterized the extremal cacti having the largest Wiener and hyper-Wiener indices in $\mathcal{C}_{n,k}$. Motivated by the results of chemical indices and their applications, it is worth noting that it is an interesting problem to characterize the cacti in $\mathcal{C}_{n,k}$ with maximum and minimum vertex PI indices. The concept of vertex PI index yields the following propostion.

Proposition 1.5.6. *Let $G \in \mathcal{C}_{n,k}$ with $n \geq k \geq 0$, then*
(i) If G is C_3, C_4 or C_5, then $PI(G) = 0$, 8, 10.
(ii) If G is C_3 attaching a pendent edge e(say $C_3 \cup e$), then $PI(G) = 4$.

In our work, we determine the graphs with the largest and smallest vertex PI indices in $\mathcal{C}_{n,k}$, and provide the extremal cacti in Figs $1, 2$ of Figure 1.5.1, which extend Das and Gutman's result [22] by excluding the number of edges and cliques for the cacti. (In Figs 1 and 2, $\circ$ means that the vertex may exist.)

Fig. 1

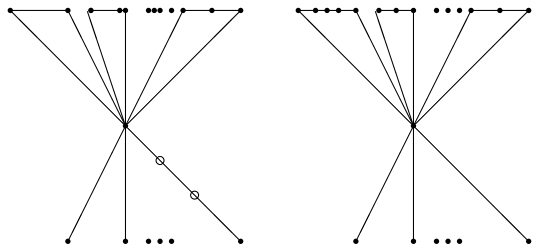

Fig. 2

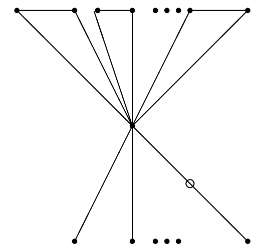

Figure 1.5.1: The cacti with extremal PI indices

Theorem 1.5.7 (Wang, Wang and Wei [80]). *Let $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_4, C_5\}$ with $n \geq k \geq 0$, then $PI(G) \leq (n - 1 + \lfloor \frac{n-k-1}{3} \rfloor)(n-2)$, where the equality holds if and only if G is a tree for $n \leq k+3$ and otherwise, one of the following statements holds(See Fig. 1):*

(i) All cycles have length 4 and there are at most $k+2$ cut edges.

(ii) All cycles have length 4 except one of length 6 and there are exact k pendent edges.

Theorem 1.5.8 (Wang, Wang and Wei [80]). *Let $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_4\}$ with $n \geq k \geq 0$, then $PI(G) \geq (n-1)(n-2) - 2\lfloor \frac{n-k-1}{2} \rfloor$, where the equality holds if and only if G is a tree for $n \leq k+2$ and otherwise, all cycles have length 3 and there are at most $k+1$ cut edges (See Fig. 2).*

1.6 DOMINATION AND INDEPENDENT DOMINATION

A classical problem in domination-related theory that attracted many scholars' attention is the N-Queens Problem on an $n \times n$ chess board from the mid-1860s. De Jaenisch [1] attempted to determine the minimum number of queens required to cover an $n \times n$ chess board, so that no two queens attack each other. A solution exists for all natural numbers n except 2 and 3. In 1892, two typical chess board problems were given by W.W. Rouse Ball as follows.

- **Covering:** Determine the minimum number of chess pieces of a given type that are necessary to cover (attack) every square of an $n \times n$ chess board.

- **Independent Covering:** Determine the smallest number of mutually nonattacking chess pieces of a given type that are necessary to dominate every square of an $n \times n$ board.

Based on these two typical chess board problems, the following concepts are prospoosed.

Definition 1.6.1. *A vertex set $D \subseteq V(G)$ is a dominating set if every vertex of $V(G) - D$ is adjacent to some vertices of D. The minimum cardinality of a dominating set of G is called the domination number, denoted by $\gamma(G)$.*

Definition 1.6.2. *A vertex set $I \subseteq V(G)$ is an independent dominating set if I is both an independent set and a dominating set in G, where an independent set is a set of vertices in a graph such that no two of which are adjacent. The minimum cardinality of an independent dominating set of G is called the independent domination number, denoted by $i(G)$.*

Definition 1.6.3. *Let G be a graph. The ratio of domination number and independent domination number is defined as*

$$\frac{i(G)}{\gamma(G)}.$$

1.6.1 Motivation on the ratio of domination numbers

In general, it is very difficult to find the domination and independent domination numbers of a graph. Note that $i(G) \geq \gamma(G)$. This implies $i(G)/\gamma(G) \geq 1$. A natural problem is to determine an upper bound for $i(G)/\gamma(G)$. Hedetniemi and Mitchell [43] in 1977 showed that if L is a line graph of a tree, then $i(L)/\gamma(L) = 1$, where the line graph $L(G)$ of a connected graph G is a graph such that each vertex of $L(G)$ represents an edge of G and two vertices of $L(G)$ are adjacent if and only if their corresponding edges share a common endpoint in G. Since a line graph does not have an induced subgraph isomorphic to $K_{1,3}$, Allan and Laskar [1] extended the previous result and obtained that if a graph G is a $K_{1,3}$-free graph, then $i(G)/\gamma(G) = 1$. In 2012, Goddard et al.[21] continued the similar approach and proved that $i(G)/\gamma(G) \leq 3/2$ if G is a cubic graph. In 2013, Southey and Henning [25] improved the previous bound to $i(G)/\gamma(G) \leq 4/3$ for a connected cubic graph G other than $K_{3,3}$. Additionally, Rad and Volkmann [67] obtained an upper bound of $i(G)/\gamma(G)$ related to the maximum degree $\Delta(G)$ for any graph G and proposed a conjecture below.

Theorem 1.6.1. (Rad and Volkmann [67]) If G is a graph, then

$$\frac{i(G)}{\gamma(G)} \leq \begin{cases} \frac{\Delta(G)}{2}, & \text{if } 3 \leq \Delta(G) \leq 5, \\ \Delta(G) - 3 + \frac{2}{\Delta(G)-1}, & \text{if } \Delta(G) \geq 6. \end{cases}$$

Conjecture 1.6.4. [67] If G is a graph with $\Delta(G) \geq 3$, then

$$i(G)/\gamma(G) \leq \Delta(G)/2.$$

In 2014, Furuya et al. [25] proved that $i(G)/\gamma(G) \leq \Delta(G) - 2\sqrt{\Delta(G)} + 2$ and gave a class of graphs which achieve the new upper bound. However, when $\Delta(G) \neq 4$, $\Delta(G) - 2\sqrt{\Delta(G)} + 2 > \Delta(G)/2$. On the other hand, it is still very interesting to determine other class of graphs, for which Conjecture 2 holds. One of the special class of graphs achieved this bound is as follows.

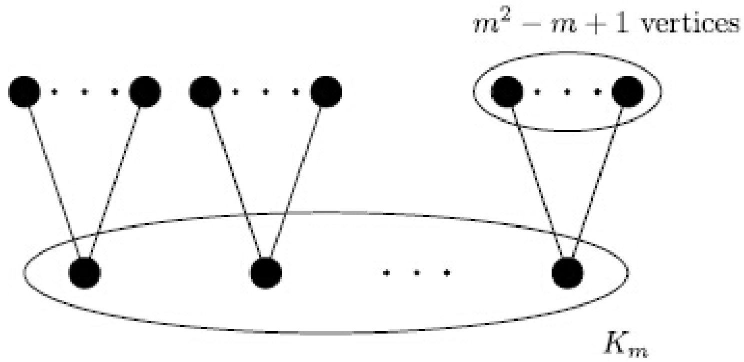

Figure 1.6.1: One of the counterexamples of Furuya et al.

Motivated by Conjecture 1.6.4 and previous results, we show that:

Theorem 1.6.2 (Wang and Wei [79]). *Let G be a bipartite graph with $\Delta(G) \geq 2$, then*

$$\frac{i(G)}{\gamma(G)} \leq \frac{\Delta(G)}{2}.$$

1.7 DISSERTATION STRUCTURE

In chapter 1, we introduce the outline of this work. All notation and definitions that will be used in the following sections are given. The motivations and the history of the main results are prospsed as well. The remaining chapters of this dissertation are organized as follows.

Chapters 2 covers the degree-based topological index with respective sharp graphs. In Chapter 3, we study a distance-based topological index and provide the extremal bounds for k-trees and cactus graphs. We explore another classic problem regarding domination number and independent domination number in Chapter 4. We find the relationship between these two domination numbers. Furthermore, we prove a related conjecture for bipartite graphs.

In addition, the future research plan to improve and expand the current results is provided in Chapter 5.

2 MULTIPLICATIVE ZAGREB INDICES

In this chapter, we provide the extremal k-trees and cactus graphs about the important topological indices (Multiplicative Zagreb indices). First of all, we introduce a developed method from two analytic lemmas to derive our results. Based on the calculations, the two lemmas are as follows.

Lemma 2.0.1. *The function* $f(x) = \dfrac{x}{x+m}$ *is strictly increasing for* $x \in [0, \infty)$*, where* m *is a positive integer.*

Lemma 2.0.2. *The function* $f(x) = \dfrac{x^x}{(x+m)^{x+m}}$ *is strictly decreasing for* $x \in [0, \infty)$*, where* m *is a positive integer.*

2.1 K-TREES

In this section, we present the main results again and provide the complete proofs.

Theorem 2.1.1 (Wang and Wei [76])**.** *If* T_n^k *is a k-tree on* $n \geq k$ *vertices, then*

$$\prod\nolimits_{1,c}(S_{k,n-k}) \leq \prod\nolimits_{1,c}(T_n^k) \leq \prod\nolimits_{1,c}(P_n^k),$$

the left-side and the right-side equalities are reached if and only if $T_n^k \cong S_{k,n-k}$ *and* $T_n^k \cong P_n^k$*, respectively.*

Theorem 2.1.2 (Wang and Wei [76])**.** *If* T_n^k *is a k-tree on* $n \geq k$ *vertices, then*

$$\prod\nolimits_2(P_n^k) \leq \prod\nolimits_2(T_n^k) \leq \prod\nolimits_2(S_{k,n-k}),$$

the left-side and the right-side equalities are reached if and only if $T_n^k \cong P_n^k$ *and* $T_n^k \cong S_{k,n-k}$*, respectively.*

Furthermore, if we let $G[\{v_1, v_2 ... v_k\}]$ denote the initial k-clique, then just by the definition of k-trees, one can get some useful propositions.

Proposition 2.1.3. *For the k-star, the degree of vertex v_i can be characterized as follows:* $d(v_i) = n - k$*, for* $i \in [1, k]$*;* $d(v_i) = k$*, for* $i \in [k + 1, n]$.

Proposition 2.1.4. *For the k-path, the degree of vertex v_i can be characterized as follows:*
(1) If $4 \leq n \leq 2k$*,* $d(v_i) = k+i-1$*, for* $i \in [1, n-k-1]$*;* $d(v_i) = n-1$*, for* $i \in [n-k, k+1]$*;* $d(v_i) = k + n - i$*, for* $i \in [k + 2, n]$*.*
(2) If $n \geq 2k + 1$*,* $d(v_i) = k + i - 1$*, for* $i \in [1, k]$*;* $d(v_i) = 2k$*, for* $i \in [k + 1, n - k]$*;* $d(v_i) = k + n - i$*, for* $i \in [n - k + 1, n]$*.*

One can deduce the first generalized multiplicative Zagreb indices and second multiplicative Zagreb indices of the k-path and k-star using induction and the above observations as shown below.

Proposition 2.1.5. *Let $S_{k,n-k}$ be a k-star on $n \geq k + 1$ vertices, then*
(1) $\prod_{1,c}(S_{k,n-k}) = (n - k)^{ck} k^{c(n-k)}$;
(2) $\prod_2(S_{k,n-k}) = (n - k)^{k(n-k)} k^{k(n-k)}$.

Proposition 2.1.6. *Let P_n^k be a k-path on $n \geq k + 1$ vertices, then*
(1.1) $\prod_{1,c}(P_n^k) = (n - 1)^c \prod_{i=k}^{n-2} i^{2c}$*, if* $n \in [k + 1, 2k]$*;*
(1.2) $\prod_{1,c}(P_n^k) = (2k)^{c(n-2k)} \prod_{i=k}^{2k-1} i^{2c}$*, if* $n \geq 2k + 1$*;*
(2.1) $\prod_2(P_n^k) = (n - 1)^{n-1} \prod_{i=k}^{n-2} i^{2i}$*, if* $n \in [k + 1, 2k]$*;*
(2.2) $\prod_2(P_n^k) = (2k)^{2k(n-2k)} \prod_{i=k}^{2k-1} i^{2i}$*, if* $n \geq 2k + 1$*.*

Prior to the proof of main results, we give some lemmas that are critical in the proof of our main results.

Lemma 2.1.7. For any k-tree $G \ncong S_{k,n-k}$, let $u \in S_2$, $N(u) \cap S_1 = \{v_1, v_2 ... v_s\}$, where $s \geq 1$ is an integer. Then

(1) For any i with $1 \leq i \leq s$, there exists a vertex $v \in N(u) - \{v_1, v_2 ... v_s\}$ of degree at least k in $G[V(G) - \{v_1, v_2 ... v_s\}]$ such that $vv_i \notin E(G)$.

(2)There exists a k-tree G^* such that $\prod_{1,c}(G^*) < \prod_{1,c}(G)$ and $\prod_2(G^*) > \prod_2(G)$.

Proof. For (1), let $G' = G[V(G) - \{v_1, v_2 ... v_s\}]$ and $S = N(u) - \{v_1, v_2 ... v_s\}$, we obtain that $d_{G'}(u) = |S| = k$ and $G[S]$ is a k-clique by $u \in S_2$. Since $G \ncong S_n^k$, $d_{G'}(v) \geq k$ for all $v \in S$. And by the facts that $N(v_i) \subseteq (N(u) - \{v_1, v_2 ... v_s\}) \cup \{u\}$ with $|N(v_i)| = k$ and $|(N(u) - \{v_1, v_2 ... v_s\}) \cup \{u\}| = k+1$, we have for any $i \in [1, s]$, there exists a vertex $v \in S$ such that $vv_i \notin E(G)$.

For (2), choose v_1 and by (1) there exists a vertex $v \in N(u) - \{v_1, v_2 ... v_s\}$ with $d_{G'}(v) \geq k$ such that $vv_1 \notin E(G)$. If $d_{G'}(v) = k$, and by $uv \in E(G')$, we obtain G' is a $k+1$-clique. Let $x \in S$ be the vertex such that $d(x) = min_{v \in S}\{d(v)\}$, and let v_t be the vertex such that $v_t x \in E(G)$, $v_t y \notin E(G)$ for some $t \in [1, s]$ and $y \in S$, that is, $d(x) - 1 < d(y)$. Construct a new graph G^* such that $V(G^*) = V(G)$, and $E(G^*) = E(G) - \{v_t x\} + \{v_t y\}$. Denote $G_0 = G[V(G) - \{x, y\}]$, since $d(x) - 1 < d(y)$, and by the definition of $\prod_{1,c}(G)$, $\prod_2(G)$, Lemma 2.0.1 and Lemma 2.0.2, we have

$$\begin{aligned}
\frac{\prod_{1,c}(G)}{\prod_{1,c}(G^*)} &= \frac{[\prod_{w \in V(G_0)} d(w)^c] d(y)^c d(x)^c}{[\prod_{w \in V(G_0)} d(w)^c][d(y)+1]^c[d(x)-1]^c} \\
&= \frac{d(y)^c d(x)^c}{[d(y)+1]^c[d(x)-1]^c} \\
&= \frac{\frac{d(y)^c}{[d(y)+1]^c}}{\frac{[d(x)-1]^c}{d(x)^c}} \\
&> 1.
\end{aligned}$$

Also,

$$
\begin{aligned}
\frac{\prod_2(G)}{\prod_2(G^*)} &= \frac{[\prod_{w\in V(G_0)} d(w)^{d(w)}]d(y)^{d(y)}d(x)^{d(x)}}{[\prod_{w\in V(G_0)} d(w)^{d(w)}][d(y)+1]^{d(y)+1}[d(x)-1]^{d(x)-1}} \\
&= \frac{d(y)^{d(y)}d(x)^{d(x)}}{[d(y)+1]^{d(y)+1}[d(x)-1]^{d(x)-1}} \\
&= \frac{[\frac{d(y)^{d(y)}}{[d(y)+1]^{d(y)+1}}]}{[\frac{[d(x)-1]^{d(x)-1}}{d(x)^{d(x)}}]} \\
&< 1.
\end{aligned}
$$

Thus, we find that the k-tree G^* satisfies $\prod_{1,c}(G^*) < \prod_{1,c}(G)$ and $\prod_2(G^*) > \prod_2(G)$, we are done.

If $d_{G'}(v) \geq k+1$, reorder the subindices of $\{v_1, v_2 ... v_s\}$ such that $vv_i \notin E(G)$ with $i \in [1, s_1]$, where $s_1 \leq s$, and by the fact that $G[N(u) - \{v_1, v_2 ... v_s\}]$ is a k-clique, we have $d(u) = k+s$ and $d(v) \geq k+1+s-s_1$, that is, $d(v) \geq d(u) - s_1 + 1$. Construct a new graph G^* such that $V(G^*) = V(G)$, and $E(G^*) = E(G) - \{uv_i\} + \{vv_i\}$, for all $i \in [1, s_1]$. Since $G[N(u) - \{v_1, v_2 ... v_s\} + \{u\}]$ is a $(k+1)$-clique, and for any i, $N(v_i) \subseteq N_{G-\{v_1, v_2 ... v_s\}}(u) \cup \{u\}$, we deduce that G^* is a k-tree. Denote $G_0 = G[V(G) - \{u, v\}]$. Since $d(v) \geq d(u) - s_1 + 1$, and by the definition of $\prod_{1,c}(G)$, $\prod_2(G)$, Lemma 2.0.1 and Lemma 2.0.2, we have

$$
\begin{aligned}
\frac{\prod_{1,c}(G)}{\prod_{1,c}(G^*)} &= \frac{[\prod_{w\in V(G_0)} d(w)^c]d(v)^c d(u)^c}{[\prod_{w\in V(G_0)} d(w)^c][d(v)+s_1]^c[d(u)-s_1]^c} \\
&= \frac{d(v)^c d(u)^c}{[d(v)+s_1]^c[d(u)-s_1]^c} \\
&= \frac{[\frac{d(v)^c}{[d(v)+s_1]^c}]}{[\frac{[d(u)-s_1]^c}{d(u)^c}]} \\
&> 1.
\end{aligned}
$$

Also,

$$
\begin{aligned}
\frac{\prod_2(G)}{\prod_2(G^*)} &= \frac{[\prod_{w\in V(G_0)} d(w)^{d(w)}]d(v)^{d(v)}d(u)^{d(u)}}{[\prod_{w\in V(G_0)} d(w)^{d(w)}][d(v)+s_1]^{d(v)+s_1}[d(u)-s_1]^{d(u)-s_1}} \\
&= \frac{d(v)^{d(v)}d(u)^{d(u)}}{[d(v)+s_1]^{d(v)+s_1}[d(u)-s_1]^{d(u)-s_1}} \\
&= \frac{[\dfrac{d(v)^{d(v)}}{[d(v)+s_1]^{d(v)+s_1}}]}{[\dfrac{[d(u)-s_1]^{d(u)-s_1}}{d(u)^{d(u)}}]} \\
&< 1.
\end{aligned}
$$

Hence, we find that the k-tree G^* satisfies $\prod_{1,c}(G^*) < \prod_{1,c}(G)$ and $\prod_2(G^*) > \prod_2(G)$, we are done. □

Lemma 2.1.8. Let G be a k-tree. If either $\prod_{1,c}(G)$ attains the maximal or $\prod_2(G)$ attains the minimal, then every hyper pendent edge is a k-path.

Proof. Let $\mathcal{P}$= $G[V(S)\cup V(C)]$ be a hyper pendent edge, where $G[S] = G[\{x_1, x_2 ... x_k\}]$ is a cut k-clique and $V(C) = \{u_1, u_2 ... u_p\}$ with p is a positive ingeter such that u_1 is the only vertex of $\mathcal{P}$ in $S_1(G)$ and for $i \in [1, p-1]$, u_i is the vertex added following by u_{i+1} through the process of the definition of k-trees.

Fact 1. *For any hyper pendent edge* $\mathcal{P}$= $G[V(S)\cup V(C)]$ *as represented above,* $\{u_1, u_2 ... u_p\}$ *is a simplicial elimination ordering of* $\mathcal{P}$.

Proof. By contradiction, assume that $\{u_1, u_2 ... u_p\}$ is not a simplicial elimination ordering of $\mathcal{P}$. Let u_t be the first vertex from u_1 to u_p such that $\{u_t, u_{t+1}\} \in S_t$ for $t \in [2, p-1]$. Then $u_t u_{t+1} \notin E(G)$ and $\{u_t, u_{t+1}\}$ can not be in some k-cliques. And by the definition of k-trees, there must be at least two vertices that belongs to S_1 in $V(C)$, a contradiction. □

By Fact 1, we know $\{u_1, u_2 ... u_p\}$ is a simplicial elimination ordering of $\mathcal{P}$. For $p \leq 2$, $\mathcal{P}$ is a k-path by the definition of k-paths; For $p \geq 3$, if $\mathcal{P}$ is a k-path, then we are done. Otherwise, let u_s be the first vertex from u_p to u_1 such that $G[V(S) \cup \{u_p, u_{p-1} ... u_{s+1}, u_s\}]$ is not a k-path. Since $G[V(S) \cup \{u_p, u_{p-1} ... u_{s+1}\}]$ is a k-path, for each $i \in [s+1, p]$, let

$N_{G-\{u_1,u_2...u_{i-1}\}}(u_i) = \{u_{i+1}, u_{i+2}......u_{min\{p,i+k\}}, x_1, x_2...x_{max\{0,k-p+i\}}\}$, and by Definition 2 and the symmetry of $G[S]$, we have $|N(u_s) \cap \{u_{s+1}, u_{s+2}...u_{min\{p,s+k\}}\}| = min\{p-s-1, k-1\}$, where $1 \leq s \leq p-1$.

For $p \leq k+s$, suppose that u_t is the vertex such that $u_t \notin N(u_s)$ with $s+2 \leq t \leq p$. Let $N_{G-\{u_1,u_2...u_{s-1}\}}(u_s) = \{u_{s+1}, u_{s+2}...u_{t-1}, u_{t+1}...u_p, x_1, x_2...x_{k-p+s+1}\}$, and let $|N(x_{k-p+s+1}) \cap \{u_1, u_2...u_{s-1}\}| = m$ for $m \in [0, s-1]$. By the defition of k-paths, we have $u_t u_i \notin E(G)$ for $i \in [1, s]$, and then $d(u_t) = k+t-s-1$ and $d(x_{k-p+s+1}) > k+p-s+m-1$. Now construct a new graph G^* such that $V(G^*) = V(G), E(G^*) = E(G) - \{u_s x_{k-p+s+1}, u_i x_{k-p+s+1}\} + \{u_s u_t, u_i u_t\}$ with $i \in [0, m]$, then G^* is a k-tree. Since $t \leq p$, we have $d(x_{k-p+s+1}) > d(u_t)+m+1$, and by the definition of $\prod_{1,c}(G)$, $\prod_2(G)$, Lemma 2.0.1 and Lemma 2.0.2, we get

$$\begin{aligned}
\frac{\prod_{1,c}(G)}{\prod_{1,c}(G^*)} &= \frac{d(u_t)^c d(x_{k-p+s+1})^c}{[d(u_t)+m+1]^c [d(x_{k-p+s+1})-m-1]^c} \\
&= \frac{[\frac{d(u_t)}{d(u_t)+m+1}]^c}{[\frac{d(x_{k-p+s+1})-m-1}{d(x_{k-p+s+1})}]^c} \\
&< 1,
\end{aligned}$$

$$\begin{aligned}
\frac{\prod_2(G)}{\prod_2(G^*)} &= \frac{d(u_t)^{d(u_t)} d(x_{k-p+s+1})^{d(x_{k-p+s+1})}}{[d(u_t)+m+1]^{d(u_t)+m+1} [d(x_{k-p+s+1})-m-1]^{d(x_{k-p+s+1})-m-1}} \\
&= \frac{\frac{d(u_t)^{d(u_t)}}{[d(u_t)+m+1]^{d(u_t)+m+1}}}{\frac{[d((x_{k-p+s+1})-m-1]^{d((x_{k-p+s+1})-m-1}}{d(x_{k-p+s+1})^{d(x_{k-p+s+1})}}} \\
&> 1.
\end{aligned}$$

Thus, $\prod_{1,c}(G^*) > \prod_{1,c}(G)$ and $\prod_2(G^*) < \prod_2(G)$, a contradiction.

For $p \geq k+s+1$, let $|N(u_{k+s+1}) \cap \{u_1, u_2...u_{s-1}\}| = m$ for $m \in [0, s-1]$. Since $G[V(S) \cup \{u_p, u_{p-1}...u_{s+1}\}]$ is a k-path, we have $G[\{u_{s+1}, u_{s+2}...u_{s+k+1}\}]$ is a $(k+1)$-clique. Suppose that u_t is the vertex such that $u_t \notin N(u_s)$ with $s+2 \leq t \leq s+k$, let $N_{G-\{u_1,u_2...u_{s-1}\}}(u_s) = \{u_{s+1}, u_{s+2}...u_{t-1}, u_{t+1}...u_{s+k+1}\}$. Now we construct a new graph G^* such that $V(G^*) =$

$V(G)$, $E(G^*) = E(G) - \{u_s u_{k+s+1}, u_i u_{k+s+1}\} + \{u_s u_t, u_i u_t\}$ for $i \in [0, m]$. Then G^* is a k-tree and $d(u_{k+s+1}) = 2k + m$, $d(u_t) = k + t - s - 1$. Since $t \leq s + k$, we have $d(u_{k+s+1}) > d(u_t) + m + 1$, and by the definition of $\prod_{1,c}(G)$, $\prod_2(G)$, Lemma 2.0.1 and Lemma 2.0.2, we get

$$\begin{aligned}
\frac{\prod_{1,c}(G)}{\prod_{1,c}(G^*)} &= \frac{d(u_t)^c d(u_{k+s+1})^c}{[d(u_t) + m + 1]^c [d(u_{k+s+1}) - m - 1]^c} \\
&= \frac{[\frac{d(u_t)}{d(u_t) + m + 1}]^c}{[\frac{d(u_{k+s+1}) - m - 1}{d(u_{k+s+1})}]^c} \\
&< 1,
\end{aligned}$$

$$\begin{aligned}
\frac{\prod_2(G)}{\prod_2(G^*)} &= \frac{d(u_t)^{d(u_t)} d(u_{k+s+1})^{d(u_{k+s+1})}}{[d(u_t) + m + 1]^{d(u_t)+m+1} [d(u_{k+s+1}) - m - 1]^{d(u_{k+s+1})-m-1}} \\
&= \frac{\frac{d(u_t)^{d(u_t)}}{[d(u_t) + m + 1]^{d(u_t)+m+1}}}{\frac{[d((u_{k+s+1}) - m - 1]^{d(u_{k+s+1})-m-1}}{d(u_{k+s+1})^{d(u_{k+s+1})}}} \\
&> 1.
\end{aligned}$$

Thus, $\prod_{1,c}(G^*) > \prod_{1,c}(G)$ and $\prod_2(G^*) < \prod_2(G)$, a contradiction. Hence, for any $s \in [1, p]$ $N_{G-\{u_1, u_2 \ldots u_{s-1}\}}(u_s) = \{u_{s+1}, u_{s+2} \ldots u_{min\{p, k+s\}}, x_1, x_2 \ldots x_{max\{0, k-p+s\}}\}$, that is, $\mathcal{P}$ is a k-tree. $\square$

Lemma 2.1.9. Let G be a k-tree, if either $\prod_{1,c}(G)$ attains the maximal or $\prod_2(G)$ attains the minimal, then $|S_1(G)| = 2$.

Proof. We know that $|S_1(G)| \geq 2$ for $n \geq k + 2$, and by Lemma 2.1.8, every hyper pendent edge is a k-path for $\prod_{1,c}(G)$ to attain the maximal or $\prod_2(G)$ to attain the minimal. If $|S_1(G)| = 2$, we are done; Suppose that $|S_1(G)| \geq 3$, it suffices to prove that there exists a graph G' such that $|S_1(G')| = |S_1(G)| - 1$ with $\prod_{1,c}(G') > \prod_{1,c}(G)$ and $\prod_2(G') < \prod_2(G)$.

Fact 2. *For any k-tree G satisfying the conditions of Lemma 3, if $|S_1(G)| \geq 3$, then there exists a k-clique $G[S]$ such that $w(G - S) \geq 3$.*

Proof. We will proceed by induction on $n = |G|$. For $n = k+3$, it is trivial; For $n \geq k+4$, assume that the fact is true for the k-tree G with $n < k+p$, and consider $n = k+p$. If $|S_1(G)| \geq 4$, choose any vertex $v \in S_1(G)$, or $|S_1(G)| = 3$ and $|S_2(G)| \geq 2$, choose the vertex $v \in S_1(G)$ such that $N(w) \cap S_1(G) = \{v\}$ for some $w \in S_2(G)$, then construct a new graph G' such that $G' = G - v$. Since $S_2(G)$ is an dependent set and $G[N(v)]$ is a k-clique for any $v \in S_1(G)$, we obtain $|S_1(G')| \geq 3$. By the induction hypothesis, there exists a k-clique $G[S]$ in G' such that $w(G' - S) \geq 3$. Thus, by adding back v, $G[S]$ is still a k-clique in G and $w(G - S) \geq 3$, we are done. Next, we only consider $|S_1(G)| = 3$ and $|S_2(G)| = 1$.

Let $S_1(G) = \{v_1, v_2, v_3\}$ and $G_0 = G - \{v_1, v_2, v_3\}$, we have G_0 is a $(k+1)$-clique, denoted by $G[\{x_1, x_2 ... x_{k+1}\}]$. If there exists $N(v_i) = N(v_j)$, for some $i, j \in [1,3]$ with $i \neq j$, and take $S = N(v_i)$, then $w(G - S) \geq 3$, we are done; If $N(v_i) \neq N(v_j)$, for any $i, j \in [1,3]$ with $i \neq j$, then reorder the index of x_i such that $N(v_1) = \{x_1, x_2 ... x_k\}$, $N(v_2) = \{x_2, x_3 ... x_{k+1}\}$ and $N(v_3) = \{x_1, x_3 ... x_{k+1}\}$. Construct a new graph G^* such that $V(G^*) = V(G)$, $E(G^*) = E(G) - \{v_1x_1\} + \{v_1v_2\}$, then G^* is still a k-tree and $d_G(x_1) = k+2$, $d_{G^*}(x_1) = k+1$, $d_G(v_1) = d_G(v_2) = k$ and $d_{G^*}(v_2) = k+1$. By the definition of $\prod_{1,c}(G)$, $\prod_2(G)$, Lemma 2.0.1 and Lemma 2.0.2, we have

$$\begin{aligned}
\frac{\prod_{1,c}(G)}{\prod_{1,c}(G^*)} &= \frac{d(v_2)^c d(x_1)^c}{[d(v_2)+1]^c [d(x_1)-1]^c} \\
&= [\frac{k(k+2)}{(k+1)^2}]^c \\
&< 1,
\end{aligned}$$

$$\begin{aligned}
\frac{\prod_2(G)}{\prod_2(G^*)} &= \frac{d(v_2)^{d(v_2)} d(x_1)^{d(x_1)}}{[d(v_2)+1]^{d(v_2)+1} [d(x_1)-1]^{d(x_1)-1}} \\
&= \frac{(k+2)^{k+2} k^k}{(k+1)^{2(k+1)}} \\
&= \frac{[\frac{k^k}{(k+1)^{k+1}}]}{[\frac{(k+1)^{k+1}}{(k+2)^{k+2}}]} \\
&> 1.
\end{aligned}$$

Thus, we find a graph G^* with $\prod_{1,c}(G^*) > \prod_{1,c}(G)$ and $\prod_2(G^*) < \prod_2(G)$, a contradiction with that $\prod_{1,c}(G)$ attains the maximal or $\prod_2(G)$ attains the minimal, we are done. $\square$

Choose a k-clique $G[S]$ with $w(G-S) \geq 3$ such that there are two components of $G-S$: C_1, C_2 with $|C_1| = p, |C_2| = q$ and $p+q$ being minimal, for $p \geq q$. Let $u_1 \in V(C_1)$, $v_1 \in V(C_2)$ with $\{u_1, v_1\} \subseteq S_1(G)$. Let $N_{G-\{v_1,v_2...v_{i-1}\}}(v_i) = \{v_{i+1}, v_{i+2}...v_{min\{k+1,q\}}, x_1, x_2...x_{max\{0,k-q+i\}}$, $N_{G-\{u_1,u_2...u_{j-1}\}}(u_j) = \{u_{j+1}, u_{j+2}...u_{min\{k+1,p\}}, y_1, y_2...y_{max\{0,k-p+i\}}\}$ for $i \geq 1, j \geq 1$, where $\{v_1, v_2...v_q\}$ and $\{u_1, u_2...u_p\}$ are simplicial elimination orderings of $G[S \cup V(C_1)]$ and $G[S \cup V(C_2)]$, respectively. We will prove Lemma 2.1.9 by induction on q.

(1) If $q = 1$, then $d(v_1) = k$. Choose $x_t \in N(v_1)$, let $|N(x_t) \cap \{u_1, u_2...u_p\}| = m$ for $m \in [1,k]$, we get $d(x_t) > k+1+m$ by $w(G-S) \geq 3$, and then $d(x_t) > d(v_1)+m+1$. Now construct a new graph G^* such that $V(G^*) = V(G), E(G^*) = E(G) - \{u_i x_t\} + \{u_i v_1\}$ for $i \in [1,m]$, then G^* is a k-tree and $|C_1| + |C_2| = p$ with $G[\{x_1, x_2...x_{t-1}, x_{t+1}...x_k, v_1\}]$ is a k-clique in G^*. Since $d(x_t) > d(v_1)+m+1$, by the definition of $\prod_{1,c}(G)$, $\prod_2(G)$, Lemma 2.0.1 and Lemma 2.0.2, we have

$$\begin{aligned}
\frac{\prod_{1,c}(G)}{\prod_{1,c}(G^*)} &= \frac{d(v_1)^c d(x_t)^c}{[d(v_1)+m]^c [d(x_t)-m]^c} \\
&= \frac{[\dfrac{d(v_1)}{d(v_1)+m}]^c}{[\dfrac{d(x_t)-m}{d(x_t)}]^c} \\
&< 1,
\end{aligned}$$

$$\begin{aligned}
\frac{\prod_2(G)}{\prod_2(G^*)} &= \frac{d(v_1)^{d(v_1)} d(x_t)^{d(x_t)}}{[d(v_1)+m]^{d(v_1)+m} [d(x_t)-m]^{d(x_t)-m}} \\
&= \frac{\dfrac{d(v_1)^{d(v_1)}}{[d(v_1)+m]^{d(v_1)+m}}}{\dfrac{[d((x_t)-m]^{d((x_t)-m}}{d(x_t)^{d(x_t)}}} \\
&> 1.
\end{aligned}$$

Then, $\prod_{1,c}(G^*) > \prod_{1,c}(G)$ and $\prod_2(G^*) < \prod_2(G)$. Thus, let $G' = G^*$, $|S_1(G')| = |S_1(G)| - 1$, $\prod_{1,c}(G') > \prod_{1,c}(G)$ and $\prod_2(G') < \prod_2(G)$, and we are done.

(2) Assume that $q = s$, there exists a k-tree G' such that $|S_1(G')| = |S_1(G)| - 1$, $\prod_{1,c}(G') > \prod_{1,c}(G)$, $\prod_2(G') < \prod_2(G)$ and we consider $q = s + 1$.

If $q \leq k$, we have $d(v_q) = k + q - 1$ by the fact that $G[S \cup V(C_2)]$ is a k-path. Choose $x_t \in N(v_1)$, we know $x_t \in N(v_i)$ for all $i \in [1, p]$ by $G[S \cup V(C_2)]$ is a k-path. Let $|N(x_t) \cap \{u_1, u_2 ... u_p\}| = m$ for $m \in [1, k]$, we have $d(x_t) > k+q+m$ by $w(G-S) \geq 3$, and then $d(x_t) > d(v_q) + m + 1$. Now construct a new graph G^* such that $V(G^*) = V(G), E(G^*) = E(G) - \{u_i x_t\} + \{u_i v_q\}$ for $i \in [1, m]$, then G^* is a k-tree and $|C_1| + |C_2| = p + q - 1$ with $G[\{x_1, x_2 ... x_{t-1}, x_{t+1} ... x_k, v_q\}]$ is a k-clique in G^*. Since $d(x_t) > d(v_q) + m + 1$, by the definition of $\prod_{1,c}(G)$, $\prod_2(G)$, Lemma 2.0.1 and Lemma 2.0.2, we have

$$\begin{aligned}
\frac{\prod_{1,c}(G)}{\prod_{1,c}(G^*)} &= \frac{d(v_q)^c d(x_t)^c}{[d(v_q)+m]^c [d(x_t)-m]^c} \\
&= \frac{[\dfrac{d(v_q)}{d(v_q)+m}]^c}{[\dfrac{d(x_t)-m}{d(x_t)}]^c} \\
&< 1,
\end{aligned}$$

$$\begin{aligned}
\frac{\prod_2(G)}{\prod_2(G^*)} &= \frac{d(v_q)^{d(v_q)} d(x_t)^{d(x_t)}}{[d(v_q)+m]^{d(v_q)+m} [d(x_t)-m]^{d(x_t)-m}} \\
&= \frac{\dfrac{d(v_q)^{d(v_q)}}{[d(v_q)+m]^{d(v_q)+m}}}{\dfrac{[d((x_t)-m]^{d((x_t)-m}}{d(x_t)^{d(x_t)}}} \\
&> 1.
\end{aligned}$$

Then, $\prod_{1,c}(G) < \prod_{1,c}(G^*)$, $\prod_2(G) > \prod_2(G^*)$ and $q = s$ in G^*, then by the induction hypothesis, there exists a k-tree G' such that $|S_1(G')| = |S_1(G)| - 1$, $\prod_{1,c}(G') > \prod_{1,c}(G)$ and $\prod_2(G') < \prod_2(G)$, we are done.

If $q \geq k + 1$, we have $N(u_1) = \{u_2, u_3 ... u_{k+1}\}$, $N(v_1) = \{v_2, v_3 ... v_{k+1}\}$ by the facts that $p \geq q$ and $G[S \cup V(C_1)]$, $G[S \cup V(C_2)]$ are k-paths. We construct a new graph G^* such that $V(G^*) = V(G), E(G^*) = E(G) - \{v_1v_i\} + \{u_jv_1\}$ for $i \in [2, k+1]$, $j \in [1, k]$. And the definition of $\prod_{1,c}(G)$, $\prod_2(G)$, Lemma 2.0.1 and Lemma 2.0.2, we obtain

$$\begin{aligned}
\frac{\prod_{1,c}(G)}{\prod_{1,c}(G^*)} &= \frac{\prod_{i=2}^{k+1} d(v_i)^c \prod_{j=1}^{k} d(u_j)^c}{\prod_{i=2}^{k+1}[d(v_i)-1]^c \prod_{j=1}^{k,}[d(u_j)+1]^c} \\
&= 1, \\
\frac{\prod_2(G)}{\prod_2(G^*)} &= \frac{\prod_{i=2}^{k+1} d(v_i)^{d(v_i)} \prod_{j=1}^{k} d(u_j)^{d(u_j)}}{\prod_{i=2}^{k+1}[d(v_i)-1]^{d(v_i)-1} \prod_{j=1}^{k}[d(u_j)+1]^{d(u_j)+1}} \\
&= 1.
\end{aligned}$$

Then, $\prod_{1,c}(G) = \prod_{1,c}(G^*)$, $\prod_2(G) = \prod_2(G^*)$ and $q = s$ in G^*, then by the induction hypothesis, there exists a k-tree G' such that $|S_1(G')| = |S_1(G)| - 1$, $\prod_{1,c}(G') > \prod_{1,c}(G)$ and $\prod_2(G') < \prod_2(G)$, we are done. $\square$

Next we turn to prove the main results of this section.

Proof of Theorem 2.1.1. For any k-tree T_n^k, if $|S_1(T_n^k)| = n - k$, then $T_n^k \cong S_{k,n-k}$, we are done. And if $|S_1(T_n^k)| \leq n - k - 1$, we can recursively use Lemma 2.1.7 to make $\prod_{1,c}(T_n^k)$ decreasing until $|S_1(T_n^k)| = n - k$. Thus, we have $T_n^k \cong S_{k,n-k}$ for $\prod_{1,c}(T_n^k)$ to arrive the minimal value.

By Lemma 2.1.8, if $\prod_{1,c}(T_n^k)$ get the maximal, then every hyper pendent edge is a k-path, and by Lemma 2.1.9, $|S_1(T_n^k)| = 2$, implying that $T_n^k \cong P_n^k$ for $\prod_{1,c}(T_n^k)$ to arrive the maximal value. $\square$

Proof of Theorem 2.1.2. For any k-tree T_n^k, if $|S_1(T_n^k)| = n - k$, then $T_n^k \cong S_{k,n-k}$,we are done. And if $|S_1(T_n^k)| \leq n - k - 1$, we can recursively use Lemma 2.1.7 to make $\prod_2(T_n^k)$ increasing until $|S_1(T_n^k)| = n-k$, then we have $T_n^k \cong S_{k,n-k}$ for $\prod_2(T_n^k)$ to arrive the maximal value.

By Lemma 2.1.8, if $\prod_2(T_n^k)$ get the minimal, every hyper pendent edge is a k-path, and by Lemma 2.1.9, $|S_1(T_n^k)| = 2$. Then this k-tree is a k-path, that is, $T_n^k \cong P_n^k$ for $\prod_2(T_n^k)$ to arrive the minimal value. $\square$

2.2 CACTUS GRAPHS

In this section, we rewrite the results and give the complete proofs. Theorem 2.2.1 gives the lower bounds of the first generalized Zagreb index of cactus graphs and states the corresponding extremal graphs.

Theorem 2.2.1 (Wang and Wei [77]). *For any graph G in $\mathcal{C}_n^k$,*

$$\prod_{1,c}(G) \geq \begin{cases} 3^{kc}2^{(n-2k)c}, & \text{if} \quad k = 0, 1, \\ 2^{(n-k-1)c}k^c, & \text{if} \quad k \geq 2, \end{cases}$$

the equalities hold if and only if their degree sequences are $\underbrace{3, 3, ..., 3}_{k}, \underbrace{2, 2, ..., 2}_{n-2k}, \underbrace{1, 1, ..., 1}_{k}$ *and* $k, \underbrace{2, 2, ..., 2}_{n-k-1}, \underbrace{1, 1, ..., 1}_{k}$, *respectively.*

Theorems 2.2.2 and 2.2.3 provide the sharp upper bounds on the first generalized multiplicative Zagreb indices of cactus graphs and characterize the extremal graphs.

Theorem 2.2.2 (Wang and Wei [77]). *For any graph G in $\mathcal{C}_n^k$ with $n \leq k + 3$,*

$$\prod_{1,c}(G) \leq \begin{cases} k^c & \text{if} \quad n = k + 1, \\ (\lceil \frac{k}{2} \rceil + 1)^c(\lfloor \frac{k}{2} \rfloor + 1)^c & \text{if} \quad n = k + 2, \\ (\lceil \frac{k}{3} \rceil + 2)^c(\lfloor \frac{k}{3} \rfloor + 2)^c(k - \lceil \frac{k}{3} \rceil - \lfloor \frac{k}{3} \rfloor + 2)^c & \text{if} \quad n = k + 3, \end{cases}$$

the equalities hold if and only if their degree sequences are $k, \underbrace{1, 1, ..., 1}_{k}$; $\lceil \frac{k}{2} \rceil + 1, \lfloor \frac{k}{2} \rfloor + 1, \underbrace{1, 1, ..., 1}_{k}$ *and* $\lceil \frac{k}{3} \rceil + 2, \lfloor \frac{k}{3} \rfloor + 2, k - \lceil \frac{k}{3} \rceil - \lfloor \frac{k}{3} \rfloor + 2, \underbrace{1, 1, ..., 1}_{k}$, *respectively.*

Theorem 2.2.3 (Wang and Wei [77]). *For any graph G in $\mathcal{C}_n^k$ with $n \geq k + 4$ and $t \geq 0$,*

$$\prod_{1,c}(G) \leq \begin{cases} 16^c & \text{if} \quad k = 0, n = 4, \\ 2^{(3t+6)c} & \text{if} \quad k = 0, n = 2t + 5, \\ 2^{(3t+4)c}9^c & \text{if} \quad k = 0, n = 2(t + 3), \end{cases}$$

the equalities hold if and only if their degree sequences are $2,2,2,2$*;* $\underbrace{4,4,...,4}_{t+1},\underbrace{2,2,...,2}_{t+4}$ *and* $\underbrace{4,4,...,4}_{t},3,3,\underbrace{2,2,...,2}_{t+4}$*, respectively;*

For $k \neq 0$*, if* $\prod_{1,c}(G)$ *attains the maximal value, then one of the following statements holds: For any nonpendant vertices* u,v*, either (i)* $|d(u)-d(v)| \leq 1$ *or (ii)* $d(u) \in \{2,3,4\}$ *and* G *contains no cycles of length greater than 3, no dense paths of length greater than 1 except for at most one of them with length 2, and no paths of length greater 0 that connects only two cycles except for at most one of them with length 1.*

Theorem 2.2.4 gives sharp lower bounds on the second multiplicative Zagreb indices of cactus graphs and characterizes the extremal graphs.

Theorem 2.2.4 (Wang and Wei [77])**.** *For any graph* G *in* $\mathcal{C}_n^k$ *with* $\gamma = \frac{k-2}{n-k}$*,*

$$\prod_2(G) \geq \begin{cases} 3^{3k}2^{2(n-2k)} & if \quad k=0,1, \\ (2+\lceil\gamma\rceil)^{(2+\lceil\gamma\rceil)[k-2-\lfloor\gamma\rfloor(n-k)]}(2+\lfloor\gamma\rfloor)^{(2+\lfloor\gamma\rfloor)[n-2k+2+\lfloor\gamma\rfloor(n-k)]} & if \quad k \geq 2, \end{cases}$$

the equalities hold if and only if their degree sequences are $\underbrace{3,3,...,3}_{k},\underbrace{2,2,...,2}_{n-2k},\underbrace{1,1,...,1}_{k}$ *and* $\underbrace{2+\lceil\gamma\rceil,2+\lceil\gamma\rceil,...,2+\lceil\gamma\rceil}_{k-2-\lfloor\gamma\rfloor(n-k)},\underbrace{2+\lfloor\gamma\rfloor,2+\lfloor\gamma\rfloor,...,2+\lfloor\gamma\rfloor}_{n-2k+2+\lfloor\gamma\rfloor(n-k)},\underbrace{1,1,...,1}_{k}$*, respectively.*

Theorem 2.2.5 states sharp upper bounds on the second multiplicative Zagreb indices of cactus graphs and characterizes the extremal graphs.

Theorem 2.2.5 (Wang and Wei [77])**.** *For any graph* G *in* $\mathcal{C}_n^k$*,*

$$\prod_2(G) \leq \begin{cases} (n-2)^{n-2}2^{2(n-k-1)} & if \quad n-k \equiv 0(mod\,2), \\ (n-1)^{n-1}2^{2(n-k-1)} & if \quad n-k \equiv 1(mod\,2), \end{cases}$$

the equalities hold if and only if their degree sequences are $n-2,\underbrace{2,2,...,2}_{n-k-1},\underbrace{1,1,...,1}_{k}$ *and* $n-1,\underbrace{2,2,...,2}_{n-k-1},\underbrace{1,1,...,1}_{k}$*, respectively.*

Before we prove the theorems, we first give some lemmas that will be used later. By the definition of Multiplicative Zagreb index, one can obtain the following lemmas.

Lemma 2.2.6. For $G \in \mathcal{C}_n^k$ with $k \leq 1$ and $n \geq 3$, if $\prod_{1,c}(G)$ or $\prod_2(G)$ attains the minimal value, then G is an unicyclic graph.

Proof. For $k = 0$ or 1, by the choice of G, one can obtain that G contains at least one cycle. Otherwise, G is a tree which has at least two pendant vertices. Assume that there exists at least two cycles in G, and choose two cycles $C_1 = x_1x_2...x_1, C_2 = y_1y_2...y_1$ and a path $P = z_1z_2...z_p$ such that $V(P) \cap V(C_1) = \{z_1\}, V(P) \cap V(C_2) = \{z_p\}$ and P has no common vertices with any other cycles except C_1, C_2. Let $N(z_1) \cap V(C_1) = \{x_{11}, x_{12}\}$ and $N(z_p) \cap V(C_1) = \{x_{p1}, x_{p2}\}$, and set $G' = (G - \{x_{11}z_1, x_{p1}z_p\}) \cup \{x_{11}x_{p1}\}$, then $d_{G'}(z_1) = d(z_1) - 1, d_{G'}(z_p) = d(z_p) - 1$. By the definitions of $\prod_{1,c}(G)$ and $\prod_2(G)$, we have $\prod_{1,c}(G') < \prod_{1,c}(G)$ and $\prod_2(G') < \prod_2(G)$, a contradiction to the choice of G. Thus, Lemma 2.2.6 is ture. $\square$

Lemma 2.2.7. Let G' be a proper subgraph of a connected graph G. Then $\prod_{1,c}(G') < \prod_{1,c}(G), \prod_2(G') < \prod_2(G)$. In particular, for $G \in \mathcal{C}_n^k$ with $k \geq 2$, if $\prod_{1,c}(G)$ or $\prod_2(G)$ attains the minimal value, then G is a tree.

Proof. Since G' is a proper subgraph of G, by the definitions of $\prod_{1,c}(G)$ and $\prod_2(G)$, one can easily obtain that $\prod_{1,c}(G') < \prod_{1,c}(G)$ and $\prod_2(G') < \prod_2(G)$. For $k \geq 2$, we proceed to prove it by contradiction. For $k \geq 2$, assume that G is not a tree. Let C be a cycle of G and $P_1 = u_1u_2...u_p$ and $P_2 = v_1v_2...v_q$ be two pendant paths such that $V(P_1) \cap V(C) = \{u_1\}$ and $d(v_q) = 1$. Let $w_1 \in N(u_1) \cap V(C_1)$ and $G'' = (G - \{u_1w_1, v_1v_2\}) \cup \{v_2w_1\}$, then $d_{G''}(u_1) = d(u_1) - 1, d_{G''}(v_1) = d(v_1) - 1$ and $G'' \in \mathcal{C}_n^k$. By the definitions of $\prod_{1,c}(G)$ and $\prod_2(G)$, we have $\prod_{1,c}(G'') < \prod_{1,c}(G)$, $\prod_2(G'') < \prod_2(G)$ and Lemma 2.2.7 is true. $\square$

Lemma 2.2.8. If $\prod_2(G)$ attains the minimal value with $k \geq 2$, then any non-pendant vertices u, v of a connected graph G have the property: $|d(u) - d(v)| \leq 1$.

Proof. Since $k \geq 2$, by Lemma 2.2.7, we have that G must be a tree. On the contrary, if there are two non-pendant vertices $u, v \in V(G)$ such that $d(u) - d(v) \geq 2$, let $x \in N(u) - N(v)$ and $G' = (G - \{ux\}) \cup \{vx\}$, by $d_{G'}(u) = d(u) - 1, d_{G'}(v) = d(v) + 1, d(v) \leq d(u) - 2 < d(u) - 1$, we deduce that

$$\frac{\prod_2(G)}{\prod_2(G')} = \frac{d(v)^{d(v)} d(u)^{d(u)}}{[d(v)+1]^{d(v)+1}[d(u)-1]^{d(u)-1}} = \frac{\left[\frac{d(v)^{d(v)}}{[d(v)+1]^{d(v)+1}}\right]}{\left[\frac{[d(u)-1]^{d(u)-1}}{d(u)^{d(u)}}\right]} > 1,$$

that is, $\prod_2(G') < \prod_2(G)$, a contradiction with the choice of G. Thus, Lemma 2.2.8 is true. □

Lemma 2.2.9. If $\prod_{1,c}(G)$ or $\prod_2(G)$ attains the maximal value, then all cycles of G have length 3 except for at most one of them with length 4.

Proof. On the contrary, let C_m be a cycle of G with $C_m = v_1 v_2 \ldots . v_m v_1$ and $m \geq 5$, $G' = (G - \{v_3 v_4\}) \cup \{v_1 v_3, v_1 v_4\}$. Since G' has k pendant vertices, then $G' \in \mathcal{C}_n^k$. By the definitions of $\prod_{1,c}(G)$, $\prod_2(G)$ and $d_{G'}(v_1) = d(v_1) + 2$, we have

$$\frac{\prod_{1,c}(G)}{\prod_{1,c}(G')} = \frac{d(v_1)^c}{[d(v_1)+2]^c} < 1, \frac{\prod_2(G)}{\prod_2(G')} = \frac{d(v_1)^{d(v_1)}}{[d(v_1)+2]^{d(v_1)+2}} < 1,$$

that is, $\prod_{1,c}(G) < \prod_{1,c}(G')$ and $\prod_2(G) < \prod_2(G')$, a contradiction with the choice of G. We can proceed this process until all of the cycles have length 3 or 4.

Suppose that there exist two cycles of length 4, say $C_1 = x_1 x_2 x_3 x_4 x_1, C_2 = y_1 y_2 y_3 y_4 y_1$ in G. Since G is a cactus, then there exists a vertex $x_t \in V(C_1)$ (say x_4) such that there are no paths connecting x_4 and y_1, x_4 and y_2 in $G - \{x_1 x_4, x_3 x_4\}$. Otherwise, if every vertex of $V(C)$ is either connected with y_1 or with y_2 in $G - \{x_1 x_4, x_3 x_4\}$, then there exist a cycle that shares at least one common edge with C_1, a contradiction with the definition of cactus graph. Let $G^* = (G - \{x_1 x_4, x_3 x_4, y_1 y_4\}) \cup \{x_1 x_3, x_4 y_1, x_4 y_2, y_2 y_4\}$. Since G^* has k pendant vertices, then $G^* \in \mathcal{C}_n^k$. By the definitions of $\prod_{1,c}(G)$, $\prod_2(G)$ and $d_{G^*}(y_2) = d(y_2) + 2$, we have

$$\frac{\prod_{1,c}(G)}{\prod_{1,c}(G^*)} = \frac{d(y_2)^c}{[d(y_2)+2]^c} < 1, \frac{\prod_2(G)}{\prod_2(G^*)} = \frac{d(y_2)^{d(y_2)}}{[d(y_2)+2]^{d(y_2)+2}} < 1,$$

that is, $\prod_{1,c}(G) < \prod_{1,c}(G^*)$ and $\prod_2(G) < \prod_2(G^*)$, a contradiction with the choice of G and Lemma 4 is true. □

Lemma 2.2.10. If $\prod_{1,c}(G)$ or $\prod_2(G)$ attains the maximal value, then every dense path has length 1 except for at most one of them with length 2.

Proof. On the contrary, let C be a cycle and $P = v_1v_2...v_{p-1}v_{p_i}$ with $p \geq 2$ and $j \geq 1$ be a dense path such that $V(C) \cap V(P) = \{v_1\}$ and $d(v_{p_i}) = 1$. If $p \geq 4$, let $G' = G \cup \{v_1v_{p-1}\}$. Then $G' \in G[n,k]$ and $d_{G'}(v_1) = d(v_1)+1, d_{G'}(v_{p-1}) = d(v_{p-1})+1$. Thus, by the definition, we have $\prod_{1,c}(G') > \prod_1(G)$ and $\prod_2(G') > \prod_2(G)$, a contradiction with the choice of G. We can proceed this process until $p \leq 3$, that is, all of the dense paths have the length as 1 or 2.

If there exist two such paths of length 2, say $P_1 = x_1x_2x_{3j}$, $P_2 = y_1y_2y_{3j'}$ with $x_1 \in V(C_2), y_1 \in V(C_3)$ such that $d(x_{3j}) = d(y_{3j'}) = 1$ and $j, j' \geq 1$, then let $G^* = (G - \{y_1y_2, y_2y_{31}\}) \cup \{y_1y_{31}, x_1y_2, x_2y_2\}$. Since G^* has k pendant vertices, then $G^* \in G[n,k]$. By the definitions of $\prod_{1,c}(G)$, $\prod_2(G)$ and $d_{G^*}(x_1) = d(x_1)+1, d_{G^*}(x_2) = d(x_2)+1$, we have $\prod_{1,c}(G^*) > \prod_1(G)$ and $\prod_2(G^*) > \prod_2(G)$, a contradiction with the choice of G and Lemma 2.2.10 is true. □

Lemma 2.2.11. If $\prod_{1,c}(G)$ or $\prod_2(G)$ attains the maximal value, then G can not have both a dense path of length 2 and a cycle of length 4.

Proof. On the contrary, let C_1 be a cycle, $P = y_1y_2y_{3i}$ be a dense path such that $V(C_1) \cap V(P) = \{y_1\}$ and $d(y_{3i}) = 1$ for $i \geq 1$, C_2 be a cycle of length 4, say $C_2 = x_1x_2x_3x_4x_1$. By the definition of the cactus, there exists $x_t \in V(C_2)$ (say x_2) such that there is no paths connecting x_2 and y_1, x_2 and y_1 in $G - \{x_1x_2, x_2x_3\}$. Let $G' = (G - \{x_1x_2, x_2x_3\}) \cup \{x_2y_1, x_2y_2, x_1x_3\}$, then G' has k pendent vetices, $d_{G'}(y_1) = d(y_1)+1$ and $d_{G'}(y_2) = d(y_2)+1$.

By the definitions of $\prod_{1,c}(G)$, $\prod_2(G)$, we have $\prod_{1,c}(G') > \prod_1(G)$ and $\prod_2(G') > \prod_2(G)$, a contradiction with the choice of G and Lemma 2.2.11 is true. $\square$

Lemma 2.2.12. Let C be a cycle of G in $\mathcal{C}_n^k$ and $u, v \in V(C)$, if $min\{d(u), d(v)\} > 2$, then there exist a graph G' such that $\prod_2(G') > \prod_2(G)$.

Proof. Since $min\{d(u), d(v)\} \geq 3$, without loss of generality, let $d(u) \geq d(v) \geq 3$. Then there exists $x \in N(v) - V(C) - N(u)$. Otherwise, there will be two cycles containing at least two common vertices. Let $G' = (G - \{vx\}) \cup \{ux\}$, we have $d(u) \geq d(v) > d(v) - 1$. Then we have

$$\frac{\prod_2(G)}{\prod_2(G')} = \frac{d(u)^{d(u)}d(v)^{d(v)}}{[d(u)+1]^{d(u)+1}[d(v)-1]^{d(v)-1}} = \frac{[\frac{d(u)^{d(u)}}{[d(u)+1]^{d(u)+1}}]}{[\frac{[d(v)-1]^{d(v)-1}}{d(v)^{d(v)}}]} < 1.$$

Thus, $\prod_2(G') > \prod_2(G)$ and Lemma 2.2.12 is true. $\square$

Lemma 2.2.13. If $\prod_2(G)$ attains the maximal value, then any three cycles have a common vertex.

Proof. By the definition of the cactus, any two cycles have at most one common vertex. Now assume that there exist two disjoint cycles C_1, C_2 contained in G such that the path P connecting C_1 and C_2 is as short as possible. For convenience, let $P = u_1u_2...u_p$, $V(P) \cap V(C_1) = \{u_1\}$ and $V(P) \cap V(C_2) = \{u_p\}$.

If the path P has no common edges with any other cycle(s) contained in G and $|E(P)| \geq 2$, let the new graph $G' = G \cup \{u_1u_p\}$, then $G' \in G[n,k]$, $d_{G'}(u_1) = d(u_1) + 1$, and $d_{G'}(u_2) = d(u_2) + 1$. By the definition of $\prod_2(G)$, we have $\prod_2(G') > \prod_2(G)$. If $|E(P)| = 1$, without loss of generality, let $d(u_1) \geq d(u_2)$ and $C_2 = u_2v_2v_3...u_2$, we have $v_2 \notin N(u_1)$. Otherwise, there are two cycles who have the common edge contradicted with the definition of the cactus. Let $G^* = (G - \{u_2v_2\}) \cup \{u_1v_2\}$, we have $G^* \in G[n,k]$, $d_{G^*}(u_1) = d(u_1) + 1$ and $d_{G^*}(u_2) = d(u) - 1$. Since $d(u_1) \geq d(u_2) > d(u_2) - 1$, then

$$\frac{\prod_2(G)}{\prod_2(G^*)} = \frac{d(u_1)^{d(u_1)}d(u_2)^{d(u_2)}}{[d(u_1)+1]^{d(u_1)+1}[d(u_2)-1]^{d(u_2)-1}} = \frac{[\frac{d(u_1)^{d(u_1)}}{[d(u_1)+1]^{d(u_1)+1}}]}{[\frac{[d(u_2)-1]^{d(u_2)-1}}{d(u_2)^{d(u_2)}}]} < 1,$$

that is, $\prod_2(G^*) > \prod_2(G)$, a contradiction with the choice of G.

If P has some common edges with some other cycle, say C_3, by the choice of C_1, C_2 and the definition of cactus graph, we have $\{u_1\} = C_3 \cap C_1$ and $\{u_p\} = C_3 \cap C_2$. Since $min\{d(u_1), d(u_p)\} \geq 3$, by Lemma 2.2.12, we can get that there exist G^{**} such that $\prod_2(G^{**}) > \prod_2(G)$, a contradiction with the choice of G.

Thus, any two cycles of G have one common vertex. By the definition of cactus graph, we have that any three cycles have exactly one common vertex and Lemma 2.2.13 is true. □

Lemma 2.2.14. Let T be a tree attached to a vertex v_0 of a cycle of G. If $\prod_2(G)$ attains the maximal value, then $d(v) \leq 2$ for any $v \in V(T) - \{v_0\}$.

Proof. Choose a graph G such that $\prod_2(G)$ achieves the maximal value. On the contrary, assume that $u \in V(T) - \{v_0\}$ is of degree $r \geq 3$ and closest to a pendant vertex. For $d(u, v_0) \geq 2$, let $G' = G \cup \{uv_0\}$, we have $G' \in G[n, k]$, $d_{G'}(u) = d(u) + 1$ and $d_{G'}(v_0) = d(v_0) + 1$. By the definition of $\prod_2(G)$, we can obtain that $\prod_2(G') > \prod_2(G)$, a contradiction with the choice of G. For $d(u, v_0) = 1$, let $\{y_1, y_2, ..., y_{r-2}\}$ be the $r - 2$ neighbors of u such that $d(y_i, v_0) > d(u, v_0)$, y be a neighbor of v_0 which belongs to a cycle C_0.

Since v_0uy_1 is a pendant path of length 2, by Lemma 2.2.11, we have that every cycle has length 3. Let $C_0 = v_0w_1yv_0$, $G'' = (G - \{uy_1\}) \cup \{v_0y_1\}$ and $G''' = (G - \{v_0y\}) \cup \{uy\}$. Then $G'', G''' \in G[n, k]$, $d_{G''}(u) = d(u) - 1, d_{G''}(v_0) = d(v_0) + 1$ and $d_{G'''}(u) = d(u) + 1, d_{G'''}(v_0) = d(v_0) - 1$. By the definition of $\prod_2(G)$, Lemma 2.0.1 and Lemma 2.0.2, we can obtain

$$\frac{\prod_2(G)}{\prod_2(G'')} = \frac{d(u)^{d(u)}d(v_0)^{d(v_0)}}{[d(u)-1]^{d(u-1)}[d(v_0)+1]^{d(v_0)+1}} = \frac{[\frac{d(v_0)^{d(v_0)}}{[d(v_0)+1]^{d(v_0)+1}}]}{[\frac{[d(u)-1]^{d(u)-1}}{d(u)^{d(u)}}]} < 1, \text{if } d(v_0) \geq d(u),$$

$$\frac{\prod_2(G)}{\prod_2(G''')} = \frac{d(u)^{d(u)}d(v_0)^{d(v_0)}}{[d(u)+1]^{d(u+1)}[d(v_0)-1]^{d(v_0)-1}} = \frac{[\frac{d(u)^{d(u)}}{[d(u)+1]^{d(u)+1}}]}{[\frac{[d(v_0)-1]^{d(v_0)-1}}{d(v_0)^{d(v_0)}}]} < 1, \text{if } d(v_0) < d(u),$$

that is, $\prod_2(G'') > \prod_2(G)$ and $\prod_2(G''') > \prod_2(G)$, a contradiction with the choice of G. Thus, Lemma 2.2.14 is true. □

Lemma 2.2.15. If $\prod_2(G)$ attains the maximal value, then all attached trees are attached to a common vertex v_0.

Proof. On the contrary, suppose that there exist two trees T_1, T_2 attached to different vertices v_1, v_2 of some cycles, say C_1, C_2, such that $V(C_1) \cap V(T_1) = \{v_1\}, V(C_2) \cap V(T_2) = \{v_2\}$. By Lemma 2.2.13, all the cycles have a common vertex v_0. Without loss of generality, let $v_1 \neq v_0$, we have $d(v_0) \geq 3, d(v_1) \geq 3$. By Lemma 2.2.12, there exists G' such that $\prod_2(G') > \prod_2(G)$, a contradiction to the choice of G. Thus, Lemma 2.2.15 is true. □

Next, we turn to prove the main results. For any graph G in $\mathcal{C}_n^k$, if $n = 1$ or 2, then $\prod_{1,c}(G) = \prod_2(G) = 0$ or 1, that is, all upper and lower bounds of Multiplicative Zagreb indices have the same values, respectively. Thus, all of the Theorems are true. Now we may assume that $n \geq 3$.

Proof of Theorem 2.2.1. Choose a graph G in $\mathcal{C}_n^k$ such that $\prod_{1,c}(G)$ achieves the minimal value. For $k \leq 1$, by Lemma 2.2.6, G is an unicyclic graph. If $k = 0$, then G is a cycle, that is, the degree sequence of G is $\underbrace{2, 2, ..., 2}_{n}$; If $k = 1$, then G has only one pendant path, that is, the degree sequence of G is $3, \underbrace{2, 2, ..., 2}_{n-2}, 1$. Thus, Theorem 2.2.1 is true.

For $k \geq 2$, by the choice of G and Lemma 2.2.7, we obtain that G is a tree. If $k = 2$, then G is a path, that is, the degree sequence of G is $\underbrace{2, 2, ..., 2}_{n-2}, 1, 1$ and Theorem 2.2.1 is true; For $k \geq 3$, if there is a vertex v with $d(v) \geq k + 1$, since G is a tree, then G has more than k pendant vertices, a contradiction to the choice of G. Thus, $d(v) \leq k$ for any $v \in V(G)$. Now let v be the vertex with maximal degree Δ. If $\Delta = k$, then $G - v$ is a set of paths. Otherwise, there exists a vertex $u \in V(G) - \{v\}$ such that $d(u) \geq 3$ and since G is a tree, then G contains more than k pendant vertices, a contradiction to the choice of G. Thus, the degree sequence of G is $k, \underbrace{2, 2, ..., 2}_{n-k-1}, \underbrace{1, 1, ..., 1}_{k}$.

If $\Delta < k$, then G contains at least 2 cut vertices, say $u_1, u_2, ..., u_t$, such that $G - u_i$ has at least 3 components with $i \in [1, t]$ and $t \geq 2$. Otherwise, since G is a tree, G only contains Δ pendant vertices. Let $P = w_1 w_2 ... w_s$ be a path of $G - \{u_1, u_2, ..., u_t\}$ such that $w_s \in \{u_1, u_2, ..., u_t\} - \{v\}$ and P contains only a unique pendant vertex w_1. Set $G' = (G - \{w_{s-1} w_s\}) \cup \{w_{s-1} v\}$, we have $G' \in \mathcal{C}_n^k$, $d_{G'}(v) = d(v) + 1$ and $d_{G'}(w_s) = d(w_s) - 1$. Thus, by $\Delta \geq d(w_s) > d(w_s) - 1$, we have

$$\frac{\prod_{1,c}(G)}{\prod_{1,c}(G')} = \frac{\Delta^c d(w_s)^c}{(\Delta + 1)^c (d(w_s) - 1)^c} = \frac{\frac{\Delta^c}{(\Delta+1)^c}}{\frac{[d(w_s)-1]^c}{d(w_s)^c}} > 1,$$

that is, $\prod_{1,c}(G)$ is not minimal, a contradiction with the choice of G. If the maximal degree of G' is still less than k, then we can continue this process until $\Delta = k$, thus we can find the desired graph with the degree sequence of $k, \underbrace{2, 2, ..., 2}_{n-k-1}, \underbrace{1, 1, ..., 1}_{k}$. Therefore, Theorem 2.2.1 is true. $\square$

Proof of Theorem 2.2.2. Choose a graph G in $\mathcal{C}_n^k$ such that $\prod_{1,c}(G)$ achieves the maximal value. Let $S = \{v \in V(G), d(v) = 1\}$ and $G' = G - S$. If $|G'| = 1$, then for $k = 0$, the degree sequence of G is 0 and for $k \neq 0$, G is a star, that is, its degree sequence is $k, \underbrace{1, 1, ..., 1}_{k}$. If $|G'| = 2$ and for $k = 0$, there is no such simple connected graph; For $k \neq 0$, by *"Arithmetic-Mean and Geometric-Mean inequality: $x_1 x_2 ... x_n \leq (\frac{x_1 + x_2 + ... + x_n}{n})^n$, the equality holds if and only if $x_1 = x_2 = ... = x_n$"*, one can obtain that the degree sequence of G is $\lceil \frac{k}{2} \rceil + 1, \lfloor \frac{k}{2} \rfloor + 1, \underbrace{1, ..., 1}_{k}$. If $|G'| = 3$ and $k = 0$, by Lemma 2.2.7, we can obtain that G is a cycle of length 3, that is, its degree sequence is $2, 2, 2$. For $k \neq 0$, it is similar to the above proof, that is, the degree sequence of G is $\lceil \frac{k}{3} \rceil + 2, \lfloor \frac{k}{3} \rfloor + 2, k - \lceil \frac{k}{3} \rceil - \lfloor \frac{k}{3} \rfloor + 2, \underbrace{1, ..., 1}_{k}$. Therefore, Theorem 2.2.2 is true. $\square$

Proof of Theorem 2.2.3. Choose a graph G in $\mathcal{C}_n^k$ such that $\prod_{1,c}(G)$ achieves the maximal value. By Lemma 2.2.7 and $n - k \geq 4$, G contains some cycles. For $n - k = 4$, $G - S$ contains only one cycle C_0, where $S = \{v \in V(G), d(v) = 1\}$. If $k = 0$, by the choice of G, one can obtain that G is a cycle, that is, its degree sequence is $2,2,2,2$. If $k \neq 0$ and $|C_0| = 4$, by adding any deleted vertex back to $G - S$, one can get a new graph G_{01} with degree sequence $3,2,2,2,1$; If $k \neq 0$ and $|C_0| = 3$, by adding back any deleted vertex to $G - S$ such that it is adjacent to the pendant vertex in $G - S$, one can obtain a new graph G'_{01}. Since G_{01} and G'_{01} have the same degree sequences, by *Arithmetic-Mean and Geometric-Mean inequality*, we can continue to add any deleted vertex back to G_{01} or G'_{01} such that it is adjacent to the nonpendant vertex of smallest degree in G_{01} or G'_{01}. After adding back all of the deleted vertices, we can obtain the graph of maximal $\prod_{1,c}$-value and Theorem 2.2.3 is true. Thus we will consider the case when $n - k \geq 5$ below. By the choice of G and Lemma 2.2.9, G contains at least two cycles.

Claim 1. *The longest path connecting only two cycles has length at most 1.*

Proof. On the contrary, let $C_l, C_{l'}$ be two cycles and $P_1 = x_1x_2...x_p$ be a path such that $V(C_l) \cap V(P_1) = \{x_1\}, V(C_{l'}) \cap V(P_1) = \{x_p\}$. If $p \geq 3$, set $G' = G \cup \{x_1x_p\}$, then $d_{G'}(x_1) = d(x_1)+1$ and $d_{G'}(x_2) = d(x_2)+1$. By the definition of $\prod_{1,c}(G)$, we have $\prod_{1,c}(G') > \prod_{1,c}(G)$, a contradiction to the choice of G. Thus, $p \leq 2$ and Claim 1 is true. □

We first deal with the case when $k = 0$.

Claim 2. *Any three cycles have no common vertex if $k = 0$.*

Proof. On the contrary, let C_1, C_2, C_3 be the cycles of G such that $\cap_{i=1}^{3} V(C_i) = \{v_0\}$, and $N(v_0) \cap V(C_i) = \{v_{i1}, v_{i2}\}$ for $i \in [1,3]$. Choose v of degree 2 such that v is in an end block C_t of G and $N(v) \cap V(C_t) = \{v_{t1}, v_{t2}\}$. Set $G'' = (G - \{v_{21}v_0, v_{22}v_0\}) \cup \{v_{21}v, v_{22}v\}$, then $d_{G''}(v_0) = d(v_0) - 2$ and $d_{G''}(v) = d(v) + 2$. Since $d(v_0) - 2 \geq 4 > d(v)$, By the definitions of $\prod_{1,c}(G)$, we have

$$\frac{\prod_{1,c}(G)}{\prod_{1,c}(G'')} = \frac{d(v_0)^c d(v)^c}{[d(v_0)-2]^c [d(v)+2]^c} = \frac{[\frac{d(v)^c}{[d(v)+2]^c}]}{[\frac{[d(v_0)-2]^c}{d(v_0)^c}]} < 1,$$

that is, $\prod_{1,c}(G'') > \prod_1(G)$, a contradiction to the choice of G. □

Claim 3. *Every vertex of G has the degree 2, 3 or 4 if $k = 0$.*

Proof. We will prove it by the contradiction. If there is a vertex w_1 with $d(w_1) \geq 5$, by Claim 2, we can assume that there are two cycles $C_4, C_{4'}$ and a path P_2 such that $V(C_4) \cap V(C_{4'}) \cap V(P_2) = \{w_1\}$, since $k = 0$ and G is a cactus, there exists a vertex w_0 of an end block such that $d(w_0) = 2$, that is, $d(w_0) < d(w_1) - 2$. Without loss of generality, assume that w_0 is closer to $C_{4'}$, let $N(w_1) \cap V(C_4) = \{w_2, w_3\}$ and $G''' = (G - \{w_1w_2, w_1w_3\}) \cup \{w_0w_2, w_0w_3\}$, by the definition of $\prod_{1,c}(G)$, we have

$$\frac{\prod_{1,c}(G)}{\prod_{1,c}(G''')} = \frac{d(w_1)^c d(w_0)^c}{[d(w_1) - 2]^c [d(w_0) + 2]^c} = \frac{[\frac{d(w_0)^c}{[d(w_0)+2]^c}]}{[\frac{[d(w_1)-2]^c}{d(w_1)^c}]} < 1,$$

that is, $\prod_{1,c}(G''') > \prod_{1,c}(G)$, a contradiction to the choice of G. Thus, Claim 3 is true. $\square$

Claim 4. *There do not exist two paths of length 1 such that every path connects with only two cycles if $k = 0$.*

Proof. On the contrary, assume that there are two such paths $P_5 = z_1z_2$, $P_6 = y_1y_2$ with $z_1 \in C_6, z_2 \in C_7, y_1 \in C_8, y_2 \in C_9$ such that $N(y_1) \cap V(C_8) = \{y_{11}, y_{12}\}$ and $d(z_1) = d(z_2) = d(y_1) = d(y_2) = 3$. Let $G^* = (G - \{y_1y_2, y_1y_{11}, y_1y_{12}\}) \cup \{y_2y_{11}, y_2y_{12}, z_1y_1, z_2y_1\}$. Since $d_{G^*}(z_1) = d_{G^*}(z_2) = d_{G^*}(y_2) = 4, d_{G^*}(y_1) = 2$. By the definition of $\prod_{1,c}(G)$, we have

$$\frac{\prod_{1,c}(G)}{\prod_{1,c}(G^*)} = \frac{d(z_1)^c d(z_2)^c d(y_1)^c d(y_2)^c}{[d(z_1) + 1]^c [d(z_2) + 1]^c [d(y_1) - 1]^c [d(y_2) + 1]^c} = \frac{3^c 3^c 3^c 3^c}{4^c 4^c 2^c 4^c} < 1,$$

that is, $\prod_{1,c}(G^*) > \prod_{1,c}(G)$, a contradiction to the choice of G and Claim 4 is true. $\square$

Claim 5 *G can not have both a cycle of length 4 and a path of length 1 connecting only with two cycles if $k = 0$.*

Proof. On the contrary, let C_{10}, C_{11}, C_{12} be the cycles and $P = w_1w_2$ be a path such that $V(C_{10}) \cap V(P) = \{w_1\}$, $V(C_{11}) \cap V(P) = \{w_2\}$. If $|C_{10}| = |C_{11}| = 3$ and $|C_{12}| = 4$, then there exists a vertex $w_3 \in V(C_{12})$ such that $d(w_3) = 3$ or 4. Let $C_{12} = w_3x_2x_3x_4w_3$ and $G^{**} = (G - \{w_1w_2, x_2x_3\}) \cup \{w_2w_3, w_2x_2, w_3x_3\}$, then $d_{G^{**}}(w_1) = d(w_1) - 1 = 2, d_{G^{**}}(w_2) = d(w_2) + 1 = 4, d_{G^{**}}(w_3) = d(w_3) + 2 = 5$ or 6 and G^{**} has no pendent vetices. By the definitions of $\prod_{1,c}(G)$, we have

$$\frac{\prod_{1,c}(G)}{\prod_{1,c}(G^{**})} = \frac{d(w_1)^c d(w_2)^c d(w_3)^c}{[d(w_1)-1]^c[d(w_2)+1]^c[d(w_3)+2]^c} = \frac{3^c3^c3^c}{2^c4^c5^c}\text{or}\frac{3^c3^c4^c}{2^c4^c6^c} < 1,$$

that is, $\prod_{1,c}(G^{**}) > \prod_{1,c}(G)$, a contradiction with the choice of G.

If $|C_{10}| = |w_1w_{12}w_{13}w_{14}w_1| = 4$ and $|C_{11}| = |w_2w_{22}w_{23}w_2| = 3$, then $d(w_1) = d(w_2) = 3$, $d(w_{14}) = 2$ or 4. Let $G^{***} = (G - \{w_1w_{12}\}) \cup \{w_{12}w_{14}, w_2w_{14}\}$, we have $G^{***} \in \mathcal{C}_n^k$, $d_{G^{***}}(w_1) = d(w_1) - 1, d_{G^{***}}(w_{14}) = d(w_{14}) + 2, d_{G^{***}}(w_2) = d(w_2) + 1$. By the definitions of $\prod_{1,c}(G)$, we have

$$\frac{\prod_{1,c}(G)}{\prod_{1,c}(G^{***})} = \frac{d(w_1)^c d(w_{14})^c d(w_2)^c}{[d(w_1)-1]^c[d(w_{14})+2]^c[d(w_2)+1]^c} = \frac{3^c2^c3^c}{2^c4^c4^c}\text{or}\frac{3^c4^c3^c}{2^c6^c4^c} < 1.$$

that is, $\prod_{1,c}(G^{***}) > \prod_{1,c}(G)$, a contradiction with the choice of G and Claim 5 is true. $\square$

Thus, for $k = 0$ and $n = 5$, by the choice of G and Lemma 2.2.9, there exist two cycles of length 3, that is, its degree sequence is $4, 2, 2, 2, 2$; For $n = 6$, G can be G_l or G_s such that G_l contains two cycles of length 3 or G_s contains one cycle of length 3 and one cycle of length 4, that is, the degree sequences are $3, 3, 2, 2, 2, 2$ and $4, 2, 2, 2, 2, 2$. Since $\prod_{1,c}(G_l) > \prod_{1,c}(G_s)$, then $\prod_{1,c}(G_l)$ attains the maximal value; Similarly, for $n \geq 7$, if $n = 2t + 5$ with $t \geq 1$, then G^a contains only the cycles of length 3 and its degree sequence is $\underbrace{4, 4, .., 4}_{t+1}, \underbrace{2, 2, .., 2}_{t+4}$; If $n = 2(t+3)$, then G^b contains some cycles of length 3 and one path of length 1 that connects only two cycles, that is, its degree sequence is $\underbrace{4, 4, .., 4}_{t}, 3, 3, \underbrace{2, 2, .., 2}_{t+4}$.

Now we consider the case when $k \neq 0$ and define the following algorithm, say Pro : Step 1. Build G_{T_0} by deleting all the dense paths such that G_{T_0} satisfies the case of $k = 0$, that is, G_{T_0} is either G^a or G^b; Step 2. Build G_{T_i} by adding a deleted path to $G_{T_{i-1}}$ such that it is adjacent to a non-pendant vertex of smallest degree in $G_{T_{i-1}}$, $i \geq 1$; Step 3. Stop, if there is no remaining deleted paths; Go to Step 2, if otherwise.

By the choice of G and Lemma 2.2.10, all of the dense paths of G have length 1 except for at most one of them with length 2. If all of the dense paths of G have length 1, by *Arithmetic-Mean and Geometric-Mean inequality*, we can directly use *Pro* to get a new graph G_T of maximal $\prod_{1,c}$-value. Thus, for $k < 4+t$, G_T contains no cycles of length greater than 3, no dense paths of length greater than 1, no paths of length greater 0 that connects only two cycles except for at most one of them with length 1 and $d_{G_T}(w_a) \in \{2,3,4\}$, where w_a is any nonpendant vertex of G_T; For $k \geq 4+t$, we have $|d_{G_T}(w_b) - d_{G_T}(w_c)| \leq 1$, where w_b, w_c are any nonpendant vertices of G_T, that is, the statement (i) or (ii) is true. If there is one of the dense paths of G with length 2, then set $P_1 = u_1u_2u_{31}$, $P_2 = u_1u_2u_{32}, ..., P_{r-1} = u_1u_2u_{3(r-1)}$ with $d(u_{3i}) = 1, i \in [1, r-1]$. By *Arithmetic-Mean and Geometric-Mean inequality*, we can use *Pro* to get a new graph G_T such that $\prod_{1,c}(G_T) \geq \prod_{1,c}(G)$.

By the proof of the case for $k = 0$, if G_T contains a path $P_T = w_{T1}w_{T2}$ connecting only two cycles, say C_{T1}, C_{T2}, such that $V(C_{T1}) \cap V(P_T) = \{w_{T1}\}, V(C_{T2}) \cap V(P_T) = \{w_{T2}\}$, then set $G_1 = (G_T - \{u_2u_i, i \in [1, r-1]\}) \cup \{u_{31}w_{T1}, u_{31}w_{T2}, u_{31}u_j, i \in [2, r-1]\}$. Since $G_1 \in \mathcal{C}_n^k$, $d_{G_1}(w_{T1}) = d(w_{T1}) + 1, d_{G_1}(w_{T2}) = d(w_{T2}) + 1, d(u_2) = r, d_{G_1}(u_2) = 1, d(u_{31}) = 1$ and $d_{G_1}(u_{31}) = r$, by the definition of $\prod_{1,c}(G)$, we have

$$\frac{\prod_{1,c}(G)}{\prod_{1,c}(G_1)} = \frac{d(w_{T1})^c d(w_{T2})^c d(u_{31})^c d(u_2)}{[d(w_{T1})+1]^c [d(w_{T2})+1]^c d(u_{31})^c d_1(u_2)} < 1,$$

that is, $\prod_{1,c}(G_1) > \prod_{1,c}(G)$, a contradiction to the choice of G.

If G_T contains no such path P_T and $|d(u_2) - d(v_T)| \leq 1$ for any nonpendant vertices v_T, v'_T of G_T, when $|d(v_T) - d(v'_T)| \leq 1$, then the statement (i) is true; When there exist v_T, v'_T such that $|d(v_T) - d(v'_T)| > 1$, by the construction of G_T, we have $d(v_T), d(v'_T) \in \{2,3,4\}$ and G contains no dense paths of length greater than 1 except for at most one of them with length 2, that is, the statement (ii) is true. Otherwise, if there exists a vertex v_T such that $|d(u_2) - d(v_T)| > 1$, then without loss of generality, choose C_{T3} and C_{T4} such that $V(C_{T3}) \cap V(C_{T4}) = \{v_T\}$ and let $N(v_T) = \{v_{ci}, i \geq 4\}$ such that $v_{c1}, v_{c2} \in V(C_{T3})$,

$v_{c3}, v_{c4} \in V(C_{T3})$. When $d(v_T) - d(u_2) > 1$, set $G_2 = (G_T - \{v_T v_{c1}, v_T v_{c2}, u_2 u_{3i}, i \geq 1\}) \cup \{u_{31}v_{c1}, u_{31}v_{c2}, u_{31}v_T, u_{31}u_{3i}, i \geq 2\}$, then $d_{G_2}(u_2) = 1, d_{G_2}(u_{31}) = d(u_2) + 1$ and $d_{G_2}(v_T) = d(v_T) - 1$. When $d(u_2) - d(v_T) > 1$, that is, $d(u_2) > 3$, set $G_3 = (G_T - \{v_T v_{c1}, v_T v_{c2}, u_2 u_{3i}, i \geq 1\}) \cup \{u_{31}v_{c1}, u_{31}v_{c2}, u_{31}v_T, u_{32}v_T, u_{33}v_T, u_{31}u_{3i}, i \geq 4\}$, then $d_{G_3}(u_2) = 1, d_{G_3}(u_{31}) = d(u_2) - 1$ and $d_{G_3}(v_T) = d(v_T) + 1$. Since $G_2, G_3 \in \mathcal{C}_n^k$, by the definition of $\prod_{1,c}(G)$ and Fact 1, we have

$$\frac{\prod_{1,c}(G)}{\prod_{1,c}(G_2)} = \frac{d(u_{31})^c d(u_2)^c d(v_T)^c}{[d(u_2)+1]^c 1^c [d_2(v_T)-1]^c} < 1, \frac{\prod_{1,c}(G)}{\prod_{1,c}(G_3)} = \frac{d(u_{31})^c d(u_2)^c d(v_T)^c}{[d(u_2)-1]^c 1^c [d(v_T)+1]^c} < 1,$$

that is, $\prod_{1,c}(G_2) > \prod_{1,c}(G)$, $\prod_{1,c}(G_3) > \prod_{1,c}(G)$, a contradition to the choice of G. Therefore, Theorem 2.2.3 is true. $\square$

Proof of Theorem 2.2.4. Choose a graph G in $\mathcal{C}_n^k$ such that $\prod_2(G)$ achieves the minimal value. By Lemma 2.2.6, G is an unicyclic graph for $k \leq 1$. If $k = 0$, then G is a cycle, that is, its degree sequence is $\underbrace{2, 2, ..., 2}_{n}$; If $k = 1$, then G has only one pendant path, that is, its degree sequence is $3, \underbrace{2, 2, ..., 2}_{n-2}, 1$.

For $k \geq 2$, by Lemma 2.2.7, we only need to consider G as a tree. Since $\sum_{v \in V(G)} d(v) = 2(n-1)$, then the average degree of G except the pendant vertices is $\frac{\sum_{v \in V(G)} d(v) - k}{n-k} = \frac{2(n-1)-k}{n-k} = 2 + \frac{k-2}{n-k} = 2 + \gamma$. By Lemma 2.2.8, if all of nonpendant vertices have degree $2 + \lfloor \gamma \rfloor$ or $2 + \lceil \gamma \rceil$, then $\prod_2(G)$ attains the minimal value. Set the number of the vertices with degree $2 + \lfloor \gamma \rfloor$ to be y_1, the number of the vertices with degree $2 + \lceil \gamma \rceil$ to be y_2, we have $y_1 + y_2 + k = n$ and $(2 + \lfloor \gamma \rfloor)y_1 + (2 + \lceil \gamma \rceil)y_2 + k = 2(n-1)$. If $\lfloor \gamma \rfloor = \lceil \gamma \rceil$, then Theorem 2.2.4 is true; If $\lceil \gamma \rceil - \lfloor \gamma \rfloor = 1$, by solving the above equations, we have $y_1 = n - 2k + 2 + \lfloor \gamma \rfloor (n-k), y_2 = k - 2 - \lfloor \gamma \rfloor (n-k)$, that is, its degree sequence is $\underbrace{2 + \lceil \gamma \rceil, 2 + \lceil \gamma \rceil, ..., 2 + \lceil \gamma \rceil}_{k-2-\lfloor \gamma \rfloor (n-k)}, \underbrace{2 + \lfloor \gamma \rfloor, 2 + \lfloor \gamma \rfloor, ..., 2 + \lfloor \gamma \rfloor}_{n-2k+2+\lfloor \gamma \rfloor (n-k)}, \underbrace{1, 1, ..., 1}_{k}$. Therefore, Theorem 2.2.4 is true. $\square$

Proof of Theorem 2.2.5. Choose G in $\mathcal{C}_n^k$ such that $\prod_2(G)$ achieves the maximal value. By Lemma 2.2.9, the lengths of all cycles in G are 3 except for at most one of them with length 4; By Lemmas 2.2.10 and 2.2.14, every pendant path has length of 1 except for at most one of them with length 2. By Lemma 2.2.11, G can not have both a dense path of length 2 and a cycle of length 4; By Lemma 2.2.13, any three cycles have a common vertex v_0; By Lemma 2.2.15, any tree attachs to the same vertex u. Now we show that $u = v_0$. Otherwise, if $u \neq v_0$ and $d(v_0) \geq d(u)$, let C^* be the cycle that contains u and $G' = (G - \{uy|y \in N(u) - V(C^*)\}) \cup \{v_0y|N(u) - V(C^*)\}$ with $|N(u) - V(C^*)| = t_1$, by $d_{G'}(u) = d(u) - t_1, d_{G'}(v_0) = d(v_0) + t_1$, we have

$$\frac{\prod_2(G)}{\prod_2(G')} = \frac{d(v_0)^{d(v_0)} d(u)^{d(u)}}{[d(v_0) + t_1]^{d(v_0)+t_1} [d(u) - t_1]^{d(u)-t_1}} = \frac{\frac{d(v_0)^{d(v_0)}}{[d(v_0)+t_1]^{d(v_0)+t_1}}}{\frac{[d(u)-t_1]^{d(u)-t_1}}{d(u)^{d(u)}}} < 1,$$

that is, $\prod_2(G') > \prod_2(G)$, a contradiction with the choice of G; If $d(u) > d(v_0)$, let $G'' = (G - \{v_0y|y \in N(v_0) - V(C^*)\}) \cup \{uy|y \in N(v_0) - V(C^*)\}$ with $|N(u) - V(C^*)| = t_2$, by $d_{G''}(v_0) = d(v_0) - t_2, d_{G''}(u) = d(u) + t_2$, we have

$$\frac{\prod_2(G)}{\prod_2(G'')} = \frac{d(u)^{d(u)} d(v_0)^{d(v_0)}}{[d(u) + t_2]^{d(u)+t_2} [d(v_0) - t_2]^{d(v_0)-t_2}} = \frac{\frac{d(u)^{d(u)}}{[d(u)+t_2]^{d(u)+t_2}}}{\frac{[d(v_0)-t_2]^{d(v_0)-t_2}}{d(v_0)^{d(v_0)}}} < 1,$$

that is, $\prod_2(G'') > \prod_2(G)$, a contradiction with the choice of G. Therefore, we can obtain the construction of G as follows: If $n - k \equiv 0 (\mathrm{mod}\ 2)$, then the degree sequence of G is $n-2, \underbrace{2, 2, ..., 2}_{n-k-1}, \underbrace{1, 1, ..., 1}_{k}$; if $n - k \equiv 1 (\mathrm{mod}\ 2)$, then the degree sequence of G is $n - 1, \underbrace{2, 2, ..., 2}_{n-k-1}, \underbrace{1, 1, ..., 1}_{k}$. Thus, Theorem 2.2.5 is true. $\square$

3 PADMAKAR-IVAN(PI) INDEX

In this chapter, we provide the extremal k-trees and cactus graphs regarding to an interesting topological index (Padmakar–Ivan index).

3.1 K-TREES

In this section, we will answer the question that whether or not a k-star or a k-path attains the maximal or minimal bound for PI-indices of k-trees. The related results are listed again: Theorems 3.1.1 and 3.1.2 give the exact PI-values of k-stars, k-paths and k-spirals.

Theorem 3.1.1 (Wang and Wei, [78]). *For any k-star S_n^k and k-path P_n^k with $n = kp + s$ vertices, where $p \geq 0$ is an integer and $s \in [2, k+1]$,*

$$(i) PI(S_n^k) = k(n-k)(n-k-1),$$
$$(ii) PI(P_n^k) = \tfrac{k(k+1)(p-1)(3kp+6s-2k-4)}{6} + \tfrac{(s-1)s(3k-s+2)}{3}.$$

Theorem 3.1.2 (Wang and Wei, [78]). *For any k-spiral $T_{n,c}^{k*}$ with $n \geq k$ vertices, where $c \in [1, k-1]$,*

$$PI(T_{n,c}^{k*}) = \begin{cases} \frac{(n-k)(n-k-1)(4k-n+2)}{3} & \text{if} \quad n \in [k, 2k-c], \\ \frac{3c(n-2k+c-1)(n-2k+c)+(k-c)(2c^2+3nc-4kc+3kn-4k^2-6k+3n-2)}{3} & \text{if} \quad n \geq 2k-c+1. \end{cases}$$

Theorem 3.1.3 proves that k-stars achieve the maximal values of PI-values for k-trees.

Theorem 3.1.3 (Wang and Wei, [78]). *For any k-tree T_n^k with $n \geq k \geq 1$, $PI(T_n^k) \leq PI(S_n^k)$.*

Theorem 3.1.4 shows that k-paths do not attain the minimal values and certain PI-values of k-spirals are less than that of the PI-values of k-paths.

Theorem 3.1.4 (Wang and Wei, [78]). *For any k-spiral $T^{k*}_{n,c}$ with $n \geq k \geq 1$, then*

$$\begin{aligned} &(i) \quad PI(P_n^k) \geq PI(T^{k*}_{n,c}) \;\; \textit{if} \;\; c \in [1, \tfrac{k+1}{2}), \\ &(ii) \quad PI(P_n^k) \leq PI(T^{k*}_{n,c}) \;\; \textit{if} \;\; c \in [\tfrac{k+1}{2}, k-1]. \end{aligned}$$

In order to consider the PI-value of any k-tree G, let $G' = G \cup \{u\}$ be a k-tree obtained by adding a new vertex u to G. For any $v_1, v_2 \in V(G)$, let $d(v_1, v_2)$ be the distance between v_1 and v_2 in G, $d'(v_1, v_2)$ be the distance between v_1 and v_2 in G'. Now we define a function that measures the difference of PI-values of any edge relating a vertex from G to G' as follows: $f : \{w \in V(G'), xy \in E(G)\}$ to $\{1, 0\}$ as follows:

$$f(w, xy) = \begin{cases} 0 & \text{if} \quad w = u \text{ and } d'(x,w) = d'(y,w), \\ 0 & \text{if} \quad w \in V(G) \text{ and } d(x,w) - d'(x,w) = d(y,w) - d'(y,w), \\ 1 & \text{if} \quad \textit{otherwise}. \end{cases}$$

Using the construction of k-trees, we can derive the following lemmas.

Lemma 3.1.5. Let xy be any edge of a k-tree G with at least $n \geq k+1$ vertices, then $PI(xy) \leq n - k - 1$.

Proof. Since every vertex of any k-tree G with at least $k+1$ vertices must be in some $(k+1)$-cliques, that is, $|N(x) \cap N(y)| \geq k-1$ for any $xy \in E(G)$, then $PI(xy) \leq n - (k-1) - 2 = n - k - 1$. □

Lemma 3.1.6. Let xy be any edge of a k-tree G with n vertices and $G' = G \cup \{u\}$ be a k-tree obtained by adding u to G, then $f(w, xy) \leq 1$. Furthermore, if $w \in V(G)$, then $f(w, xy) = 0$.

Proof. By adding u to G, since G' is a k-tree, we can get that the distance of any pair of vertices of G will increase at most 1, then $f(w, xy) \leq 1$. If $w \in V(G)$, then there exists a shortest path P_{xw} or P_{yw} such that $u \notin V(P_{xw})$ or $V(P_{yw})$, that is, $f(w, xy) = 0$. $\square$

Lemma 3.1.7. For any k-path G with n vertices, where $n \geq k+2$, let $S_1(G) = \{v_1, v_n\}$ and $\{v_1, v_2, ..., v_n\}$ be the simplicial elimination ordering of G. Then $d(v_i, v_j) = \lceil \frac{j-i}{k} \rceil$, for $i < j$ and $i, j \in [1, n]$. Furthermore, if $n = kp + s$ with $p \geq 1, s \in [2, k+1]$, then

$$d(v, v_{kp+s}) = \begin{cases} p+1 & \text{if} \quad v \in \{v_1, v_2, ..., v_{s-1}\}, \\ p-i & \text{if} \quad v \in \{v_{ki+s}, v_{ki+s+1}, ..., v_{k(i+1)+s-1}\}, i \in [0, p-1]. \end{cases}$$

Proof. If $j - i \leq k$, then v_i, v_j must be in the same $(k+1)$-clique of G, and we have $d(v_i, v_j) = 1$; If $j - i \geq k+1$, then $P_{v_iv_j} = v_i v_{i+k} v_{i+2k} ... v_{i+(\lfloor \frac{j-i}{k} \rfloor - 1)k} v_{i+\lfloor \frac{j-i}{k} \rfloor k} v_j$ is one of the shortest paths between v_i and v_j. Thus, $d(v_i, v_j) = \lceil \frac{j-i}{k} \rceil$ and Lemma 3.1.7 is true. $\square$

Lemma 3.1.8. For any k-spiral $T_{n,c}^{k*}$ with n vertices and $v_i, v_j \in V(T_{n,c}^{k*})$ for $i < j$,

$$d(v_i, v_j) = \begin{cases} 1 & \text{if} \quad j - i \leq k - c, i, j \in [1, n-c], \\ 1 & \text{if} \quad i \text{ or } j \in [n-c+1, n], \\ 2 & \text{if} \quad j - i \geq k - c + 1, i, j \in [1, n-c]. \end{cases}$$

Proof. If $j - i \leq k - c$ with $i, j \in [1, n-c]$, by Definition 4, we can get that v_i, v_j must be in the same $(k+1)$-clique of G and $d(v_i, v_j) = 1$; If i or $j \in [n-c+1, n]$, without loss of generality, say v_i such that $i \in [n-c+1, n]$, then $N[v_i] = V(T_{n,c}^{k*})$, that is, $d(v_i, v_j) = 1$; If $j - i \geq k - c + 1$ with $i, j \in [1, n-c]$, then $v_i \notin N(v_j)$ and $P_{v_iv_j} = v_i v_n v_j$ is one of the shortest paths between v_i and v_j, that is, $d(v_i, v_j) = 2$. Thus, Lemma 3.1.8 is true. $\square$

We next give the proofs of the main results using induction. For any k-tree T_n^k, if $n = k$ or $k+1$, then T_n^k is a k or $(k+1)$-clique, that is, $PI(T_n^k) = 0$. Thus, all of the theorems are true and we will only consider the case when $n \geq k+2$ below.

Proof of Theorem 2.1.1. For (i), let $V(S_n^k) = \{u_1, u_2, ..., u_n\}$, $G[\{u_1, ..., u_k\}]$ be a k-clique and $N(u_{l_0}) = \{u_1, u_2, ..., u_k\}$ for $l_0 \geq k+1$. Just by the definition of k-stars, we can get that for $i, j \in [1, k]$, $N[u_i] = N[u_j] = V(S_n^k)$, then $PI(u_iu_j) = n_{u_iu_j}(u_i) + n_{u_iu_j}(u_j) = 0$; For $i \in [1, k]$ and $l_0 \in [k+1, n]$, $|N[u_i] - N[u_{l_0}]| = n-k-1$, then $PI(u_iu_l) = n-k-1$. Thus, we can get $PI(S_n^k) = \sum_{i,j\in[1,k]} PI(u_iu_j) + \sum_{i\in[1,k],l_0\in[k+1,n]} PI(u_iu_{l_0}) = k(n-k)(n-k-1)$.

For (ii), we will proceed by induction on $|P_n^k| = n \geq k+2$. If $n = k+2$, let $\{v_1, v_2, ..., v_{k+2}\}$ be the simplicial elimination ordering of P_{k+2}^k. By Lemma 3.1.7, we can get that $PI(v_1v_i) = 1, PI(v_iv_{i'}) = 0$ and $PI(v_iv_{k+2}) = 1$ for $i, i' \in [2, k+1]$. Thus, $PI(P_{k+2}^k) = \sum_{i=2}^{k+1} PI(v_1v_i) + \sum_{i=2}^{k+1} PI(v_iv_{k+2}) = 2k$. Assume that Theorem 3.1.1 is true for a k-path with at most $kp+s-1$ vertices, where $p \geq 1, 2 \leq s \leq k+1$. Let P_n^k be a k-path such that $|P_n^k| = kp+s$, $V(P_n^k) = \{v_1, v_2, ..., v_{kp+s}\}$ and $\{v_1, v_2, ..., v_{kp+s}\}$ be the simplicial elimination ordering of P_n^k. Set $P_{n-1}^k = P_n^k - \{v_{kp+s}\}$, then $\{v_1, v_2, ..., v_{kp+s-1}\}$ is the simplicial elimination ordering of P_{n-1}^k and for any edge $v_iv_j \in E(P_n^k)$, $d(v_i, v_j)$ or $d'(v_i, v_j)$ is the distance of v_i and v_j in P_{n-1}^k or P_n^k, respectively.

Let $\alpha = [\frac{k(k+1)(p-1)(3kp+6s-2k-4)}{6} + \frac{(s-1)s(3k-s+2)}{3}] - [\frac{k(k+1)(p-1)(3kp+6s-2k-10)}{6} + \frac{(s-2)(s-1)(3k-s+3)}{3}] = pk^2 + pk - k^2 - 3k + 2ks - s^2 + 3s - 2$. If we can show that by adding v_{kp+s} to P_{n-1}^k, $PI(P_n^k) = PI(P_{n-1}^k) + \alpha$, then Theorem 3.1.1 is true.

Set $w = v_{kp+s}$, $A_1 = \{v_1v_s, v_1v_{s+1}, ..., v_1v_{k+1}\}, A_2 = \{v_2v_s, ..., v_2v_{k+2}\}, ..., A_{s-1} = \{v_{s-1}v_s, ..., v_{s-1}v_{k+s-1}\}$ and $B_1 = \{v_1v_2, v_1v_3, ..., v_1v_{s-1}\}, B_2 = \{v_2v_3, ..., v_2v_{s-1}\}, ..., B_{s-2} = \{v_{s-2}v_{s-1}\}, B_{s-1} = \phi$. By the definition of k-paths and Lemma 3.1.7, we have $d'(v_1, v_{kp+s}) = p+1$, $d'(v_s, v_{kp+s}) = p$ and $d'(v_1, v_{kp+s}) = p+1, d'(v_2, v_{kp+s}) = p+1$, that is, $d'(v_1, v_{kp+s}) \neq d'(v_s, v_{kp+s})$ and $d'(v_1, v_{kp+s}) = d'(v_2, v_{kp+s})$. Thus, $f(w, v_1v_s) = 1$ and $f(w, v_1v_2) = 0$. Similarly, for any edge $v_{h_1}v_{h_2} \in \cup_{i=1}^{s-1} A_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v_{kp+s}) \neq d'(v_{h_2}, v_{kp+s})$, that is, $f(w, v_{h_1}v_{h_2}) = 1$; For $v_{h_1}v_{h_2} \in \cup_{i=1}^{s-1} B_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v_{kp+s}) = d'(v_{h_2}, v_{kp+s})$, that is, $f(w, v_{h_1}v_{h_2}) = 0$. Thus, we can get that

$$f(v_{kp+s}, xy) = \begin{cases} 1 & \text{if} \quad xy \in \cup_{i=1}^{s-1} A_i, \\ 0 & \text{if} \quad xy \in \cup_{i=1}^{s-1} B_i. \end{cases}$$

For $t \in [0, p-2]$, set $A_{kt+s} = \{v_{kt+s}v_{k(t+1)+s}\}$, $A_{kt+s+1} = \{v_{kt+s+1}v_{k(t+1)+s}, v_{kt+s+1}v_{k(t+1)+s+1}\}$, ..., $A_{k(t+1)+s-1} = \{v_{k(t+1)+s-1}v_{k(t+1)+s}, v_{k(t+1)+s-1}v_{k(t+1)+s+1}, ..., v_{k(t+1)+s-1}v_{k(t+2)+s-1}\}$, and $B_{kt+s} = \{v_{kt+s}v_{kt+s+1}, ..., v_{kt+s}v_{k(t+1)+s-1}\}, B_{kt+s+1} = \{v_{kt+s+1}v_{kt+s+2}, ..., v_{kt+s+1}v_{k(t+1)+s-1}\}, ..., B_{k(t+1)+s-2} = \{v_{k(t+1)+s-2}v_{k(t+1)+s-1}\}, B_{k(t+1)+s-1} = \phi$. For $t = 0$ and by Lemma 3.1.7, we have $d'(v_s, v_{kp+s}) = p$, $d'(v_{k+s}, v_{kp+s}) = p-1$ and $d'(v_s, v_{kp+s}) = p, d'(v_{s+1}, v_{kp+s}) = p$, that is, $d'(v_s, v_{kp+s}) \neq d'(v_{k+s}, v_{kp+s})$ and $d'(v_s, v_{kp+s}) = d'(v_{s+1}, v_{kp+s})$. Thus, $f(w, v_sv_{k+s}) = 1$ and $f(w, v_sv_{s+1}) = 0$. Similarly, for any edge $v_{h_1}v_{h_2} \in \cup_{i=kt+s}^{k(t+1)+s-1} A_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v_{kp+s}) \neq d'(v_{h_2}, v_{kp+s})$, that is, $f(w, v_{h_1}v_{h_2}) = 1$; For $v_{h_1}v_{h_2} \in \cup_{i=kt+s}^{k(t+1)+s-1} B_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v_{kp+s}) = d'(v_{h_2}, v_{kp+s})$, that is, $f(w, v_{h_1}v_{h_2}) = 0$. Thus, we can get that

$$f(v_{kp+s}, xy) = \begin{cases} 1 & \text{if} \quad xy \in \cup_{i=kt+s}^{k(t+1)+s-1} A_i, \\ 0 & \text{if} \quad xy \in \cup_{i=kt+s}^{k(t+1)+s-1} B_i. \end{cases}$$

Next we only consider the edges in the $(k+1)$-clique $P_n^k[N[v_{kp+s}]]$. For any edge $v_{h_1}v_{h_2}$ with $h_1, h_2 \in [k(p-1)+s, kp+s-1]$, we have $d'(v_{h_1}, v_{kp+s}) = d'(v_{h_2}, v_{kp+s}) = 1$, that is, $f(w, v_{h_1}v_{h_2}) = 0$. For any edge v_hv_{kp+s} with $h \in [k(p-1)+s, kp]$, by Lemma 3.1.7, we can obtain that $d'(v_1, v_h) = p, d'(v_1, v_{kp+s}) = p+1$, $d'(v_{h-k}, v_h) = 1, d'(v_{h-k}, v_{kp+s}) = 2$ and when $h \neq k(p-1)+s$, $d'(v_{k(p-1)+s}, v_h) = 1, d'(v_{k(p-1)+s}, v_{kp+s}) = 1$, that is, $d'(v_1, v_h) \neq d'(v_1, v_{kp+s})$, $d'(v_{h-k}, v_h) \neq d'(v_{h-k}, v_{kp+s})$ and $d'(v_{k(p-1)+s}, v_h) = d'(v_{k(p-1)+s}, v_{kp+s})$. Similarly, we get that for $j \in [1, p-1], j' \in [1, p]$ and $l \neq h$,

$$\begin{cases} d'(v_l, v_h) \neq d'(v_l, v_{kp+s}) & \text{if} \quad l \in [1, s-1] \cup [h-jk, k(p-j)+s-1], \\ d'(v_l, v_h) = d'(v_l, v_{kp+s}) & \text{if} \quad l \in [k(p-j')+s, h-j'k+k-1] \cup [h+1, kp+s-1]. \end{cases}$$

Thus, if $v_h = v_{k(p-1)+s}$, then $d'(v_l, v_{k(p-1)+s}) \neq d'(v_l, v_{kp+s})$ with $l \in [1, s-1] \cup \{\cup_{j=1}^{p-1}[k(p-1)+s-jk, (p-j)k+s-1]\} = [1, (p-1)k+s-1]$ and $d'(v_l, v_{k(p-1)+s}) = d'(v_l, v_{kp+s})$ with $l \in [(p-1)k+s+1, kp+s]$, that is, $PI(v_{k(p-1)+s}v_{kp+s}) = (p-1)k+s-1$; Similarly, we can obtain that $PI(v_{k(p-1)+s+1}v_{kp+s}) = (p-1)(k-1)+s-1; PI(v_{k(p-1)+s+2}v_{kp+s}) = (p-1)(k-2)+s-1; ...; PI(v_{kp}v_{kp+s}) = (p-1)s+s-1$.

For any edge $v_h v_{kp+s}$ with $h \in [kp+1, kp+s-1]$, by Lemma 3.1.7, we can obtain that $d'(v_{h-k}, v_h) = 1, d'(v_{h-k}, v_{kp+s}) = 2$ and $d'(v_{k(p-1)+s}, v_h) = 1, d'(v_{k(p-1)+s}, v_{kp+s}) = 1$, that is, $d'(v_{h-k}, v_h) \neq d'(v_{h-k}, v_{kp+s})$ and $d'(v_{k(p-1)+s}, v_h) = d'(v_{k(p-1)+s}, v_{kp+s})$. Similarly, we get that for $j'' \in [1, p]$ and $l \neq h$,

$$\begin{cases} d'(v_l, v_h) \neq d'(v_l, v_{kp+s}) & \text{if} \quad l \in [h-j''k, k(p-j'')+s-1], \\ d'(v_l, v_h) = d'(v_l, v_{kp+s}) & \text{if} \quad l \in [k(p-j'')+s, h-j''k+k-1] \cup [h+1, kp+s-1]. \end{cases}$$

Thus, if $v_h = v_{kp+1}$, then $d'(v_l, v_{kp+1}) \neq d'(v_l, v_{kp+s})$ for $l \in \cup_{j''=1}^{p}[kp+1-j''k, k(p-j'')+s-1]$ and $d'(v_l, v_{kp+1}) = d'(v_l, v_{kp+s})$ with $l \in \{\cup_{j''=1}^{p}[k(p-j'')+s, k(p+1-j'')]\} \cup [h+1, kp+s-1]$, that is, $PI(v_{kp+1}v_{kp+s}) = (s-1)p$; Similarly, we have $PI(v_{kp+1}v_{kp+s}) = (s-2)p; ...; PI(v_{kp+s-2}v_{kp+s}) = 2p; PI(v_{kp+s-1}v_{kp+s}) = p$.

Set $w \in V(P_{n-1}^k)$, if $xy \in E(P_n^k)$ with x or $y \neq v_{kp+s}$, by Lemma 3.1.6, we have $f(w, xy) = 0$. Thus,

$$\begin{aligned} PI(P_n^k) - PI(P_{n-1}^k) &= \textstyle\sum_{xy \in \cup_{i=1}^{k(p-1)+s-1}(A_i \cup B_i)} f(w, xy) + PI(v_{k(p-1)+s}v_{kp+s}) \\ &\quad + PI(v_{k(p-1)+s+1}v_{kp+s}) + ... + PI(v_{kp+s-1}v_{kp+s}) \\ &= [(k+2-s) + (k+3-s) + ... + k] + (1+2+...+k)(p-1) \\ &\quad + [k(p-1)+s-1] + [(k-1)(p-1)+s-1] + [(k-2)(p-1)+s \\ &\quad -1] + ... + [s(p-1)+s-1] + [(s-1)p + (s-2)p + ... + 2p + p] \\ &= pk^2 + pk - k^2 - 3k + 2ks - s^2 + 3s - 2 \\ &= \alpha. \end{aligned}$$

Thus, $PI(P_n^k) = \frac{k(k+1)(p-1)(3kp+6s-2k-4)}{6} + \frac{(s-1)s(3k-s+2)}{3}$, for $|P_n^k| = kp+s$ and Theorem 3.1.1 is true. $\square$

Proof of Theorem 3.1.2. We will proceed by induction on $n \geq k+2$. If $n = k+2$, by the definition of the spiral, we have $T_{n,c}^{k*}$ is also a k-path, that is, $PI(T_{n,c}^{k*}) = 2k$. If $n \geq k+3$, assume that Theorem 3.1.2 is true for the k-spiral with at most $n-1$ vertices, we will consider $T_{n,c}^{k*}$ with n vertices. Let $T_{n,c}^{k*}$ be a k-spiral with $V(T_{n,c}^{k*}) = V(T_{n-1,c}^{k*}) \cup \{v\}$ and $E(T_{n,c}^{k*}) = E(T_{n-1,c}^{k*}) \cup \{vv_{n-1}, vv_{n-2}, ..., vv_{n-k}\}$ such that $v_1, v_2, ..., v_{n-c-1}$ is the simplicial ordering of P_{n-c-1}^{k-c}, where $T_{n-1,c}^{k*} = P_{n-c-1}^{k-c} + K_c$ with $V(T_{n-1,c}^{k*}) = \{v_1, v_2, ..., v_{n-1}\}$ and $E(T_{n-1,c}^{k*}) = E(P_{n-c-1}^{k-c}) \cup E(K_c) \cup \{v_1v_l, v_2v_l, ..., v_{n-c-1}v_l\}$ for $l \in [n-c, n-1]$. For any edge $v_iv_j \in E(T_{n,c}^{k*})$, $d(v_i, v_j)$ or $d'(v_i, v_j)$ is the distance of v_i and v_j in $T_{n-1,c}^{k*}$ or $T_{n,c}^{k*}$, respectively.

For $k+2 \leq n \leq 2k-c$, let $\gamma = \frac{(n-k)(n-k-1)(4k-n+2)}{3} - \frac{(n-k-1)(n-k-2)(4k-n+3)}{3} = (n-k-1)(3k-n+2)$. If we can show that by adding v to $T_{n-1,c}^{k*}$, $PI(T_{n,c}^{k*}) = PI(T_{n-1,c}^{k*}) + \gamma$, then Theorem 3.1.2 is true.

Set $w = v$ and let $l \in [n-c, n-1]$, by Lemma 3.1.8, we have $d'(v_l, v) = 1$ and $d'(v_i, v) = 2$ for $i \in [1, n-k-1]$, that is, $f(w, v_lv_i) = 1$; $d'(v_l, v) = d'(v_i, v) = 1$ for $i \in [n-k, n-1]$, that is, $f(w, v_lv_i) = 0$. Set $C_1 = \{v_1v_2, v_1v_3, ..., v_1v_{n-k-1}\}, C_2 = \{v_2v_3, v_2v_4, ..., v_2v_{n-k-1}\}, ..., C_{n-k-2} = \{v_{n-k-2}v_{n-k-1}\}, C_{n-k-1} = \phi$, $D_1 = \{v_1v_{n-k}, v_1v_{n-k+1}, ..., v_1v_{k-c+1}\}$, $D_2 = \{v_2v_{n-k}, v_2v_{n-k+1}, ..., v_2v_{k-c+2}\}, ..., D_{n-k-1} = \{v_{n-k-1}v_{n-k}, v_{n-k-1}v_{n-k+1}, ..., v_{n-k-1}v_{n-c-1}\}$. By Lemma 3.1.8, we have $d'(v_1, v) = d'(v_2, v) = 2$ and $d'(v_{n-k}, v) = 1$, that is, $f(w, v_1v_2) = 0$ and $f(w, v_1v_{n-k}) = 1$. Similarly, for $v_{h_1}v_{h_2} \in \cup_{i=1}^{n-k-1} C_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v) = d'(v_{h_2}, v) = 2$, that is, $f(w, v_{h_1}v_{h_2}) = 0$; For $v_{h_1}v_{h_2} \in \cup_{i=1}^{n-k-1} D_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v) = 2$ and $d'(v_{h_2}, v) = 1$, that is, $f(w, v_{h_1}v_{h_2}) = 1$. Set $C_{n-k} = \{v_{n-k}v_{n-k+1}, v_{n-k}v_{n-k+2}, ..., v_{n-k}v_{n-c-1}\}, C_{n-k+1} = \{v_{n-k+1}v_{n-k+2}, v_{n-k+1}v_{n-k+3}, ..., v_{n-k+1}v_{n-c-1}\}, ..., C_{n-c-2} = \{v_{n-c-2}v_{n-c-1}\}$. By Lemma 3.1.8, we have $d'(v_{n-k}, v) = d'(v_{n-k-1}, v) = 1$, that is, $f(w, v_{n-k}v_{n-k-1}) = 0$. Similarly, for $v_{h_1}v_{h_2} \in \cup_{i=n-k}^{n-c-2} C_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v) = d'(v_{h_2}, v) = 1$, that is, $f(w, v_{h_1}v_{h_2}) = 0$.

Set $E_1 = \{vv_i, i \in [n-k, n-c-1]\}$, by Lemma 3.1.8, we have $d'(v_i, v) = 2, d'(v_i, v_{n-k}) = 1$ for $i \in [1, n-k-1]$ and $d'(v_j, v) = d'(v_j, v_{n-k}) = 1$ for $i \in [n-k+1, n]$. Thus, $PI(v_{n-k}v) = n-k-1$. Similarly, $PI(v_{n-k+1}v) = PI(v_{n-k+2}v) = ... = PI(v_{k-c+1}v) = n-k-1$. Also, by Lemma 3.1.8, we have $d'(v_i, v) = 2, d'(v_i, v_{k-c+2}) = 1$ for $i \in [2, n-k-1]$, $d'(v_1, v) = d'(v_1, v_{k-c+2}) = 2$ and $d'(v_j, v) = d(v_j, v_{k-c+2}) = 1$ for $j \in [n-k, n]$. Thus, $PI(v_{k-c+2}v) = n-k-2$. Similarly, we have $PI(v_{k-c+3}v) = n-k-3, PI(v_{k-c+4}v) = n-k-4, ..., PI(v_{n-c-1}v) = 1$. Set $E_2 = \{vv_l, l \in [n-c, n-1]\}$, since $N[v_l] - N[v] = n-k-1$, then $PI(vv_l) = n-k-1$. Set $E_3 = \{v_iv_l, i \in [1, n-c-1], l \in [n-c, n-1]\}$, by Lemma 4, we have $d'(v_i, v) = 2$ for $i \in [1, n-k-1]$, $d'(v_i, v) = 1$ for $i \in [n-k, n-c-1]$, $d'(v_l, v) = 1$ for $l \in [n-c, n-1]$. Thus, $f(w, v_iv_l) = 1$ for $i \in [1, n-k-1]$ and $f(w, v_iv_l) = 0$ for $i \in [n-k, n-c-1]$.

Set $w \in V(T_n^{k*}) - \{v\}$, if $xy \in E(T_{n,c}^{k*})$ with x or $y \neq v$, by Lemma 3.1.6, we have $f(w, xy) = 0$. Thus,

$$\begin{aligned}
PI(T_n^{k*}) - PI(T_{n-1}^{k*}) &= \textstyle\sum_{xy \in \cup_{i=1}^{n-c-2} C_i} f(w, xy) + \sum_{xy \in_{i=1}^{n-k-1} D_i} f(w, xy) \\
&\quad + \textstyle\sum_{xy \in E_1 \cup E_2} PI(xy) + \sum_{xy \in E_3} f(w, xy) \\
&= 0 + [(2k-n-c+2) + (2k-n-c+3) + ... + (k-c)] \\
&\quad + [1 + 2 + ... + (n-k-2) + (n-k-1)(2k-n-c+2)] \\
&\quad + c(n-k-1) + c(n-k-1) \\
&= (n-k-1)(3k-n+2) \\
&= \gamma,
\end{aligned}$$

Theorem 3.1.2 is true.

For $n \geq 2k-c+1$, let $\sigma = \frac{3c(n-2k+c-1)(n-2k+c)+(k-c)(2c^2+3nc-4kc+3kn-4k^2-6k+3n-2)}{3} - \frac{3c(n-2k+c-2)(n-1-2k+c)+(k-c)(2c^2+3(n-1)c-4kc+3k(n-1)-4k^2-6k+3n-2)}{3} = k^2 - 4kc + c^2 + 2nc - 3c + k$. If we can show that by adding v to $T_{n-1,c}^{k*}$, $PI(T_{n,c}^{k*}) = PI(T_{n-1,c}^{k*}) + \sigma$, then Theorem 3.1.2 is true.

Set $w = v$, by Lemma 3.1.8, we have $d'(v_l, v) = 1$ for $l \in [n-c, n-1]$, $d'(v_i, v) = 2$ for $i \in [1, n-k-1]$ and $d'(v_j, v) = 1$ for $j \in [n-k, n-c-1]$. Thus, $f(w, v_l v_i) = 1$ and $f(w, v_l v_j) = 0$. Set $C_1 = \{v_1v_2, v_1v_3, ..., v_1v_{k-c+1}\}, C_2 = \{v_2v_3, v_2v_4, ..., v_2v_{k-c+2}\}, ..., C_{n-2k+c-1} = \{v_{n-2k+c-1}v_{n-2k+c}, v_{n-2k+c-1}v_{n-2k+c+1}, ..., v_{n-2k+c-1}v_{n-k-1}\}, C_{n-2k+c} = \{v_{n-2k+c}v_{n-2k+s+1}, v_{n-2k+c}v_{n-2k+s+2}, ..., v_{n-2k+c}v_{n-k-1}\}, C_{n-2k+c+1} = \{v_{n-2k+c+1}v_{n-2k+c+2}, v_{n-2k+c+1}v_{n-2k+c+3}, ..., v_{n-2k+c+1}v_{n-k-1}\}, ..., C_{n-k-1} = \phi, D_{n-2k+c} = \{v_{n-2k+c}v_{n-k}\}, D_{n-2k+c+1} = \{v_{n-2k+c+1}v_{n-k}, v_{n-2k+c+1}v_{n-k+1}\}, ..., D_{n-k-1} = \{v_{n-k-1}v_{n-k}, v_{n-k-1}v_{n-k+1}, ..., v_{n-k-1}v_{n-c-1}\}$.

By Lemma 3.1.8, we can get that $d'(v_1, v) = d'(v_2, v) = 2$ and $d'(v_{n-k}, v) = 1$, that is, $f(w, v_1v_2) = 0$ and $f(w, v_1v_{n-k}) = 1$. Similarly, for $v_{h_1}v_{h_2} \in \cup_{i=1}^{n-k-1} C_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v) = d'(v_{h_2}, v) = 2$, that is, $f(w, v_{h_1}v_{h_2}) = 0$; For $v_{h_1}v_{h_2} \in \cup_{i=n-2k+c}^{n-k-1} D_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v) = 2$ and $d'(v_{h_2}, v) = 1$, that is, $f(w, v_{h_1}v_{h_2}) = 1$. Set $C_{n-k} = \{v_{n-k}v_{n-k+1}, v_{n-k}v_{n-k+2}, ..., v_{n-k}v_{n-c-1}\}, C_{n-k+1} = \{v_{n-k+1}v_{n-k+2}, v_{n-k+1}v_{n-k+3}, ..., v_{n-k+1}v_{n-c-1}\}, ..., C_{n-c+2} = \{v_{n-c-2}v_{n-c-1}\}$. By Lemma 3.1.8, we can get that $d'(v_{n-k}, v) = d'(v_{n-k+1}, v) = 1$, that is, $f(w, v_{n-k}v_{n-k+1}) = 0$. Similarly, for $v_{h_1}v_{h_2} \in \cup_{i=n-k}^{n-c-2} C_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v) = d'(v_{h_2}, v) = 1$, that is, $f(w, v_{h_1}v_{h_2}) = 0$.

Set $E_1 = \{vv_i, i \in [n-k, n-c-1]\}$, by Lemma 3.1.8, we have $d'(v, v_{n-k-1}) = 2, d'(v_{n-c-1}, v_{n-k-1}) = 1, d'(v, v_i) = d'(v_{n-c-1}, v_i) = 1$ for $i \in [n-k, n-c-2] \cup [n-c, n-1]$ and $d'(v, v_j) = d(v_{n-c-1}, v_j) = 2$ for $j \in [1, n-k-2]$. Thus, $PI(vv_{n-c-1}) = 1$. Similarly, we have $PI(vv_{n-c-2}) = 2, PI(vv_{n-c-3}) = 3, ..., PI(vv_{n-k}) = k-c$. Set $E_2 = \{vv_l, l \in [n-c, n-1]\}$, since $N[v_l] - N[v] = n-k-1$, then $PI(vv_l) = n-k-1$. Set $E_3 = \{v_iv_l, i \in [1, n-c-1], l \in [n-c, n-1]\}$, by Lemma 3.1.8, we have $d'(v, v_i) = 2, d'(v, v_l) = 1$ for $i \in [1, n-k-1]$ and $d'(v, v_i) = d'(v, v_l) = 1$ for $i \in [n-k, n-c-1]$. Thus, $f(w, v_iv_l) = 1$ for $i \in [1, n-k-1]$ and $f(w, v_iv_l) = 0$ for $i \in [n-k, n-c-1]$.

Set $w \in V(T_n^{k*}) - \{v\}$, if $xy \in E(T_{n,c}^{k*})$ with x or $y \neq v$, by Lemma 3.1.6, we have $f(w, xy) = 0$. Thus,

$$\begin{aligned}
PI(T_n^{k*}) - PI(T_{n-1}^{k*}) &= \textstyle\sum_{xy \in \cup_{i=1}^{n-c-2} C_i} f(w, xy) + \sum_{xy \in_{i=n-2k+c}^{n-k-1} D_i} f(w, xy) + \sum_{xy \in E_1 \cup E_2} PI(xy) \\
&\quad + \textstyle\sum_{xy \in E_3} f(w, xy) \\
&= 0 + [1 + 2 + 3 + ... + (k - c)] + [1 + 2 + 3 + ... + (k - c)] \\
&\quad + c(n - k - 1) + c(n - k - 1) \\
&= k^2 - 4kc + c^2 + 2nc - 3c + k \\
&= \sigma.
\end{aligned}$$

Thus, Theorem 3.1.2 is true. □

Proof of Theorem 3.1.3. For $n \geq k + 2$, we will proceed by introduction on $|T_n^k| = n$. If $n = k + 2$, T_n^k is also a k-path, that is, $PI(T_n^k) = 2k$. If $n \geq k + 3$, assume that Theorem 3.1.3 is true for the k-tree with at most $n - 1$ vertices, let $v \in S_1(T_n^k)$ and $T_{n-1}^k = T_n^k - v$, by the induction of hypothesis, we have $PI(T_{n-1}^k) \leq PI(S_{n-1}^k) = k(n - k - 1)(n - k - 2)$. By adding back v, let $N(v) = \{x_1, x_2, ..., x_k\}$ and $w = v$. Since $T_n^k[v, x_1, x_2, ..., x_k]$ is a $(k + 1)$-clique, then $f(w, x_i x_j) = 0$ for $i, j \in [1, k]$. By Lemma 3.1.5 and Lemma 3.1.6, we can obtain that $PI(vx_i) \leq n - k - 1$ with $i \in [1, k]$ and $f(w, xy) \leq 1$ for any edge $xy \in E(T_n^k) - E(T_n^k[v, x_1, x_2, ..., x_k])$. Next, set $w \in V(T_n^k) - \{v\}$, by Lemma 3.1.6, if $xy \in E(T_n^k)$ with x or $y \neq v$, we have $f(w, xy) = 0$. Since $|E(T_n^k) - E(T_n^k[v, x_1, x_2, ..., x_k])| = k(n-k-1)$, we have

$$\begin{aligned}
PI(T_n^k) &= \textstyle PI(T_{n-1}^k) + \sum_{xy \in E(T_n^k - \{vx_i, i \in [1,k]\})} f(w, xy) + \sum_{i=1}^k PI(vx_i) \\
&\leq PI(S_{n-k}^k) + k(n - k - 1) + k(n - k - 1) \\
&= k(n - k - 1)(n - k - 2) + k(n - k - 1) + k(n - k - 1) \\
&= k(n - k)(n - k - 1) \\
&= PI(S_n^k).
\end{aligned}$$

Thus, Theorem 3.1.3 is true. □

Proof of Theorem 3.1.4. For $k=1$, every tree with the same number of vertices has the same PI-value. So Theorem 3.1.4 is obvious in this case; For $k \geq 2$, if $k+2 \leq n \leq 2k-c$, let $n = kp+s$ with $p=1$ and $s=n-k$, by Theorem 3.1.1, we have $PI(P_n^k) - PI(T_{n,c}^{k*}) = \frac{(s-1)s(3k-s+2)}{3} - \frac{(n-k)(n-k-1)(4k-n+2)}{3} = \frac{(n-k-1)(n-k)[3k-(n-k)+2]}{3} - \frac{(n-k)(n-k-1)(4k-n+2)}{3} = 0$, and Theorem 3.1.4 is true. If $n \geq 2k-c+1$, $p = \frac{n-s}{k}$ and by Theorem 3.1.1 and 3.1.2, define the new functions as follows: For $z \geq 2k-c+1$, $1 \leq c \leq k-1$ and $2 \leq s \leq k+1$,

$$
\begin{aligned}
g(z) &= \tfrac{(k+1)(z-s-k)(3z+3s-2k-4)}{6} + \tfrac{s(s-1)(3k-s+2)}{3}, \\
h(z,c) &= c(z-2k+c-1)(z-2k+c) + \tfrac{(k-c)(2c^2+3zc-4kc+3kz-4k^2-6k+3z-2)}{3}, \\
l(z,c) &= g(z) - h(z,c) \\
&= (\tfrac{k}{2} + \tfrac{1}{2} - c)z^2 + (-c^2 + 2c + 4kc - \tfrac{11k^2}{6} - \tfrac{5k}{2} - \tfrac{2}{3})z \\
&+ \tfrac{ks^2}{2} - \tfrac{k^2 s}{6} - \tfrac{ks}{2} + \tfrac{5k^3}{3} + \tfrac{5k^2}{3} + \tfrac{s^2}{2} + \tfrac{4k}{3} - \tfrac{s^3}{3} - 6k^2c + 3kc^2 - \tfrac{c^3}{3} - 4kc + c^2 - \tfrac{2c}{3}, \\
l_z(z) &= l_z(z,c) \\
&= (k+1-2c)z - c^2 + 2c + 4kc - \tfrac{11k^2}{6} - \tfrac{5k}{2} - \tfrac{2}{3}.
\end{aligned}
$$

Then, it is enough to determine that whether or not $l(z,c) \geq 0$ is true. By some caculations, we can obtain the following fact.

Note 1. *$z_1 = 2k-c+1$, $z_2 = 2k-c+2$ are the two roots of $l(z,c) = 0$ with $c \neq \frac{k+1}{2}$.*

Proof: For any $c \in [1, k-1]$, let $z_1 = 2k-c+1$, $z_2 = 2k-c+2$, we have $l(2k-c+1, c) = 0, l(2k-c+2, c) = 0$. If $c \neq \frac{k+1}{2}$, then Note 1 is true. □

For fixed $c \in [1, \frac{k+1}{2})$, that is, $\frac{k}{2} + \frac{1}{2} - c > 0$, then the function of $l(z,c)$ about z is open up. Since z is an integer and by Fact 2, then $l(z,c) \geq 0$ for $z \geq 2k-c+1$ and Theorem 8 is true; If $c = \frac{k+1}{2}$ and $k \geq 1$, we have $l_z(z) = \frac{1-k^2}{12} \leq 0$, that is, $l(z, \frac{k+1}{2})$ is decreasing about z. By the proof of Note 2, we have $l(2k-c+1, c) = 0$. For $z \geq 2k-c+1$, we can get that $l(z, \frac{k+1}{2}) \leq l(2k-c+1, \frac{k+1}{2}) = 0$ and Theorem 8 is true; For fixed $c \in (\frac{k+1}{2}, k-1]$, that is, $\frac{k}{2} + \frac{1}{2} - c < 0$, then the function of $l(z,c)$ about z is open down. Since z is an integer and by Note 1, we can obtain that $l(z,c) \leq 0$ for $z \geq 2k-c+1$ and Theorem 3.1.4 is true. □

Remark. The k-stars attain the maximal values of PI-values for k-trees, but the k-paths do not attain the minimal values and not all PI-values of k-spirals are less than the values of other type of k-trees. This fact indicates two interesting problems that what is the minimum PI-value for k-trees and which type of k-trees will achieve the minimum PI-value?

3.2 CACTUS GRAPHS

The next figure gives some examples of the extremal graphs in the main results of this section. Here are the two main results and their proofs.

Fig. 1 Fig. 2

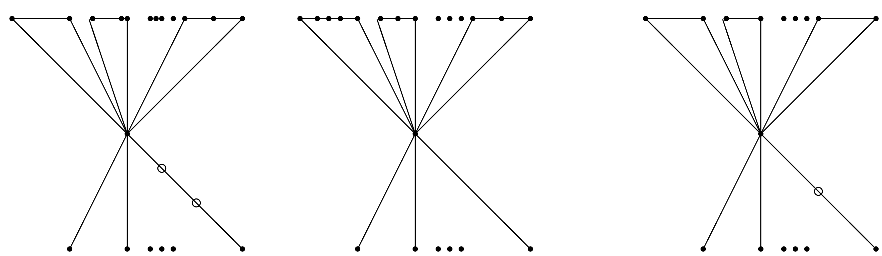

Figure 3.2.1: The cacti with extremal PI indices

Theorem 3.2.1 (Wang, Wang and Wei [80]). *Let* $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_4, C_5\}$ *with* $n \geq k \geq 0$, *then* $PI(G) \leq (n - 1 + \lfloor \frac{n-k-1}{3} \rfloor)(n-2)$, *where the equality holds if and only if* G *is a tree for* $n \leq k+3$ *and otherwise, one of the following statements holds(See Fig. 1):*

(i) All cycles have length 4 *and there are at most* $k+2$ *cut edges.*

(ii) All cycles have length 4 *except one of length* 6 *and there are exact* k *pendent edges.*

Theorem 3.2.2 (Wang, Wang and Wei [80]). *Let* $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_4\}$ *with* $n \geq k \geq 0$, *then* $PI(G) \geq (n-1)(n-2) - 2\lfloor \frac{n-k-1}{2} \rfloor$, *where the equality holds if and only if* G *is a tree for* $n \leq k+2$ *and otherwise, all cycles have length* 3 *and there are at most* $k+1$ *cut edges (See Fig. 2).*

Next we provide some lemmas which are important in the proof of our main results.

Lemma 3.2.3. *Let $G \in \mathcal{C}_{n,k}$ and $e \in E(G)$. Then*

(i) $PI(e) \leq n-2$, the equality holds if e is a cut edge or an edge of an even cycle.

(ii) If e is an edge of an odd cycle C_o, then $PI(e) \leq n-3$. Furthermore, if $G = C_o$, then $PI(e) = n-3$.

(iii) For each odd cycle C of G, $PI(C) = (n-2)(|C|-1)-2$.

Proof. Assume that $e = uv \in E(G)$. Since $PI(e)$ counts at most $n-2$ vertices, then $PI(e) \leq n-2$. If e is a cut edge, then $G-e$ contains two components G_1 and G_2. Thus, all vertices of G_1 are closer to one of $\{u, v\}$, say u, and all vertices of G_2 are closer to v. Thus, $PI(e) = n_e(u) + n_e(v) = n-2$ if e is a cut edge. Let $C = v_1v_2...v_av_1$ be a cycle of G and $v_lv'_l \in E(C)$. Since G is a cactus, then $G - E(C)$ contains a components $B_1, B_2, ..., B_a$ such that $v_i \in V(B_i)$. If a is even, then $d(v_l, v_i) \neq d(v'_l, v_i)$ for $1 \leq i \leq a$, and $d(v_l, u_i) \neq d(v'_l, u_i)$ with $u_i \in V(B_i)$. We obtain that $PI(e) = n-2$ if C is even. Thus, (i) is true.

For $C = C_o$, a is odd. Then there exists a unique vertex $v_t \in V(C)$ such that $d(v_l, v_t) = d(v'_l, v_t)$, that is, $PI(e) \leq n-3$. When $G = C_o$, we see $PI(e) = n-3$. Thus, (ii) is true.

For (iii), a is odd and $\sum_{i=1}^{a} |B_i| = n$. Note that if $d(v_l, v_t) = d(v'_l, v_t)$ with $v_t \in V(C)$, then $d(v_l, u_t) = d(v'_l, u_t)$ with $u_t \in V(B_t)$. Similarly, if $d(v_l, v_t) \neq d(v'_l, v'_t)$ with $v'_t \in V(C)$, then $d(v_l, u'_t) \neq d(v'_l, u'_t)$ with $u'_t \in V(B_t)$. Thus, $PI(v_lv'_l) = n-2-|B_t|$ with $t \neq l, l'$. It induces that

$$\begin{aligned} PI(C) &= \textstyle\sum_{e \in E(C)} PI(e) = \sum_{i=1}^{a} (n-2-|B_i|) \\ &= a(n-2) - \textstyle\sum_{i=1}^{a} |B_i| \\ &= |C|(n-2) - n \\ &= (|C|-1)(n-2) - 2 \end{aligned}$$

and Lemma 3.2.3 is true. □

Lemma 3.2.4. *Let C be a cycle of G. Define Transformation 1: $G_1 = G - xy$ with $xy \in E(G) - E(C)$ and Transformation 2: $G_2 = G + x'y'$, where at least one of $\{x', y'\}$ are in $V(G) - V(C)$. If $G_1, G_2 \in \mathcal{C}_{n,k}$ and $e \in E(C)$, then $PI(e) = PI_{G_1}(e) = PI_{G_2}(e)$.*

Proof. Let $C = v_1v_2...v_av_1$, $v_lv'_l \in E(C)$. Then $G-E(C)$ contains a components $B_1, B_2, ..., B_a$ such that $v_i \in V(B_i)$. Since G is a cactus, then for $v_i \in V(C)$, if $d(v_l, v_i) = d(v'_l, v_i)$, we obtain $d(v_l, u_i) = d(v'_l, u_i)$ with $u_i \in V(B_i)$. Similarly, if $d(v_l, v_i) \neq d(v'_l, v_i)$, we obtain $d(v_l, u_i) \neq d(v'_l, u_i)$ with $u_i \in V(B_i)$. Note that G_1 and G_2 contain the same cycle C as G, and the components B^i_j of $G_i - C$ with $v_j \in V(B^i_j)$ has the property that $V(B^i_j) = V(B^{i'}_j)$. Then for $v_i \in V(C)$, if $d(v_l, v_i) = d(v'_l, v_i)$, then $d_{G_1}(v_l, v_i) = d_{G_1}(v'_l, v_i)$ and $d_{G_2}(v_l, v_i) = d_{G_2}(v'_l, v_i)$, $d_{G_1}(v_l, u_i) = d_{G_1}(v'_l, u_i)$ with $u_i \in V_{G_1}(B_i)$ and $d_{G_2}(v_l, u_i) = d_{G_2}(v'_l, u_i)$ with $u_i \in V_{G_1}(B_i)$. Similarly, if $d(v_l, v_i) \neq d(v'_l, v_i)$, then $d_{G_1}(v_l, v_i) \neq d_{G_1}(v'_l, v_i)$ and $d_{G_2}(v_l, v_i) \neq d_{G_2}(v'_l, v_i)$, $d_{G_1}(v_l, u_i) \neq d_{G_1}(v'_l, u_i)$ with $u_i \in V_{G_1}(B_i)$ and $d_{G_2}(v_l, u_i) \neq d_{G_2}(v'_l, u_i)$ with $u_i \in V_{G_2}(B_i)$. Thus, $PI(e) = PI_{G_1}(e) = PI_{G_2}(e)$ and Lemma 3.2.4 is true. □

Lemma 3.2.5. *If $G \in \mathcal{C}_{n,k}$ contains t_1 cycles of lengths $\{l_1, l_2, ..., l_{t_1}\}$ and $t_2 \geq k$ cut edges, then $PI(G)$ is unique and these cycles can be shared a common vertex u_0, $k-1$ pendent edges can be adjacent to u_0 and a path of length $t_2 - k + 1$ can be adjacent to u_0. (See Fig. 2)*

Proof. By Lemma 3.2.3(i) and (iii), PI values with cycles of fixed lengths and fixd number of cut edges are determined. Then

$$PI(G) = \sum_{C \text{ is a cycle of G}} \sum_{e \in E(C)} PI(e) + \sum_{e \text{ is an cut edge of G}} PI(e)$$

is unique. By recombining these cycles and cut edges, t_1 cycles can have a common vertex u_0, $k-1$ pendent edges can be adjacent to u_0 and a path of length $t_2 - k + 1$ can be adjacent to u_0. Thus, Lemma 3.2.5 is true. □

Lemma 3.2.6. *Let $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_5\}$, if $PI(G)$ attains the maximal value, then the length of each cycle, if any, is even.*

Proof. If G has a cycle, then $n \geq 3$. Assume that there is an odd cycle $C_{2t+1} = u_1u_2...u_{2t}u_{2t+1}u_1$ with $t \geq 1$. If all vertices of C_{2t+1} have degree 2, then $G = C_{2t+1}$. Since $G \neq C_3, C_5$, then

$n \geq 7$. By Lemma 3.2.3(ii), $PI(e) = n - 3$ for $e \in E(C_{2t+1})$ and $PI(C_{2t+1}) = n(n-3)$. By Lemma 1(iii), $PI(G) = (n-2)(2t) - 2$. We build a new graph $G' = (G - \{u_1u_{2t+1}\}) \cup \{u_1u_{2t-2}, u_{2t+1}\}$. Then G' contains a cycle $C_1' = u_{2t-2}u_{2t-1}u_{2t}u_{2t+1}u_{2t-2}$ of length 4 and a cycle $C_2' = u_1u_2...u_{2t-2}u_1$ of length $2t-2$. By Lemma 3.2.3(i), $PI(G') = PI(C_1') + PI(C_2') = (n-2)(2t+2)$. Thus, $PI(G') > PI(G)$, contradicted that $PI(G)$ is maximal.

Thus, there is a vertex of degree at least 3 in C_{2t+1}. If the vertex of degree 3 is unique, say u_1, then there exists a pendent path $u_1v_1v_2...$. Set $G_0 = (G - \{u_1u_2\}) \cup \{u_2v_1\}$, then $G_0 \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_5\}$. By Lemma 3.2.3, we obtain $PI(G_1) > PI(G)$, a contradiction. If at least two vertices of $\{u_1, u_2, u_3\}$ has degree at least two, say u_1, u_2. Set $G_1 = G - \{u_1u_2\}$, then $G_1 \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_5\}$. By Lemma 3.2.3, we obtain $PI(G) = PI(C) + k(k+1) = k(k+3)$ and $PI(G_1) = (k+1)(k+3) > PI(G)$, a contradiction. If $t \geq 2$, we construct a new graph G_2 such that $G_2 = G - \{u_1u_{2t+1}\} \cup \{u_1u_{2t}\}$ with $d_G(u_{2t+1}) \geq 3$. Then $G_2 \in \mathcal{C}_{n,k}$, C_{2t} is an even cycle and $u_{2t}u_{2t+1}$ is a cut edge. By Lemmas 3.2.3 and 3.2.4,

$$\begin{aligned} PI(G_2) - PI(G) &= (PI(u_{2t}u_{2t+1}) + PI(C_{2t})) - PI(C_{2t+1}) \\ &= (n-2)(2t+1) - [(n-2)(2t) - 2] \\ &> 0, \end{aligned}$$

contradicted that $PI(G)$ is maximal. Therefore, each cycle, if any, is even and Lemma 3.2.6 is true. $\square$

Lemma 3.2.7. *Let $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_5\}$ with $n \geq k+4$, if $PI(G)$ attains the maximal value, then all cycles are length 4 except at most one of them is 6.*

Proof. By Lemma 3.2.6, all cycles are even. If there exists an cycle $C = u_1u_2...u_{2t}u_1$ with $t \geq 4$. Set $G_1 = (G - \{u_1u_{2t}\}) \cup \{u_1u_4, u_4u_{2t}\}$. Then $G_1 \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e\}$ and $|E(G_1)| = |E(G)| + 1$. Since each edge of G_1 is either a cut edge or an edge of an even cycle, then $PI(G_1) > PI(G)$ by Lemma 3.2.3(i), that is, the length of cycles are at most 6. Now suppose that there are two cycles of length 6. By Lemma 3.2.5, we can assume these two cycles share a common vertex u_1, say $C_1 = u_1u_2...u_6u_1$ and $C_2 = u_1v_2...v_6u_1$. Set

$G_2 = G - \{u_1u_2, u_3u_4, u_1v_2\} \cup \{u_1u_4, u_2v_2, u_3v_3, u_1v_3\}$. Then $G_2 \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e\}$ and $|E(G_2)| = |E(G)| + 1$. Since each edge of G_2 is either a cut edge or an edge of an even cycle, then $PI(G_1) > PI(G)$, that is, there are at most one cycle of length 6 and Lemma 3.2.7 is true. $\square$

Lemma 3.2.8. *Let $G \in \mathcal{C}_{n,k} - \{C_4\}$, if $PI(G)$ attains the minimal value, then the length of each cycle, if any, is odd.*

Proof. Suppose G has an even cycle $C_{2t} = u_1u_2...u_{2t}u_1$, then $n \geq k+4$ and $t \geq 2$. If all vertices of G have degree 2, then $G = C_{2t}$ and $n = 2t$. By Lemma 3.2.3(i), $PI(G) = n(n-2) = 2t(2t-2)$. Since $G \neq C_4$ and $t \geq 3$, set $G_1 = (G - \{u_1u_2\}) \cup \{u_1u_4, u_2u_4\}$. Then $G_1 \in \mathcal{C}_{n,k} - \{C_4\}$, $C_{1,3} = u_2u_3u_4u_2$ is an odd cycle and $C_{1,2t-2} = u_1u_4u_5...u_{2t}u_1$ is an even cycle. By Lemma 3.2.3(i) and (iii), $PI(G_1) = PI(C_{1,3}) + PI(C_{1,2t-2}) = (n-2)2-2+(n-2)(2t-2) = 2t(2t-2) - 2 < PI(G)$, contradicted that $PI(G)$ is minimal. If there exists a vertex u_2 with $d(u_2) \geq 3$, then we construct a new graph $G_2 = (G - \{u_1u_2\}) \cup \{u_1u_3\}$. Then $G_2 \in \mathcal{C}_{n,k}$, u_2u_3 is a cut edge and $C' = u_1u_3u_4...u_{2t}u_1$ is an odd cycle. By Lemma 3.2.3 and 3.2.5,

$$\begin{aligned}
PI(G_2) - PI(G) &= (PI_{G_2}(u_2u_3) + PI_{G_2}(C')) - PI(C_{2t}) \\
&= [(n-2) + (n-2)(2t-2) - 2] - 2t(n-2) \\
&= -n < 0.
\end{aligned}$$

Thus, $PI(G_2) < PI(G)$, contradicted that $PI(G)$ is minimal. Therefore, each cycle, if any, is odd and Lemma 3.2.8 is true. $\square$

Lemma 3.2.9. *Let $G \in \mathcal{C}_{n,k} - \{C_4\}$ with $n \geq k+3$, if $PI(G)$ attains the minimal value, then all cycles have length 3.*

Proof. By Lemma 3.2.8, we only consider all cycles of G are odd. Suppose that there is an odd cycle of length greater than 3, say $C_{2t+1} = u_1u_2...u_{2t+1}u_1$ with $t \geq 2$. Set a new graph $G_1 = (G - \{u_{2t-1}u_{2t}\}) \cup \{u_1u_{2t-1}, u_1u_{2t}\}$. Then $G_1 \in \mathcal{C}_{n,k}$ and we will show that $PI(G_1) < PI(G)$. Let $C_1 = u_1u_2...u_{2t-1}u_1$ and $C_2 = u_1u_{2t}u_{2t+1}u_1$. By Lemma 1($iii$),

$PI(C) = (n-2)(|C|-2) - 2 = 2t(n-2) - 2$ and $PI(C_1) + PI(C_2) = [(n-2)(|C_1|-2) - 2] + [(n-2)(|C_2|-2) - 2] = 2t(n-2) - 4$. Thus, $PI(C_1) + PI(C_2) < PI(C)$. By Lemma 3.2.4, $PI(G_1) - PI(G) = PI(C_1) + PI(C_2) - PI(C) < 0$ and Lemma 3.2.9 is true. $\square$

Now, we prove the main results of this section.

Proof of Theorem 3.2.1. All length of cycles, if any, are even by Lemma 3.2.6. Since $e \in E(G)$ is either a cut edge or an edge of an even cycle, then $PI(e) = n-2$ by Lemma 1(i). Thus, $PI(G) = |E(G)|(n-2)$ and it needs to maximize $|E(G)|$. For $n \leq k+3$, $\lfloor \frac{n-k-1}{3} \rfloor = 0$ and $PI(G) = (n-1)(n-2)$. Thus, Theorem 3.2.1 is true. For $n \geq k+4$, all length of cycles are 4 except at most one of them is 6 by Lemma 3.2.7. By Lemma 3.2.5, all cycles of G have a common vertex u_0, $k-1$ pendent edges are adjacent to u_0 and a path of length $t_2 - k + 1$ is adjacent to u_0.

Assume that there exists a cycle $C_6 = u_0u_1u_2u_3u_4u_5u_0$ and G contains more than $k+1$ cut edges. Then G has a path $u_0v_1v_2...$ of length more than 2. Set $G_1 = (G - \{u_2u_3\}) \cup \{u_2v_1, u_0u_3\}$, then $G_2 \in \mathcal{C}_{n,k}$ and $|E(G_2)| = |E(G)| + 1$. Since $e \in E(G_1)$ is either an cut edge or an edge of an even cycle, then $PI(e) = n-2$ and $PI(G_1) = (n-2)|E(G_1)| > PI(G) = (n-2)|E(G)|$, contradicting to the fact that $PI(G)$ is maximal. Thus, G contains exact k pendent edges. Next we will show that if all length of cycles are 4, then G contains at most $k+2$ cut edges. Otherwise, there exist a path $u_0v_1v_2...$ of length at least 4 by Lemma 3.2.5. Set $G_2 = G \cup \{u_0v_3\}$, then $G_2 \in \mathcal{C}_{n,k}$ and $|E(G_2)| = |E(G)| + 1$. Since $e \in E(G_1)$ is either an cut edge or an edge of an even cycle, then $PI(e) = n-2$ and $PI(G_2) = (n-2)|E(G_2)| > PI(G) = (n-2)|E(G)|$, contradicted that $PI(G)$ is maximal. Note that for $n \geq k+4$, the number of cycles of G is $\lfloor \frac{n-k-1}{3} \rfloor$ and the number of edges of G is $n - 1 + \lfloor \frac{n-k-1}{3} \rfloor$. Thus, $PI(G) = (n - 1 + \lfloor \frac{n-k-1}{3} \rfloor)(n-2)$ and Theorem 3.2.1 is true. $\square$

Proof of Theorem 3.2.2. For $n \leq k+2$, $\lfloor \frac{n-k-1}{2} \rfloor = 0$ and $PI(G) = (n-1)(n-2)$ by Lemma 3.2.3. Thus, Theorem 3.2.2 is true. For $n \geq k+3$, the length of each edge of G is 3 by Lemma 3.2.9. Next we will show that G contains at most $k+1$ cut edges.

Assume that G contains at least $k+2$ cut edges. By Lemma 3.2.5, all cycles of G have a common vertex u_0, $k-1$ pendent edges are adjacent to u_0 and a path of length at least $(k+2)-k+1=3$ is adjacent to u_0. Denote the path as $u_0v_1v_2v_3....$, set $G_1 = G \cup \{u_0v_2\}$. By Lemma 3.2.3(iii) and 3.2.4, $PI(G_1) - PI(G) = PI_{G_1}(v_0u_1u_2v_0) - PI(u_0v_1) - PI(v_1v_2) = [(n-2)(3-1)-2] - (n-2) - (n-2) = -2 < 0$. Thus, $PI(G_1) < PI(G)$, contradicted that $PI(G)$ is minimal. Note that for $n \geq k+3$, the number of cycles of length 3 is $\lfloor \frac{n-k-1}{2} \rfloor$ and the number of cut edges is $n-1-2\lfloor \frac{n-k-1}{2} \rfloor$. Thus,

$$\begin{aligned} PI(G) &= 2(n-3)(\lfloor \tfrac{n-k-1}{2} \rfloor) + (n-1-2\lfloor \tfrac{n-k-1}{2} \rfloor)(n-2) \\ &= (n-1)(n-2) - 2\lfloor \tfrac{n-k-1}{2} \rfloor, \end{aligned}$$

and Theorem 3.2.2 is true. □

Remarks. The maximal and minimal values of vertex PI vertices of cacti are uniqe, but the cacti achieved the maximal and minimal vertex PI index are not unique. All cacti satisfying the statements in Theorem 3.2.1 and Theorem 3.2.2 are arrived at the corresoponding sharp values. Fig 1 and Fig 2 are special examples achieved the sharp bounds.

4 THE RATIO OF DOMINATION AND INDEPENDENT DOMINATION

In this chapter, we study the ratio of the independent domination number and the domination number for bipartite graphs. We also provide further results on such ratio for any graphs.

4.1 THE RATIO

The main theorem of the ratio between domination number and independent domination number, and the proof are as follows.

Theorem 4.1.1 (Wang and Wei [67]). *Let G be a bipartite graph with $\Delta(G) \geq 2$. Then*

$$\frac{i(G)}{\gamma(G)} \leq \frac{\Delta(G)}{2}.$$

Proof of Theorem 4.1.1. Let A, B be the two partitions of G and D be a minimum dominating set. Thus, A, B are independent sets and $\gamma(G) = |D|$. Set I_0 to be the set of isolated vertices in $G[D]$.

If $|I_0| = |D|$, then D is an independent dominating set, that is, $i(G)/\gamma(G) = 1 \leq \Delta(G)/2$. Otherwise, if $|I_0| < |D|$, then there are some edges in $G[D]$. By setting $A_1 = (D - I_0) \cap A$ and $B_1 = (D - I_0) \cap B$, we have $|A_1| + |B_1| = |D| - |I_0|$. Without loss of generality, we can assume that $|A_1| \geq |B_1|$.

Define a new vertex set $I = I_0 \cup A_1 \cup (N_G(B_1) - A_1 - N_G(I_0 \cap B))$. We first show that I is an independent dominating set. Since D is a dominating set and I_0 is the set of isolated vertices of $G[D]$, then $N_G(I_0 \cap B) \cap A_1 = \phi$ and

$$\begin{aligned}
I &= (I_0 \cap B) \cup (I_0 \cap A) \cup A_1 \cup (N_G(B_1 \cup (I_0 \cap B)) - A_1 - N_G(I_0 \cap B)) \\
&\overset{B_1 \cup (I_0 \cap B) = D \cap B}{=} (I_0 \cap B) \cup ((I_0 \cap A) \cup A_1) \cup (N_G(D \cap B) - A_1 - N_G(I_0 \cap B)) \\
&\overset{N_G(D \cap B) = A}{=} (I_0 \cap B) \cup A_1 \cup (A - A_1 - N_G(I_0 \cap B)) \\
&= (I_0 \cap B) \cup (A - N_G(I_0 \cap B)). \qquad (4.1.1)
\end{aligned}$$

Thus, I is independent. By the equation (1), $N_G(I_0 \cap B) \subseteq N_G(I)$. Since $I_0 \cap B$ is a set of isolated vertices in $G[D]$, then $A \cap D \subseteq I$ and $B - (I_0 \cap B) \subseteq N_G(I)$.Thus, I is a dominating set of G as well.

By the definition of I and $|N_G(B_1) - A_1 - N_G(I_0 \cap B)| \leq |B_1|(\Delta(G) - 1)$, we have $|I| \leq |I_0| + |A_1| + |B_1|(\Delta(G) - 1)$. Note that $|A_1| + |B_1| = |D| - |I_0|$, $|A_1| \geq |B_1| \geq 0$ and $\Delta(G) - 1 \geq 1$. If $|A_1| + |B_1|(\Delta(G) - 1)$ attains the maximal value, then B_1 is as big as possible. Also, $|B_1| \leq |A_1|$ and $|A_1| + |B_1| = |D| - |I_0|$ yield that $|B_1| \leq \frac{|D| - |I_0|}{2}$. Thus, $|I|$ achieves the maximal value if $|A_1| = |B_1| = \frac{|D| - |I_0|}{2}$, that is,

$$\begin{aligned}
|I| &\leq |I_0| + \frac{|D| - |I_0|}{2} + \frac{|D| - |I_0|}{2}(\Delta(G) - 1) \\
&= |I_0| + \frac{|D| - |I_0|}{2}\Delta(G).
\end{aligned}$$

As $\frac{\Delta(G)}{2} \geq 1$ and $\gamma(G) = |D|$, then

$$i(G) \leq |I| \leq |I_0|\frac{\Delta(G)}{2} + \frac{|D| - |I_0|}{2}\Delta(G) = |D|\frac{\Delta(G)}{2} = \gamma(G)\frac{\Delta(G)}{2}.$$

Thus,

$$\frac{i(G)}{\gamma(G)} \leq \frac{|I|}{\gamma(G)} \leq \frac{\Delta(G)}{2}.$$

$\square$

Remark. We see that the Conjecture holds for the bipartite graph G. For the examples, a balanced double star and a complete balanced bipartite graph attain the upper bound.

4.2 EXTENDED RESULTS

Due to the main result, we can obtain the special theorem. If G has no cycles, the following proposition is obvious.

Theorem 4.2.1 ([67]). *Let G be a tree with $\Delta(G) \geq 2$, then $\frac{i(G)}{\gamma(G)} \leq \frac{\Delta(G)}{2}$ and the equality holds if G is a balanced double star, where a balanced double star is a tree with exactly two vertices of same degree greater than 1.*

We now provide graphs containing some odd cycles, for which Conjecture 1.6.4 does not hold. For any large n, the graph G' consists of an odd cycle C_{2k+1} and $(2k+1)s$ vertices of degree 1 such that each vertex on C_{2k+1} is adjacent to exactly s degree-1 vertices, for $k, s \geq 1$. Then $\Delta(G') = s + 2, \gamma(G') = 2k + 1$ and $i(G') = k + (k + 1)s$. By caculations, $i(G')/\gamma(G') > \Delta(G')/2$ if $s > 2k + 2$.

Furthermore, as suggested by Dr. Hehui Wu, we provide a series of examples for $\delta \geq 2$, which disprove the Conjeture for any $\delta(G)$. The method of buiding the counterexamples is: Starting with a complete graph, several independent sets of the same size, we add the vertices between the complete graph and any independent set. In paticular, The counterexample Figure 4.2.1 to the Conjecture with $\delta = 2$ is as follows:

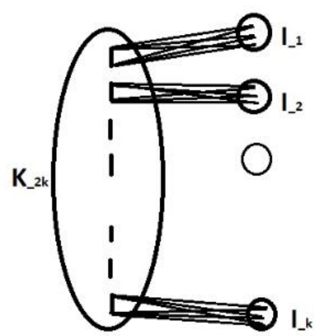

Figure 4.2.1: One of the counterexamples for $\delta = 2$

5 FUTURE RESEARCH

In this chaper, we propose some further research problems on the topological indices, domination numbers and the long cycles of chordal graphs.

5.1 TOPOLOGICAL INDICES

In my current study of topological indices, I found sharp bounds on the multiplicative Zagreb indices of k-trees in Theorems 3.4 and 3.5. For a cactus graph with given number of pendent vertices, sharp bounds on the multiplicative Zagreb indices are provided in Theorems 3.10-3.14. I will continue to explore the multiplicative Zagreb indices of k-trees with a given number of vertices of degree k. I will apply the analytic tools of Lemmas 2.0.1 and 2.0.2 to deal with the following problem.

Problem 5.1 *What are the sharp bounds of multiplicative Zagreb indices of k-trees with fixed number of vertices of degree k?*

5.2 DOMINATION NUMBERS

In my study on domination numbers, all known counterexamples to Conjecture 4.2 contain a large number of vertices with all $\delta \geq 1$ are proposed. In 2012, Goddard et al. [37] proved that $i(G)/\gamma(G) \leq 3/2$ if G is a cubic graph. In 2013, Southey and Henning [25] improved the previous bound to $i(G)/\gamma(G) \leq 4/3$ for a connected cubic graph G other than $K_{3,3}$, which is better than 3/2. Since $i(K_{4,4})/\gamma(K_{4,4}) = 2$, we consider the following problem proposed by Goddard et al.[37].

Problem 5.2 *If $G \neq K_{4,4}$ is a connected 4-regular graph, then is it true that $i(G)/\gamma(G) \leq 3/2$?*

5.3 LONG CYCLE

Every two maximum length paths in a connected graph have a common vertex. Gallai in [30] asked whether all maximum length paths share a common vertex of the graph. This perfect "Helly property" on maximum paths is not true in general. The first counter-example was constructed by H. Walther, and the smallest known counter-example is due to Zamfirescu [88]. These and many further examples in Skupien [70] all contain induced cycles longer than three with no chord. In other words, the known counter-examples are not chordal graphs. We have not been able to determine whether the maximum paths of every chordal graph have the Helly property envisioned by Gallai. However, Klavizar and Petkovisek in [53] observed that this is true in a connected split graph (split graphs are chordal graphs whose complement is also chordal). In addition we shall prove that Gallai's question has an affirmative answer for a subfamily of chordal graphs.

A graph is a chordal graph if and only if it is an intersection graph of subgraphs of a host tree. we will try to solve the following problem, which shows that the conjecture is true for the chordal graph with a host tree as a subdivision of double star.

Problem 5.3 *Given a chordal graph with a host tree as a subdivision of double star, there is a common vertex for all maximum cycles.*

6 CONCLUSION

6.1 SUMMARY AND CONCLUSIONS

In this dissertation, we study k-trees and cactus graphs. We provide the sharp upper and lower bounds of the degree-based topological indices(Multiplicative Zagreb indices) for these graphs. For a distance-based topological index (PI index), the extremal cacti of upper and lower bounds are given. Furthermore, we provide the extremal graphs with the corresponding topological indices.

We also establish and verify a proposed conjecture for the relationship between domination number and independent domination number. The corresponding counterexamples and the graphs achieving the extremal bounds are given as well.

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