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Graph Invariants of Trees with Given Degree Sequence

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GRAPH INVARIANTS OF TREES WITH GIVEN DEGREE SEQUENCE

by

RACHEL BASS

(Under the Direction of Hua Wang)

ABSTRACT

Graph invariants are functions defined on the graph structures that stay the same under taking graph isomorphisms. Many such graph invariants, including some commonly used graph indices in Chemical Graph Theory, are defined on vertex degrees and distances between vertices. We explore generalizations of such graph indices and the corresponding extremal problems in trees. We will also briefly mention the applications of our results.

GRAPH INVARIANTS OF TREES WITH GIVEN DEGREE SEQUENCE

by

RACHEL BASS

B.S., Armstrong State University, 2015

A Thesis Submitted to the Graduate Faculty of Georgia Southern University in Partial Fulfillment

of the Requirement for the Degree

MASTER OF SCIENCE

STATESBORO, GEORGIA

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Electronic Version Approved:

May 2017

DEDICATION

This thesis is dedicated to the strong and beautiful women in my life. Without these women I would not have had the courage to pursue my personal and academic goals.

My sister, Sarah Bass, has provided a steady source of support and encouragement.

My aunt, Joan Parker, reminds me to enjoy my journey even when it becomes difficult.

My grandmothers, Elisabeth Hodobas and Marguerite Bass, have left a legacy of kindness and strength. They continuously emphasized education and the importance of curiosity.

My mother, Ilona Bass, has taught me many things but most importantly my mother has shown me that what you want out of life is worth fighting for.

ACKNOWLEDGMENTS

There are many people that I wish to acknowledge.

I would like to start with my thesis advisor, Dr. Wang along with the rest of my thesis committee, Dr. Gray and Dr. Magnant. They provided me with valuable advice and guidance.

Next I would like to thank my collaborators, Dr. X-M Zhang, Dr. X-D Zhang, and Dr. Hu.

Since this thesis was part of my journey to a PhD program it is only fitting that I mention those people who also helped me get there.

Dr. Wang played an important role in my acceptance to a PhD program. He helped me complete and submit my first accepted paper and wrote many letters of recommendation.

Along with Dr. Wang, Dr. Magnant allowed me to participate in research which led to my second submitted paper.

My undergraduate advisor, Dr. Tiemeyer, was the first person to introduce me to the field of Graph Theory, the subject on which this thesis is based. Along with research, Dr. Tiemeyer helped prepare me for the continuation of my education in mathematics which included many letters of recommendation.

This list would not be complete unless I acknowledge my teaching advisors, Mrs. Barrs and Mrs. Hutcheson. They have helped me through my first year of teaching and answered a myriad of questions. Besides the teaching advice, Mrs. Barrs also wrote several letters of recommendation on my behalf.

My fellow classmates also played a crucial role in my success. In particular I would like to recognize Moriah Gibson, Charles Lanning, Taylor Nesmith, Angel Woods, Seth Gutierrez, Zach Espe, and Nicolas Smoot. These friends gave me study

support and often provided comical relief to an otherwise stressful program.

Last but certainly not least I would like to thank my family for their constant love and support.

Needless to say that without these people I would not be where I am today.

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CHAPTER 1

INTRODUCTION

1.1 Chemical Graph Theory

Chemical graph theory has become a popular area of research in mathematics. Its popularity began with the Wiener index in 1947. Harry Wiener made an observation regarding the correlation of chemical properties and the spacing of a compound [26, 27]. From his observations he created the Wiener index ,$W(G)$,

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

For instance, we may observe from Table 1.1 that there is a positive correlation between the Wiener index values and the boiling points of the chemicals.

Chemical	Wiener Index	Boiling Point
Heptane	56	98.42
3-ethylpentane	48	93.50
3-methylhexane	50	91.00
2-methylhexane	52	90.00
2,3-dimethylpentane	46	89.90
3,3-dimethylpentane	44	86.00
2,2,3-triethylbutane	42	81.70
2,4-dimethylpentane	48	80.00
2,2-dimethylpentane	46	79.00

Table 1.1: The Wiener index and boiling points of isomers of heptane.

We may notice that the Wiener index is based on distances but we can also examine indices based on vertex degrees. The most well known such index is probably

the *Randić index* [14]

$$R(T) = \sum_{uv \in E(T)} (d(u)d(v))^{-\frac{1}{2}}.$$

This concept can be naturally generalized to

$$w_\alpha(T) = \sum_{uv \in E(T)} (d(u)d(v))^\alpha$$

for $\alpha \neq 0$, also known as the *connectivity index* (see for example [6]). When $\alpha = 1$, this is also called the *weight* of a tree. In fact, Randić also proposed $w_\alpha(T)$ for $\alpha = -1$, later rediscovered and known as the *Modified Zagreb index.*

In order to study these chemical properties we must introduce the *molecular graph.* A molecular graph is the graphical representation of a chemical where $V(G)$ represents the atoms and $E(G)$ represents the bonds while the Hydrogen atoms are disregarded. As an example we may consider 2,2,3 - trimethylbutane and construct its chemical graph. Figure 1.1 shows the chemical structure of 2,2,3 - trimethylbutane.
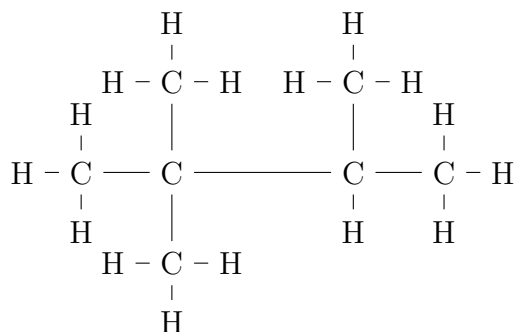
Figure 1.1: Chemical Structure of 2,2,3 - trimethylbutane

To obtain the molecular graph we replace all double and triple bonds with single bonds which creates the edges of the graph, $E(G)$ and remove all hydrogen atoms. Lastly, replace all remaining atoms with vertices to create $V(G)$. This process creates a tree as shown in Figure 1.2.

This concept appeared in [3]. One of the goals of chemical graph theory is to study graph invariants. Graph invariants are often referred to as topological indices
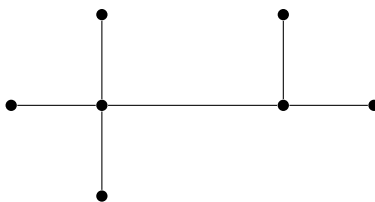
Figure 1.2: Chemical Graph of 2,2,3 - trimethylbutane

since the shape of the chemical graph determines the values of the index. These chemical indices often provide a prediction of a particular chemical property. We may consider many types of indices including those that are degree-based and distance-based. These indices will be the focus of our discussion.

1.2   Preliminaries

In this section we will list a few definitions that will be commonly referenced. More definitions will be presented throughout Chapter 2 and Chapter 3.

Definition 1.1 (Graph)**.** *A graph G is a set of vertices, denoted $V(G)$, together with a set of edges, denoted $E(G)$, that connect pairs of vertices from $V(G)$.*
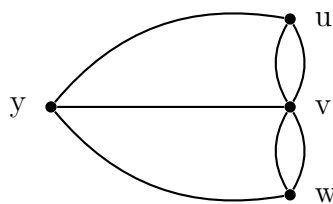
Figure 1.3: Example of a Graph

Throughout this paper we will focus on trees, a specific type of graph, which is defined below.

Definition 1.2 (Tree)**.** *A tree T is a graph in which no two vertices are connected by more than one path.*
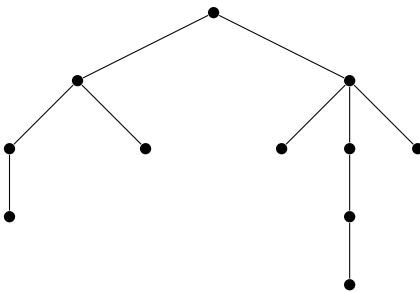
Figure 1.4: Example of a Tree

The *degree sequence* of a tree is simply the non-increasing sequence of the vertex degrees.

Definition 1.3 (Degree). *The degree of a vertex v in $V(G)$ is the number of edges incident to v in G, denoted $d(v)$.*

In Figure 1.3, $d(v) = 5$.

Definition 1.4 (Leaf). *A leaf (in a tree) is a vertex whose degree is one.*

Definition 1.5 (Distance). *The distance between two vertices in a graph is the length of the shortest path connecting them, denoted $d(u, v)$.*

In Figure 1.3, $d(u, w) = 2$.

Definition 1.6 (Eccentricity). *The eccentricity of a vertex v in G is the maximum distance from v to any other vertex in G, denoted $\varepsilon_G(v)$.*

In Figure 1.3, $\varepsilon_G(u) = 2$.

1.3   Degree-based Graph Indices

In Chapter 2 we will concentrate on the topic of degree-based graph indices.

The question of finding extremal structures with respect to various graph indices has received much attention in recent years. Among these graph indices, many are

defined on adjacent vertex degrees and are maximized or minimized by the same extremal structure. We consider a function defined on adjacent vertex degrees of a tree, T, to be $f(x, y)$ and the connectivity function associated with f,

$$R_f(T) = \sum_{uv \in E(T)} f(d(u), d(v)).$$

We first introduce the extremal tree structures, with a given degree sequence, that maximize or minimize such functions under certain conditions. When a partial ordering, called "majorization," is defined on the degree sequences of trees on n vertices, we compare the extremal trees of different degree sequences π and π'. As a consequence many extremal results follow as immediate corollaries. Our finding provides a uniform way of characterizing the extremal structures with respect to a class of graph invariants. We also briefly discuss the applications to specific indices.

1.4   A Special Case of Distance-based Graph Indices

In Chapter 3 we will concentrate on a special case of distance-based graph indices.

Among many well-known chemical indices, the connective eccentricity index of a graph G is defined as $\xi^{ce}(G) = \sum_{v \in V(G)} \frac{d_G(v)}{\varepsilon_G(v)}$ where $d_G(v)$ is the degree of v in G and $\varepsilon_G(v)$ is the eccentricity of v in G. Many extremal problems related to $\xi^{ce}(G)$ in various classes of graphs have been studied. Another interpretation of this concept, $\xi^{ce}(G) = \sum_{uv \in E(G)} \left(\frac{1}{\varepsilon(u)} + \frac{1}{\varepsilon(v)} \right)$ as the sum of reciprocals of the eccentricities of vertices motivates a natural generalization, where one can replace $\frac{1}{\varepsilon(v)}$ with $\frac{1}{g(\varepsilon(v))}$ and consequently $\xi_g^{ce}(G) = \sum_{v \in V(G)} \frac{d_G(v)}{g(\varepsilon_G(v))}$, which in turn generalizes to

$$\xi_{f,g}^{ce}(G) = \sum_{v \in V(G)} \frac{f(d_G(v))}{g(\varepsilon_G(v))}$$

for any functions f and g. We consider extremal problems related to $\xi_{f,g}^{ce}(G)$ in trees. First we show that some classic approaches can be easily adapted to prove

some general extremal results with respect to $\xi_{f,g}^{ce}(G)$. We then briefly discuss the comparison between extremal trees and the applications that follow.

CHAPTER 2

FUNCTIONS ON ADJACENT VERTEX DEGREES

2.1   Introduction

Graph invariants can be useful in many areas of applied sciences. In particular, chemical indices have been popular and powerful tools in the research of chemical graph theory. See for instance [4,5,8,9,14,27] for some applications. There have been many studies on indices defined on adjacent vertex degrees. The most well known such index is probably the *Randić index* [14]

$$R(T) = \sum_{uv \in E(T)} (d(u)d(v))^{-\frac{1}{2}}.$$

This concept can be naturally generalized to

$$w_\alpha(T) = \sum_{uv \in E(T)} (d(u)d(v))^\alpha$$

for $\alpha \neq 0$, also known as the *connectivity index* (see for example [6]). When $\alpha = 1$, this is also called the *weight* of a tree. In fact, Randić also proposed $w_\alpha(T)$ for $\alpha = -1$, later rediscovered and known as the *Modified Zagreb index.* The extremal trees for trees in general [12], trees with restricted degrees [15] and trees with given *degree sequence* (the non-increasing sequence of degrees of internal vertices) [6,22] have been characterized over the years.

Natural variations of $R(T)$ and $w_\alpha(T)$ were brought forward as the *sum-connectivity index* [39]

$$\chi(T) = \sum_{uv \in E(T)} (d(u) + d(v))^{-\frac{1}{2}}$$

and the *general sum-connectivity index* [40]

$$\chi_\alpha(T) = \sum_{uv \in E(T)} (d(u) + d(v))^\alpha.$$

Many interesting mathematical properties on these two indices, including some extremal results, can be found in $[39, 40]$ and the studies that follow.

Another variant of $R(T)$ was proposed more recently, as the *harmonic index* [8]

$$H(T) = \sum_{uv \in E(T)} \frac{2}{d(u) + d(v)},$$

which takes the sum of the reciprocal of the arithmetic mean (as opposed to the geometric mean in the case of $R(T)$) of adjacent vertex degrees. The extremal trees among simple connected graphs and general trees were characterized in [38].

Other examples of such graph invariants includes the *third Zagreb index* [17], defined as

$$\sum_{uv \in E(T)} (d(u) + d(v))^2.$$

It is easy to see that this is a special case of the general sum-connectivity index with $\alpha = 2$.

A slight variant of the third Zagreb index is the *reformulated Zagreb index* [13], defined as

$$\sum_{uv \in E(T)} (d(u) + d(v) - 2)^2.$$

Last but certainly not the least, the *Atom-Bond connectivity index* [7], defined as

$$\sum_{uv \in E(T)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}},$$

is a rather complicated example of such graph invariants that has recently received much attention (for example, see [36]).

A fundamental question in the study of such invariants asks for the extremal structures under certain constraints that maximize or minimize a chemical index. Many of such extremal structures turned out to be identical for different but similar invariants. In particular, the *greedy tree* (defined below) is often extremal among trees of a given degree sequence (the non-increasing sequence of the vertex degrees).

Definition 2.1 (Greedy Tree). *[24] With given vertex degrees, the greedy tree is achieved through the following "greedy algorithm":*

   i Label the vertex with the largest degree as v (the root);

  ii Label the neighbors of v as $v_1, v_2, ...$, assign the largest degrees available to them such that $d(v_{11}) \geq d(v_{12}) \geq ...$;

 iii Label the neighbors of v_1 (except v) as $v_{11}, v_{12}, ...$, such that they take all the largest degrees available and that $d(v_{11}) \geq d(v_{12}) \geq ...$, then do the same for $v_2, v_3, ...$;

 iv Repeat (iii) for all the newly labeled vertices. Always start with the neighbors of the labeled vertex with largest degree whose neighbors are not labeled yet.

Figure 2.1 shows an example of a greedy tree.

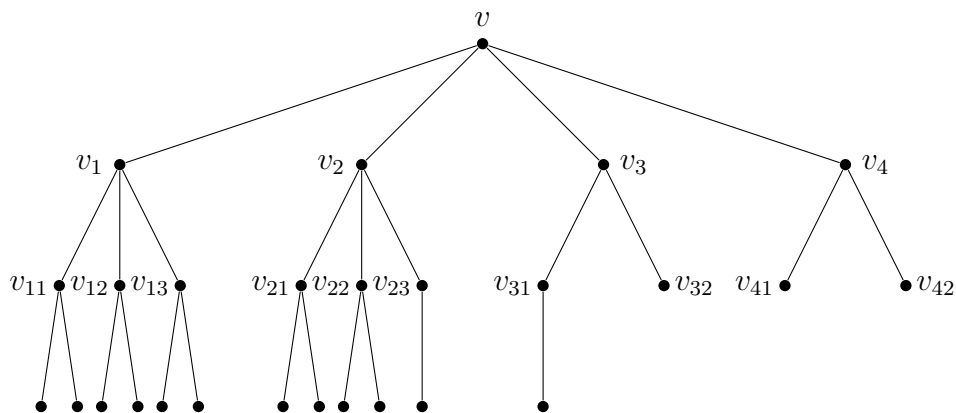Figure 2.1: A greedy tree with degree sequence $(4, 4, 4, 3, 3, 3, 3, 3, 3, 3, 2, 2, 1, \ldots, 1)$.

To facilitate our discussion, we call a bivariable function $f(x, y)$, defined on $\mathbb{N} \times \mathbb{N}$, *escalating* if

$$f(a, b) + f(c, d) \geq f(c, b) + f(a, d) \text{ for any } a \geq c \text{ and } b \geq d. \qquad (2.1)$$

Example 2.2. *The function $f(x, y) = xy$ is an escalating function.*

For a tree T, let the *connectivity function* associated with f be

$$R_f(T) = \sum_{uv \in E(T)} f(d(u), d(v)). \qquad (2.2)$$

It is worth pointing out that (2.1) is essentially a discrete version of

$$\frac{\partial^2}{\partial x \partial y} f(x, y) \geq 0.$$

It is not difficult to see, that with different f, $R_f(T)$ describes various graph invariants including many of the invariants mentioned above. The followings are shown in [24].

Theorem 2.3. *[24] For any escalating function f and $R_f(T)$ defined as in (2.2), $R_f(T)$ is maximized by the greedy tree among trees with given degree sequence.*

Similarly, a bivariable function $f(x, y)$ defined on $\mathbb{N} \times \mathbb{N}$ is *de-escalating* if

$$f(a, b) + f(c, d) \leq f(c, b) + f(a, d) \text{ for any } a \geq c \text{ and } b \geq d. \qquad (2.3)$$

Theorem 2.4. *[24] For any de-escalating function f and $R_f(T)$ defined as in (2.2), $R_f(T)$ is minimized by the greedy tree among trees with given degree sequence.*

Although greedy trees are interesting in their own right because of the close relation between vertex degrees and valences of atoms, comparing greedy trees of different degree sequences has proven to be an effective way of studying extremal tree structures in general. This is exactly the goal of this chapter. Majorization techniques are a fruitful method in the study of graph topological indicators and there is a wide literature (for example see $[1, 2, 33\text{--}35]$ etc.) about this topic.

First we recall the following partial ordering on degree sequences of trees of given order.

Definition 2.5 (Majorization)**.** *Given two nonincreasing degree sequences π and π' with $\pi = (d_1, d_2, ..., d_n)$ and $\pi' = (d'_1, d'_2, ..., d'_n)$, we say that π' majorizes π if the following conditions are met:*

1 $\sum_{i=0}^{k} d_i \leqslant \sum_{i=0}^{k} d'_i$ for $1 \leqslant k \leqslant n-1$, and

2 $\sum_{i=0}^{n} d_i = \sum_{i=0}^{n} d'_i$

We denote this by $\pi \lhd \pi'$.

For example: Let $\pi = (5, 5, 4, 4, 3, 2, 2, 1, ..., 1)$ and $\pi' = (5, 5, 5, 4, 3, 3, 2, 1, ..., 1)$. Then $\pi \lhd \pi'$.

The concept of majorization between degree sequences led to many interesting studies on various graph indices, see for instance, [1, 2]. The following fact will be of crucial importance to our argument.

Proposition 2.6. *[25] Let $\pi = (d_0, ..., d_{n-1})$ and $\pi' = (d'_0, ..., d'_{n-1})$ be two noincreasing graphical degree sequences. If $\pi \lhd \pi'$, then there exists a series of graphical degree sequences $\pi_1, ..., \pi_k$ such that $\pi \lhd \pi_1 \lhd ... \lhd \pi_k \lhd \pi'$, where π_i and π_{i+1} differ at exactly two entries, say d_j (d'_j) and d_k (d'_k) of π_i (π_{i+1}), with $d'_j = d_j + 1, d'_k = d_k - 1$ and $j < k$.*

In this chapter, we will first present our main result on the comparison between greedy trees of different degree sequences with respect to the $R_f(.)$ value. Then we will use our main theorem to deduce many extremal results as immediate consequences. We will also show some examples of the application of our findings to specific graph invariants.

2.2 Main result

In this section we prove our main result, stated in Theorems 2.7 and 2.10.

Theorem 2.7. *Given two degree sequences π and π' with $\pi \lhd \pi'$. Let T^*_π and $T^*_{\pi'}$ be the greedy trees with degree sequences π and π' respectively. For an escalating function f*

with

$$\frac{\partial f}{\partial x} \geq 0 \tag{2.4}$$

and

$$\frac{\partial^2 f}{(\partial x)^2} \geq 0, \tag{2.5}$$

we have

$$R_f(T_\pi^*) \leq R_f(T_{\pi'}^*).$$

Remark 2.8. *Although f is a discrete function, we treat it as a continuous function in order to use the above partial derivative conditions (2.4) and (2.5). This allows for a clear presentation of our conditions.*

Proof. Given the conditions (2.1), (2.4) and (2.5), we want to show

$$R_f(T_\pi^*) \leq R_f(T_{\pi'}^*)$$

for

$$(d_0, ..., d_{n-1}) = \pi \lhd \pi' = (d'_0, ..., d'_{n-1}).$$

By Proposition 2.6 we may assume the degree sequences π and π' differ at only two entries, say d_{j_0} (d'_{j_0}) and d_{k_0} (d'_{k_0}) with $d'_{j_0} = d_{j_0} + 1, d'_{k_0} = d_{k_0} - 1$ for some $j_0 < k_0$. Let T_π^* contain the vertices u_1 and u_2 with degrees $\mathcal{A} := d_{j_0}$ and $\mathcal{C} := d_{k_0}$ respectively (note that $\mathcal{A} \geq \mathcal{C}$). We introduce the followings:

- let the parent of u_1 have degree $\mathcal{B}$;

- let the children of u_1 have degrees $\mathcal{B}_1, \mathcal{B}_2, ..., \mathcal{B}_{\mathcal{A}-1}$;

- let the parent of u_2 have degree $\mathcal{D}$;

- let the children of u_2 have degrees $\mathcal{D}_1, \mathcal{D}_2, ..., \mathcal{D}_{\mathcal{C}-1}$.

Note that, from the structure of greedy trees, we have $\mathcal{D} \leq \mathcal{B}$ and $\mathcal{D}_i \leq \mathcal{B}_j$ for any $1 \leq i \leq \mathcal{C} - 1$ and $1 \leq j \leq \mathcal{A} - 1$.

Now consider the tree

$$T_{\pi'} = T_\pi^* - \{u_2 u_3\} + \{u_1 u_3\}$$

as in Figure 2.2. Note that $T_{\pi'}$ has degree sequence π' but is not necessarily a greedy tree.
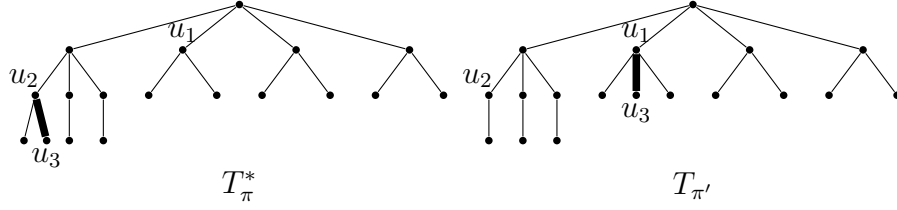
Figure 2.2: $\pi = (4, 4, 3, 3, 3, 3, 2, 2, 1, \ldots, 1)$ and $\pi' = (4, 4, 4, 3, 3, 2, 2, 2, 1, \ldots, 1)$.

From T_π^* to $T_{\pi'}$, we have altered the contribution to $R_f(.)$ associated with the vertices u_1, u_2 and u_3. Note that the degrees of u_1 and u_2 have changed to $\mathcal{A} + 1$ and $\mathcal{C} - 1$ respectively. Looking at the difference in the contributions to the function value between u_1 and its parent we have

$$f(\mathcal{A} + 1, \mathcal{B}) - f(\mathcal{A}, \mathcal{B}).$$

Similarly we have

$$- (f(\mathcal{C}, \mathcal{D}) - f(\mathcal{C} - 1, \mathcal{D}))$$

for u_2 and its parent. From the edge $u_2 u_3$ to $u_1 u_3$ we have a change in the function value of

$$f(\mathcal{A} + 1, \mathcal{D}_1) - f(\mathcal{C}, \mathcal{D}_1).$$

The change in the contributions of the function value between u_1 and its children can be represented by the sum

$$\sum_{i=1}^{\mathcal{A}-1} (f(\mathcal{A} + 1, \mathcal{B}_i) - f(\mathcal{A}, \mathcal{B}_i)).$$

Similarly, the change in contributions to the function value between u_2 and its children can be represented by the sum

$$-\left(\sum_{j=2}^{\mathcal{C}-1}(f(\mathcal{C},\mathcal{D}_j) - f(\mathcal{C}-1,\mathcal{D}_j))\right).$$

Now we have $R_f(T_{\pi'}) - R_f(T_\pi^*)$ as

$$(f(\mathcal{A}+1,\mathcal{D}_1) - f(\mathcal{C},\mathcal{D}_1)) \tag{2.6}$$

$$+((f(\mathcal{A}+1,\mathcal{B}) - f(\mathcal{A},\mathcal{B})) - (f(\mathcal{C},\mathcal{D}) - f(\mathcal{C}-1,\mathcal{D}))) \tag{2.7}$$

$$+\left(\sum_{i=1}^{\mathcal{A}-1}(f(\mathcal{A}+1,\mathcal{B}_i) - f(\mathcal{A},\mathcal{B}_i)) - \sum_{j=2}^{\mathcal{C}-1}(f(\mathcal{C},\mathcal{D}_j) - f(\mathcal{C}-1,\mathcal{D}_j))\right). \tag{2.8}$$

Next we consider each of these three terms (2.6), (2.7), and (2.8).

- First note that

$$f(\mathcal{A}+1,\mathcal{D}_1) - f(\mathcal{C},\mathcal{D}_1) \geq 0$$

as $\dfrac{\partial f}{\partial x} \geq 0$ and $\mathcal{A} \geq \mathcal{C}$.

- Next, note that

$$f(\mathcal{A}+1,\mathcal{B}) - f(\mathcal{A},\mathcal{B}) = \frac{\partial f}{\partial x}(\mathcal{A}',\mathcal{B})$$

and

$$f(\mathcal{C}+1,\mathcal{B}) - f(\mathcal{C},\mathcal{B}) = \frac{\partial f}{\partial x}(\mathcal{C}',\mathcal{B}),$$

where $\mathcal{A} \leq \mathcal{A}' \leq \mathcal{A}+1$ and $\mathcal{C} \leq \mathcal{C}' \leq \mathcal{C}+1$.

Since $\mathcal{A} \geq \mathcal{C}$, we have $\mathcal{A}' \geq \mathcal{C}'$. Then our assumption $\dfrac{\partial^2 f}{(\partial x)^2} \geq 0$ implies that

$$\frac{\partial f}{\partial x}(\mathcal{A}',\mathcal{B}) \geq \frac{\partial f}{\partial x}(\mathcal{C}',\mathcal{B})$$

and hence

$$f(\mathcal{A}+1,\mathcal{B}) - f(\mathcal{A},\mathcal{B}) \geq f(\mathcal{C},\mathcal{B}) - f(\mathcal{C}-1,\mathcal{B}).$$

Together with

$$(f(\mathcal{C}, \mathcal{B}) - f(\mathcal{C} - 1, \mathcal{B})) \geqslant (f(\mathcal{C}, \mathcal{D}) - f(\mathcal{C} - 1, \mathcal{D}))$$

(as f is escalating and $\mathcal{C} \geq \mathcal{C} - 1$, $\mathcal{B} \geq \mathcal{D}$), we have

$$(f(\mathcal{A} + 1, \mathcal{B}) - f(\mathcal{A}, \mathcal{B})) - (f(\mathcal{C}, \mathcal{D}) - f(\mathcal{C} - 1, \mathcal{D})) \geq 0.$$

- Similarly we have

$$(f(\mathcal{A} + 1, \mathcal{B}_i) - f(\mathcal{A}, \mathcal{B}_i)) - (f(\mathcal{C}, \mathcal{D}_j) - f(\mathcal{C} - 1, \mathcal{D}_j)) \geq 0$$

for any i and j. Hence any term of $\sum_{i=1}^{\mathcal{A}-1}(f(\mathcal{A}+1, \mathcal{B}_i) - f(\mathcal{A}, \mathcal{B}_i))$ is larger than every term of $\sum_{j=2}^{\mathcal{C}-1}(f(\mathcal{C}, \mathcal{D}_j) - f(\mathcal{C}-1, \mathcal{D}_j))$. Also, note that $\sum_{i=1}^{\mathcal{A}-1}(f(\mathcal{A}+1, \mathcal{B}_i) - f(\mathcal{A}, \mathcal{B}_i))$ has more terms than $\sum_{j=2}^{\mathcal{C}-1}(f(\mathcal{C}, \mathcal{D}_j) - f(\mathcal{C}-1, \mathcal{D}_j))$ since $\mathcal{A} - 1 > \mathcal{C} - 2$, and that $f(\mathcal{A} + 1, \mathcal{B}_i) - f(\mathcal{A}, \mathcal{B}_i) \geq 0$, $f(\mathcal{C}, \mathcal{D}_j) - f(\mathcal{C} - 1, \mathcal{D}_j) \geq 0$ for any i, j (since $\dfrac{\partial f}{\partial x} \geq 0$).

Therefore

$$\sum_{i=1}^{\mathcal{A}-1}(f(\mathcal{A} + 1, \mathcal{B}_i) - f(\mathcal{A}, \mathcal{B}_i)) - \sum_{j=2}^{\mathcal{C}-1}(f(\mathcal{C}, \mathcal{D}_j) - f(\mathcal{C} - 1, \mathcal{D}_j)) \geq 0.$$

Thus all three terms (2.6), (2.7) and (2.8) are non-negative. Hence

$$R_f(T_{\pi'}) - R_f(T_\pi^*) \geq 0.$$

Note that $R_f(T_{\pi'}^*) \geq R_f(T_{\pi'})$ by Theorem 2.3. Therefore

$$R_f(T_\pi^*) \leq R_f(T_{\pi'}) \leq R_f(T_{\pi'}^*).$$

$\square$

Remark 2.9. *Note that, as in condition* (2.1)*, the discrete version of the conditions* (2.4) *and* (2.5) *would be sufficient for our argument. We state Theorem 2.7 with* $\dfrac{\partial f}{\partial x}$ *and* $\dfrac{\partial^2 f}{(\partial x)^2}$ *in order to facilitate the presentation, as well as to simplify the application of the result.*

Although we formulated our main theorem in terms of the escalating functions, it is not difficult to see that the next theorem follows from the similar arguments. We omit the details.

Theorem 2.10. *Given two degree sequences π and π' with $\pi \lhd \pi'$. Let T_π^* and $T_{\pi'}^*$ be the greedy trees with degree sequences π and π' respectively. For a de-escalating function f with*

$$\frac{\partial f}{\partial x} \leq 0 \tag{2.9}$$

and

$$\frac{\partial^2 f}{(\partial x)^2} \leq 0, \tag{2.10}$$

we have

$$R_f(T_\pi^*) \geq R_f(T_{\pi'}^*).$$

2.3 General extremal structures

First we assume the function f to be escalating and satisfies conditions (2.4), (2.5), and that $R_f(.)$ is defined as in (2.2). We now immediately have the following consequences. We include a brief proof for each of them for completeness.

Corollary 2.11. *Among all trees of order n, the star maximizes $R_f(.)$.*

Proof. Among all trees of order n, it is easy to see that the degree sequence $(n - 1, 1, \ldots, 1)$ majorizes all other degree sequences. Noting that the greedy tree with this degree sequence is the star. The conclusion then follows from Theorems 2.3 and 2.7. □

Corollary 2.12. *Among all trees of order n with given maximum degree Δ, the greedy tree with degree sequence $(\Delta, \Delta, \ldots, \Delta, q, 1, \ldots, 1)$ (where $1 \leq q \leq \Delta - 1$) maximizes $R_f(.)$.*

In different literatures this extremal tree is sometimes called a "complete Δ-ary tree", "good Δ-ary tree", or "Volkmann trees".

Proof. It is easy to see that with given maximum degree, the claimed degree sequence majorizes any other degree sequence under the same condition. The conclusion then follows from Theorems 2.3 and 2.7. □

Corollary 2.13. *Among all trees of order n with s leaves, the greedy tree with degree sequence $\left(s, 2, \ldots, 2, \underbrace{1, \ldots, 1}_{s \ 1\text{'s}} \right)$ maximizes $R_f(.)$. Such a tree is often called a "star like tree".*

Proof. Given s leaves, the degree sequence must have exactly s 1's. It is easy to see that $\left(s, 2, \ldots, 2, \underbrace{1, \ldots, 1}_{s \ 1\text{'s}} \right)$ majorizes any other degree sequence with s 1's. The conclusion then follows from Theorems 2.3 and 2.7. □

Corollary 2.14. *Among all trees of order n with independence number α and degree sequence $(\alpha, 2, \ldots, 2, 1, \ldots, 1)$ maximizes $R_f(.)$.*

Proof. Let I be an independent set of T of exactly α vertices. For any leaf $u \notin I$, the unique neighbor v of u must be in I and $I \cup \{u\} - \{v\}$ is also an independent set of T. Hence there exists an independent set of α vertices that contains all leaves. Consequently there are at most α leaves. It is easy to see, under this condition, the claimed degree sequence majorizes all others. The conclusion then follows from Theorems 2.3 and 2.7. □

Corollary 2.15. *Among all trees of order n with matching number β and degree sequence $\left(n - \beta, \underbrace{2, \ldots, 2}_{\beta \ 2\text{'s}}, 1, \ldots, 1) \right)$ maximizes $R_f(.)$.*

Proof. Let M be a matching of T of exactly β edges, each of these edges contains at least one vertex of degree at least 2. Hence there are at least β vertices of degree at

least 2. Under this condition, the claimed degree sequence majorizes all others. The conclusion then follows from Theorems 2.3 and 2.7. □

Remark 2.16. *Of course, it is easy to see the analogues of the above statements for de-escalating functions satisfying conditions* (2.9) *and* (2.10). *We omit the exact statements here. Essentially f is de-escalating and $R_f(.)$ will be minimized.*

2.4   Applications

In this section we explore the application of our results to specific graph invariants.

2.4.1   Connectivity index

When $f(x, y) = x^\alpha y^\alpha$, recall that

$$R_f(T) = \sum_{uv \in E(T)} (d(u)d(v))^\alpha$$

is the connectivity index, a natural generalization of the well known Randić index. Consider the case $\alpha > 0$, we have

$$f(a, b) + f(c, d) - f(c, b) - f(a, d) = a^\alpha b^\alpha + c^\alpha d^\alpha - c^\alpha b^\alpha - a^\alpha d^\alpha = (a^\alpha - c^\alpha)(b^\alpha - d^\alpha) \geq 0$$

for any $a \geq c$ and $b \geq d$. Thus $f(x, y)$ is escalating and Theorem 2.3 holds.

Similarly, $f(x, y)$ is de-escalating for $\alpha < 0$. Consequently we immediately have the following results.

Theorem 2.17 ([15, 22]). *Among trees with given degree sequence, the connectivity index is maximized (minimized) by the greedy tree for $\alpha > 0$ ($\alpha < 0$).*

Remark 2.18. *Furthermore, if $\alpha > 1$, it is easy to verify* (2.4) *and* (2.5). *Consequently Theorem 2.7 holds and the corresponding corollaries in Section 2.3 hold.*

2.4.2   General Sum-connectivity index and the third Zagreb index

When $f(x, y) = (x + y)^\alpha$, recall that

$$R_f(T) = \chi_\alpha(T) = \sum_{uv \in E(T)} (d(u) + d(v))^\alpha$$

is the general sum-connectivity index. It is simply the sum-connectivity index when $\alpha = 1$.

We first show that $\chi_\alpha(T)$ is escalating (de-escalating) for $\alpha \geq 1$ $(0 < \alpha < 1)$.

Consider $\alpha \geq 1$ and let $a \geq c$ and $b \geq d$. To show that $f(x, y)$ is escalating it suffices to show that

$$(a + b)^\alpha - (b + c)^\alpha \geq (a + d)^\alpha - (c + d)^\alpha,$$

which is equivalent to, through some calculus, the following:

$$\int_{b+c}^{a+b} \alpha t^{\alpha-1} dt \geq \int_{c+d}^{a+d} \alpha t^{\alpha-1} dt.$$

This can be rewritten as

$$\int_c^a \alpha(t + b)^{\alpha-1} dt \geq \int_c^a \alpha(t + d)^{\alpha-1} dt,$$

which holds if and only if

$$\alpha(t + b)^{\alpha-1} \geq \alpha(t + d)^{\alpha-1}.$$

Since $\alpha \geq 1$, the last inequality is true if and only if $b \geq d$.

Similarly, if $0 < \alpha < 1$ $f(x, y)$ is de-escalating.

Consequently we have the following as a corollary to Theorem 2.3.

Theorem 2.19. *Among trees with given degree sequence, the general sum-connectivity index is maximized (minimized) by the greedy tree for $\alpha \geq 1$ $(0 < \alpha < 1)$.*

Remark 2.20. *Furthermore, if $\alpha \geq 0$, it is easy to verify (2.4) and (2.5) for $f(x,y) = (x+y)^\alpha$. Therefore Theorem 2.7 applies (when $\alpha \geq 1$ and $f(x,y)$ is escalating) and the corresponding corollaries in Section 2.3 hold.*

Remark 2.21. *Noting that the third Zagreb index is a special case of the general sum-connectivity index with $\alpha = 2$. Both Theorems 2.3 and 2.7, and their consequences from Section 2.3 apply. We skip the exact statements.*

Of course, the same can be concluded for the sum-connectivity index itself.

2.4.3 Reformulated Zagreb index

It is not difficult to see that although the reformulated Zagreb index, defined as

$$\sum_{uv \in E(T)} (d(u) + d(v) - 2)^2,$$

is not a special case of the general sum-connectivity index, it can be analyzed in very similar ways.

Letting $a \geq c$ and $b \geq d$,

$$(a + b - 2)^2 + (c + d - 2)^2 \geq (b + c - 2)^2 + (a + d - 2)^2$$

is equivalent to

$$2b(a - c) - 2d(a - c) \geq 0,$$

which holds by our conditions.

Thus $f(x,y)$ is escalating and Theorem 2.3 holds.

Theorem 2.22. *Among trees with given degree sequence, the reformulated Zagreb index is maximized by the greedy tree.*

Remark 2.23. *Furthermore, it is easy to verify (2.4) and (2.5) for $f(x,y) = (x+y-2)^2$. Therefore Theorem 2.7 applies and the corresponding corollaries in Section 2.3 hold.*

2.4.4 Atom-Bond connectivity index

When $f(x, y) = \sqrt{\dfrac{x + y - 2}{xy}}$, the Atom-Bond connectivity (ABC) index

$$\sum_{uv \in E(T)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}$$

is perhaps one of the most complicated graph invariants defined on adjacent vertex degrees. In [28] it is shown that the greedy tree achieves the minimum ABC index among trees of given degree sequence. In order to prove that $f(x, y) = \sqrt{\dfrac{x + y - 2}{xy}}$ is de-escalating, we first prove the following facts.

Lemma 2.24. *For all positive integers c and d,*

$$f(c + 1, d + 1) + f(c, d) \leq f(c, d + 1) + f(c + 1, d). \tag{2.11}$$

Proof. Since

$$
\begin{aligned}
&\left(\frac{1}{c + 1} + \frac{1}{d} - \frac{2}{(c + 1)d} \right) \left(\frac{1}{c} + \frac{1}{d + 1} - \frac{2}{c(d + 1)} \right) \\
&\qquad - \left(\frac{1}{c} + \frac{1}{d} - \frac{2}{cd} \right) \left(\frac{1}{c + 1} + \frac{1}{d + 1} - \frac{2}{(c + 1)(d + 1)} \right) \\
=\ &\left(\frac{1}{c} - \frac{1}{c + 1} \right) \left(\frac{1}{d} - \frac{1}{d + 1} \right) \\
>\ &0,
\end{aligned}
$$

we have

$$
\begin{aligned}
&(f(c, d + 1) + f(c + 1, d))^2 - (f(c + 1, d + 1) + f(c, d))^2 \\
=\ &2\sqrt{\left(\frac{1}{c + 1} + \frac{1}{d} - \frac{2}{(c + 1)d} \right) \left(\frac{1}{c} + \frac{1}{d + 1} - \frac{2}{c(d + 1)} \right)} \\
&\qquad - 2\sqrt{\left(\frac{1}{c} + \frac{1}{d} - \frac{2}{cd} \right) \left(\frac{1}{c + 1} + \frac{1}{d + 1} - \frac{2}{(c + 1)(d + 1)} \right)} \\
&\qquad + \frac{2}{cd(c + 1)(d + 1)} \\
>\ &0.
\end{aligned}
$$

Hence (2.11) holds. □

Lemma 2.25. *For any nonnegative integer k and positive integers c, d,*

$$f(c+k, d+1) + f(c, d) \le f(c, d+1) + f(c+k, d). \qquad (2.12)$$

Proof. Through repeated applications of (2.11), we have

$$
\begin{aligned}
f(c+k, d+1) - f(c+k, d) \;\le\;& f(c+k-1, d+1) - f(c+k-1, d) \\
\le\;& f(c+k-2, d+1) - f(c+k-2, d) \\
\le\;& \ldots\ldots \\
\le\;& f(c, d+1) - f(c, d).
\end{aligned}
$$

So (2.12) holds. $\qquad\square$

Proposition 2.26. *The function $f(x, y) = \sqrt{\dfrac{x+y-2}{xy}}$ is de-escalating on $\mathbb{N} \times \mathbb{N}$.*

Proof. By the definition of de-escalating functions, we need only prove the following inequality

$$f(a, b) + f(c, d) \le f(c, b) + f(a, d) \text{ for any } a \ge c \text{ and } b \ge d.$$

Let $a = c + k$ and $b = d + r$ with nonnegative integers k, r. Through repeated applications of (2.12), we have

$$
\begin{aligned}
f(a, b) - f(c, b) \;=\;& f(c+k, d+r) - f(c, d+r) \\
\le\;& f(c+k, d+r-1) - f(c, d+r-1) \\
\le\;& f(c+k, d+r-2) - f(c, d+r-2) \\
\le\;& \ldots\ldots \\
\le\;& f(c+k, d) - f(c, d) \\
=\;& f(a, d) - f(c, d).
\end{aligned}
$$

So $f(x, y) = \sqrt{\dfrac{x+y-2}{xy}}$ is de-escalating on $\mathbb{N} \times \mathbb{N}$. $\qquad\square$

By Proposition (2.26) and Theorem 2.3, we have the following statement.

Theorem 2.27. *Among trees with given degree sequence, the Atom-Bond connectivity (ABC) index is minimized by the greedy tree.*

Although the greedy tree is indeed extremal, unfortunately (2.9) and (2.10) do not both hold in order to apply Theorem 2.10.

2.5   Concluding remarks

We considered functions defined on adjacent vertex degrees and the corresponding topological indices. With certain additional conditions we show not only the characterization of extremal graphs, but also the comparison between extremal graphs with different degree sequences. This statement, based on the majorization between degree sequences, leads to many extremal results as immediate consequences. We also explored the application of our main theorem on a variety of popular graph indices.

CHAPTER 3

FUNCTIONS ON DEGREES AND ECCENTRICITIES

3.1   Introduction

In the past few decades the study of topological indices has become a very important part of mathematical chemistry. Such indices, often called chemical indices, correlate the structures of chemical compounds with the chemical's properties. A relatively new such index is called the *connective eccentricity index*, introduced in [11] and defined as

$$\xi^{ce}(G) = \sum_{v \in V(G)} \frac{d_G(v)}{\varepsilon_G(v)} = \sum_{uv \in E(G)} \left(\frac{1}{\varepsilon(u)} + \frac{1}{\varepsilon(v)} \right)$$

where $d_G(v)$ is the degree of v in G and $\varepsilon_G(v)$ is the *eccentricity of v* (the maximum distance from v to any other vertex) in G.

As a chemical index $\xi^{ce}(G)$ provides a unique aspect as it takes into consideration both the distance and the degree, as well as the adjacency between vertices. Consequently it has received much attention in recent years. In particular, the extremal problem with respect to $\xi^{ce}(G)$ has been studied for different classes of graphs [29–31].

Note that the expression $\sum_{uv \in E(G)} \left(\frac{1}{\varepsilon(u)} + \frac{1}{\varepsilon(v)} \right)$ takes the sum of reciprocals of eccentricities, a natural generalization would be to consider

$$\xi^{ce}_g(G) = \sum_{uv \in E(G)} \left(\frac{1}{g(\varepsilon(u))} + \frac{1}{g(\varepsilon(v))} \right) = \sum_{v \in V(G)} \frac{d_G(v)}{g(\varepsilon_G(v))}$$

where we consider a function g of the eccentricity in the formula. Similarly, replacing $d_G(v)$ in the last expression by a function f of the degree yields

$$\mathscr{E}(G) := \xi^{ce}_{f,g}(G) = \sum_{v \in V(G)} \frac{f(d_G(v))}{g(\varepsilon_G(v))}.$$

In this chapter we will consider the topological index $\mathscr{E}(G)$ and related extremal problems. We will limit our attention to trees. First we introduce some background information in Section 3.2. Next we find the extremal trees with respect to $\mathscr{E}(G)$

among trees with a given degree sequence in Section 3.3. We then move on to comparing the extremal structures with different degree sequences in Section 3.4 and present applications of this comparison in Section 3.5.

3.2   Preliminaries

Let $\sigma_T(v) = \dfrac{f(d_T(v))}{g(\varepsilon_T(v))}$, then

$$\mathscr{E}(G) := \xi_{f,g}^{ce}(G) = \sum_{v \in V(G)} \sigma_T(v).$$

In practice f is usually the identity function. We consider it in a more general setting where f is an increasing function. We use the notation $\mathscr{E}_{\nearrow}(G)$ if g is increasing and $\mathscr{E}_{\searrow}(G)$ if g is decreasing.

Recall that the *degree sequence* of a tree is simply the non-increasing sequence of the vertex degrees. Given the degree sequence, we first define a few special trees.

The greedy tree is known to be extremal among trees with a given degree sequence with respect to many different indices. In particular, it is known to minimize the distance (the sum of distances between vertices [23, 35] and the sum of eccentricities [18]) among trees with a given degree sequence. We will show that the greedy trees are indeed also extremal with respect to $\mathscr{E}(G)$. Our approach makes use of a number of known results, including the following concepts.

Definition 3.1 (Level-Degree Sequence [18])**.** *In a rooted tree, the list of multisets L_i of degrees of vertices at height i, starting with L_0 containing the degree of the root vertex, is called the level-degree sequence of the rooted tree.*

In a rooted tree, the outdegree of the root is equal to its degree and the outdegree of any other vertex is its degree minus one. For a given level-degree sequence the corresponding outdegrees describe the number of vertices at each level.

Definition 3.2 (Level-Greedy Tree (Figure 3.1) [16])**.** *For $i \in \{0, 1, ..., H\}$, let mul-tisets*

$\{a_{i1}, a_{i2}, ..., a_{il_i}\}$ *of nonnegative numbers be given such that $l_0 = 1$ and*

$$l_{i+1} = \sum_{j=1}^{l_i} a_{ij}.$$

Assume that the elements of each multiset are sorted, i.e. $a_{i1} \geq a_{i2} \geq ... \geq a_{il_i}$. The level-greedy tree, with height H, corresponding to this sequence of multisets is the rooted tree whose j^{th} vertex at level i has outdegree a_{ij}.

Likewise, if sorted multisets $\{a_{i1}, a_{i2}, ..., a_{il_i}\}$ of nonnegative numbers are given for $i \in \{0, 1, ..., H\}$ such that $l_0 = 2$ and

$$l_{i+1} = \sum_{j=1}^{l_i} a_{ij},$$

then the level-greedy tree corresponding to this sequence of multisets is the edge-rooted tree (i.e. there are two vertices at level 0, connected by an edge) whose j^{th} vertex at level i has outdegree a_{ij}.
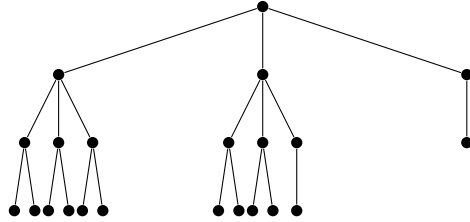

Figure 3.1: A level-greedy tree with level-degree sequence.

A caterpillar is a tree whose removal of leaves results in a path (Figure 3.2). The greedy caterpillar with a given degree sequence is defined as following.

Definition 3.3 (Greedy Caterpillar (Figure 3.3) [21])**.** *A greedy caterpillar is a cater-pillar where the path formed by the internal vertices can be labeled as $v_1 v_2 ... v_k$ such that*

$$min\{d_1, d_k\} \geq max\{d_2, d_{k-1}\}, \ min\{d_2, d_{k-1}\} \geq max\{d_3, d_{k-2}\}, ...$$
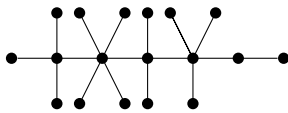
where d_i is the degree of v_i.

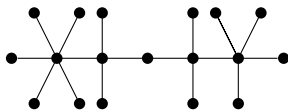Figure 3.2: A caterpillar with degree sequence $\{6, 5, 4, 4, 2, 1, ..., 1\}$.

Figure 3.3: A greedy caterpillar with degree sequence $\{6, 5, 4, 4, 2, 1, ..., 1\}$.

From these definitions it is easy see the following facts.

Proposition 3.4. *Given a degree sequence, the number of internal vertices is fixed. Furthermore:*

- *In a caterpillar with a given degree sequence, all internal vertices lie on the same path, and the eccentricity of an internal vertex does not depend on the degree of this or any other internal vertices.*

- *In a greedy caterpillar with a given degree sequence, the larger the eccentricity of an internal vertex is, the larger the degree of it is.*

3.3 Extremal trees with a given degree sequence

Theorem 3.5. *Among trees with a given degree sequence π, the greedy caterpillar minimizes $\mathscr{E}_{\nearrow}(T)$ and maximizes $\mathscr{E}_{\searrow}(T)$.*

Proof. We only consider the case of $\mathscr{E}(T) := \mathscr{E}_{\nearrow}(T)$. The other case is similar.

Let $\mathscr{T}$ be the set of trees whose degree sequence is π. Let $T \in \mathscr{T}$ be the tree such that $\mathscr{E}(T) = \min_{F \in \mathscr{T}} \mathscr{E}(F)$.

First we show that T must be a caterpillar. If not, let $P_T(u,v) = uu_1u_2...u_kv$ be a longest path in T for some $k \in \mathbb{Z}$. We then find a vertex, $u_t \in V(T)$ such that u_t is the first vertex (i.e., with smallest subscript t) with a non-leaf neighbor, w, not on $P_T(u,v)$. Note that $t \in \{2, 3, ..., k\}$ since $P_T(u,v)$ is a longest path in T. Let W denote the connected component containing w in $T - u_tw$. Now detaching W from w and reattaching it to u creates a new tree, T', with degree sequence π. See Figure 3.4.
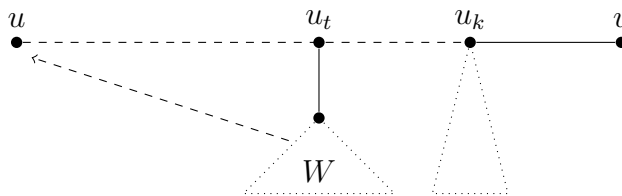

Figure 3.4: The caterpillar T and the component W.

Note that

- for any vertex $s \in (V(T) \setminus V(W)) \cup \{w\}$ we have, $\varepsilon_{T'}(s) \geq \varepsilon_T(s)$ since $P_T(u,v)$ is a longest path in T.

- for any vertex $r \in V(W) - \{w\}$ we have,

$$\varepsilon_{T'}(r) = d_{T'}(r,u) + d_T(u,v) > d_T(u,v) \geq \varepsilon_T(r)$$

  where $d_G(x,y)$ denotes the distance between vertices x and y in G.

- for any vertex $z \in V(T) \setminus \{u,w\}$, $d_{T'}(z) = d_T(z)$. For u and w we have $d_{T'}(u) = d_T(w)$ and $d_{T'}(w) = d_T(u)$.

Then $\sigma_{T'}(z) \leq \sigma_T(z)$ for any $z \in V(T) \setminus \{u,w\}$, and as $d_T(w) > 1 = d_T(u)$ and $\varepsilon_T(u) > \varepsilon_T(w)$ we have the following

$$\sigma_{T'}(u) + \sigma_{T'}(w) - \sigma_T(u) - \sigma_T(w)$$

$$= \frac{f(d_{T'}(u))}{g(\varepsilon_{T'}(u))} + \frac{f(d_{T'}(w))}{g(\varepsilon_{T'}(w))} - \frac{f(d_T(u))}{g(\varepsilon_T(u))} - \frac{f(d_T(w))}{g(\varepsilon_T(w))}$$

$$= \frac{f(d_T(w))}{g(\varepsilon_{T'}(u))} + \frac{f(d_T(u))}{g(\varepsilon_{T'}(w))} - \frac{f(d_T(u))}{g(\varepsilon_T(u))} - \frac{f(d_T(w))}{g(\varepsilon_T(w))}$$

$$\leq \frac{f(d_T(w))}{g(\varepsilon_T(u))} + \frac{f(d_T(u))}{g(\varepsilon_T(w))} - \frac{f(d_T(u))}{g(\varepsilon_T(u))} - \frac{f(d_T(w))}{g(\varepsilon_T(w))}$$

$$= (f(d_T(w)) - f(d_T(u))) \left(\frac{1}{g(\varepsilon_T(u))} - \frac{1}{g(\varepsilon_T(w))} \right) < 0.$$

Consequently $\mathscr{E}(T') < \mathscr{E}(T)$, a contradiction. Thus T must be a caterpillar.

Next we show that T is a greedy caterpillar. Since T is a caterpillar its internal vertices form a path, $P'_T(u_1, u_k) = u_1 u_2 ... u_k$. If T is not greedy, then by Proposition 3.4 there exist vertices u_i and u_j with $i, j \in \{1, 2, ..., k\}$ such that $d_T(u_i) > d_T(u_j)$ and $\varepsilon_T(u_i) < \varepsilon_T(u_j)$.

We construct a new tree, T'', by taking $D = d(u_i) - d(u_j)$ vertices and their adjacent edges from u_i and moving them to u_j. Let these moved pendant vertices be $x_1, x_2, ..., x_D$ (Figure 3.5). Note that the degree sequence of T'' is still π. It follows that

- $d_T(u_i) = d_{T''}(u_j)$ and $d_T(u_j) = d_{T''}(u_i)$.

- $\varepsilon_T(u_i) = \varepsilon_{T''}(u_i)$ and $\varepsilon_T(u_j) = \varepsilon_{T''}(u_j)$ since no vertices in $P'(u_1, u_k)$ were moved during the creation of T''.

- For any $1 \leq i \leq D$, $d_T(x_i) = 1 = d_{T''}(x_i)$ and $\varepsilon_T(x_i) < \varepsilon_{T''}(x_i)$.

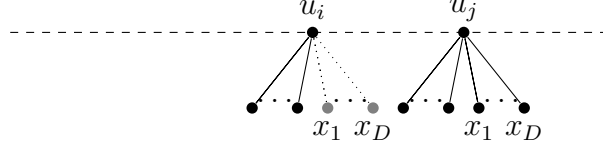Now consider $\mathscr{E}(T'') - \mathscr{E}(T)$. Among all vertices in $V(T) = V(T'')$ the value of

Figure 3.5: The caterpillar T and the vertices $x_1, x_2, ..., x_D$.

$\sigma(.)$ changed for vertices u_i, u_j, and $x_1, x_2, ..., x_D$. So we have

$$\mathscr{E}(T'') - \mathscr{E}(T)$$
$$= (\sigma_{T''}(u_i) - \sigma_T(u_i)) + (\sigma_{T''}(u_j) - \sigma_T(u_j)) + \left(\sum_{i=1}^{D} \sigma_{T''}(x_i) - \sum_{i=1}^{D} \sigma_T(x_i) \right).$$

Since $d_T(x_i) = d_{T''}(x_i)$ and $\varepsilon_T(x_i) < \varepsilon_{T''}(x_i)$, we have $\sigma_{T''}(x_i) - \sigma_T(x_i) < 0$ for any $1 \le i \le D$. As a result $\sum_{i=1}^{D} \sigma_{T''}(x_i) - \sum_{i=1}^{D} \sigma_T(x_i) < 0$. Consequently

$$\mathscr{E}(T'') - \mathscr{E}(T) < (\sigma_{T''}(u_i) - \sigma_T(u_i)) + (\sigma_{T''}(u_j) - \sigma_T(u_j))$$

$$= \frac{f(d_{T''}(u_i))}{g(\varepsilon_{T''}(u_i))} - \frac{f(d_T(u_i))}{g(\varepsilon_T(u_i))} + \frac{f(d_{T''}(u_j))}{g(\varepsilon_{T''}(u_j))} - \frac{f(d_T(u_j))}{g(\varepsilon_T(u_j))}$$

$$= \frac{f(d_{T''}(u_i))}{g(\varepsilon_{T''}(u_i))} + \frac{f(d_{T''}(u_j))}{g(\varepsilon_{T''}(u_j))} - \frac{f(d_T(u_i))}{g(\varepsilon_T(u_i))} - \frac{f(d_T(u_j))}{g(\varepsilon_T(u_j))}$$

$$= \frac{f(d_T(u_j))}{g(\varepsilon_T(u_i))} + \frac{f(d_T(u_i))}{g(\varepsilon_T(u_j))} - \frac{f(d_T(u_i))}{g(\varepsilon_T(u_i))} - \frac{f(d_T(u_j))}{g(\varepsilon_T(u_j))}$$

$$= \left(f(d_T(u_j)) - f(d_T(u_i)) \right) \left(\frac{1}{g(\varepsilon_T(u_i))} - \frac{1}{g(\varepsilon_T(u_j))} \right) < 0.$$

This is a contradiction. Hence T must be a greedy caterpillar. $\qquad\square$

In order to show that the greedy tree is extremal among trees with a given degree sequence, we first consider trees with a given level-degree sequence.

Theorem 3.6. *Among trees with a given level-degree sequence, the level-greedy tree maximizes $\mathscr{E}_{\nearrow}(T)$ and minimizes $\mathscr{E}_{\searrow}(T)$.*

Proof. We only consider the rooted case for $\mathscr{E}(T) := \mathscr{E}_\nearrow(T)$. The edge-rooted case and the $\mathscr{E}_\searrow(T)$ cases are similar.

Let T be an *optimal* tree with root v and the given level-degree sequence that maximizes $\mathscr{E}(T)$. Let T_1 be the subtree of T that is rooted at v_1, a child of v, that contains some leaves of height $h = h(T)$. and let $h' = h(T - T_1)$. For any vertex $u \in V(T - T_1)$ and any vertex $w \in V(T_1)$ such that $h_T(u) = h_T(w) = j$, we claim that

$$d_T(w) \geq d_T(u). \tag{3.1}$$

To see (3.1), first note that

$$\varepsilon_T(w) = \max\{j + h', \varepsilon_{T_1}(w)\} \leq j + h = \varepsilon_T(u). \tag{3.2}$$

Suppose for a contradiction that $d_T(u) > d_T(w)$. Let $D = d_T(u) - d_T(w)$ and create a new tree, T', by removing D of the children $u_1, \ldots, u_D$ (and their descendants) of u, and attaching them to w. By doing this we maintain the level-degree sequence while switching the degrees of u and w (Figure 3.6). In other words,

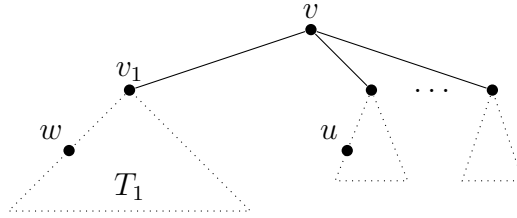$$T' = T - uu_1 - uu_2 - \ldots - uu_D + wu_1 + wu_2 + \ldots + wu_D.$$

Figure 3.6: The tree T, vertices $u \in V(T - T_1)$ and $w \in V(T_1)$.

Now from T to T', we have

- $\varepsilon_{T'}(u) = \varepsilon_T(u)$;

- $\varepsilon_T(x) \geq \varepsilon_{T'}(x)$ for all $x \in V(T)$, hence

$$\sigma_{T'}(x) = \frac{f(d_{T'}(x))}{g(\varepsilon_{T'}(x))} \geq \frac{f(d_T(x))}{g(\varepsilon_T(x))} = \sigma_T(x)$$

for any $x \in V(T) - \{u, w\}$;

- $\varepsilon_{T'}(w) \leq \varepsilon_T(w)$.

Consequently we have

$$\mathscr{E}(T') - \mathscr{E}(T) = \sigma_{T'}(u) + \sigma_{T'}(w) - \sigma_T(u) - \sigma_T(w) + \sum_{x \in V(T) - \{u,w\}} \left(\sigma_{T'}(x) - \sigma_T(x)\right).$$

Since $\sigma_{T'}(x) - \sigma_T(x) \geq 0$ for any $x \in V(T) - \{u, w\}$, we now have

$$\mathscr{E}(T') - \mathscr{E}(T) \geq \frac{f(d_{T'}(u))}{g(\varepsilon_{T'}(u))} + \frac{f(d_{T'}(w))}{g(\varepsilon_{T'}(w))} - \frac{f(d_T(u))}{g(\varepsilon_T(u))} - \frac{f(d_T(w))}{g(\varepsilon_T(w))}$$

$$\geq \frac{f(d_T(w))}{g(\varepsilon_T(u))} + \frac{f(d_T(u))}{g(\varepsilon_T(w))} - \frac{f(d_T(u))}{g(\varepsilon_T(u))} - \frac{f(d_T(w))}{g(\varepsilon_T(w))}$$

$$= \left(f(d_T(w)) - f(d_T(u))\right)\left(\frac{1}{g(\varepsilon_T(u))} - \frac{1}{g(\varepsilon_T(w))}\right) \geq 0.$$

We have a contradiction if strict inequality holds. Otherwise, T and T' would both be optimal and we can replace T with T'. We may repeat this process (starting from vertices of smaller height) until we have an optimal tree where (3.1) holds for any $w \in V(T_1)$ and $u \in V(T - T_1)$ of the same height.

What (3.1) states, is that at the same level, the vertices on the left (in T_1) are of larger degrees than the vertices on the right (not in T_1). Next we show that the vertices at the same level, from left to right, are indeed from the largest to smallest. In other words, we will show that each of T_1 and $T - T_1$ is level greedy.

- For the tree $T - T_1$, let $u', w' \in V(T - T_1)$ such that w' and u' are at the same level and w' is to the left of u'. It is easy to see that

$$\varepsilon_T(w') = h + h(w') = h + h(u') = \varepsilon_T(u'). \tag{3.3}$$

If $d_{T-T_1}(w') \geq d_{T-T_1}(u')$ then we are done. Otherwise, if $d_{T-T_1}(w') < d_{T-T_1}(u')$, let $D' = d_{T-T_1}(u') - d_{T-T_1}(w')$ and create T'' by removing D' of the children $u'_1, \ldots, u'_{D'}$ (and their descendants) of u', and attaching them to w'. That is,

$$T'' = T - u'u'_1 - u'u'_2 - \ldots - u'u'_D + w'u'_1 + w'u'_2 + \ldots + w'u'_D.$$

Now the degrees of u' and w' are switched in T''. Since their eccentricities stay the same (so do any other pair of vertices at the same level in $T - T_1$, for the same reason as (3.3)), $\mathscr{E}(T'') = \mathscr{E}(T)$. Similar to before, repeating this process (starting from vertices of smaller height) leads to an optimal tree in which $T - T_1$ is level greedy.

- Now consider the tree T_1. For two vertices r and s at the same level, note that by (3.2) we see that

$$\varepsilon_{T_1}(r) \geq \varepsilon_{T_1}(s) \text{ if and only if } \varepsilon_T(r) \geq \varepsilon_T(s).$$

This allows us to apply the exact same argument as above to T_1 and finish the proof in an inductive manner.

$\square$

To reach our conclusion on greedy trees, we need to recall some previously established concepts and results. The *semi-regular property* was first introduced in [19], where a number of variations were presented. Below is one of them.

Definition 3.7 (Semi-regular Property [19])**.** *We say that a tree satisfies the semi-regular property if, given any path with non-leaf end vertices $u, v \in V(T)$, the set of subtrees $\{T_u^1, ..., T_u^a\}$ attached to u and the set of subtrees $\{T_v^1, ..., T_v^b\}$ attached to v (such that $v \notin T_u^i$ and $u \notin T_v^j$ holds for each i and j) satisfy either*

$$a \geq b \text{ and } \min\{|V(T_u^1)|, ..., |V(T_u^a)|\} \geq \max\{|V(T_v^1)|, ..., |V(T_v^b)|\}$$

or

$$b \geq a \;\; and \;\; \max\{|V(T_u^1)|, ..., |V(T_u^a)|\} \leq \min\{|V(T_v^1)|, ..., |V(T_v^b)|\}.$$

It was also shown in [19], that a tree with a given degree sequence that satisfies the semi-regular property must be a greedy tree.

Theorem 3.8 ([19])**.** *A tree with a given degree sequence with the semi-regular property is a greedy tree.*

On the other hand, it was shown, in [16], that if the optimal tree, with any given level-degree sequence, is level-greedy, then the optimal tree must satisfy the semi-regular property.

Theorem 3.9 ([16])**.** *If the optimal tree is level-greedy (when given the level-degree sequence), then the optimal tree (when given the degree sequence) must satisfy the semi-regular property.*

Hence Theorems 3.9 and 3.8, along with Theorem 3.6, imply the following:

Theorem 3.10. *Among trees with a given degree sequence, the greedy tree maximizes $\mathscr{E}_{\nearrow}(T)$ and minimizes $\mathscr{E}_{\searrow}(T)$.*

3.4 Comparison between extremal trees of different degree sequences

In this section we compare the greedy trees of different degree sequences with respect to $\mathscr{E}_{\nearrow}(T)$ and $\mathscr{E}_{\searrow}(T)$. To do this we first define a partial ordering on the set of degree sequences of trees on a given number of vertices.

Definition 3.11 (Majorization)**.** *Given two nonincreasing degree sequences π and π' with $\pi = (d_1, d_2, ..., d_n)$ and $\pi' = (d_1', d_2', ..., d_n')$, we say that π' majors π if the following conditions are met:*

- $\sum_{i=0}^k d_i \leq \sum_{i=0}^k d_i'$ for $1 \leq k \leq n-1$

- $\sum_{i=0}^n d_i = \sum_{i=0}^n d_i'$

We denote this by $\pi \lhd \pi'$.

For example, for $\pi = (5, 5, 4, 4, 3, 3, 2, 1, ..., 1)$ and $\pi' = (5, 5, 5, 4, 3, 3, 2, 1, ..., 1)$ we have $\pi \lhd \pi'$. The following observation allows us to only compare "adjacent degree sequences".

Proposition 3.12 ([25]). *Let $\pi = (d_0, ..., d_{n-1})$ and $\pi' = (d_0', ..., d_{n-1}')$ be two noincreasing graphical degree sequences. If $\pi \lhd \pi'$, then there exists a series of graphical degree sequences $\pi_1, ..., \pi_k$ such that $\pi \lhd \pi_1 \lhd ... \lhd \pi_k \lhd \pi'$, where π_i and π_{i+1} differ at exactly two entries, say d_j (d_j') and $d_k(d_k')$ of $\pi_i(\pi_{i+1})$, with $d_j' = d_j + 1, d_k' = d_k - 1$ and $j < k$.*

We are now ready to present our main theorem of the section, which belongs to a class of "majorization results" that have shown to be very useful in the study of extremal problems.

Theorem 3.13. *Given two degree sequences (for trees) π and π' such that $\pi \lhd \pi'$. If*

$$f(x+1) - f(x) > f(y) - f(y-1)$$

when $x \geq y$, we have

$$\mathscr{E}_{\nearrow}(T_\pi^*) \leq \mathscr{E}_{\nearrow}(T_{\pi'}^*)$$

and

$$\mathscr{E}_{\searrow}(T_\pi^*) \geq \mathscr{E}_{\searrow}(T_{\pi'}^*)$$

where T_α^* denotes the greedy tree with the degree sequence α.

Proof. Again we only consider the case of $\mathscr{E}(T) := \mathscr{E}_{\nearrow}(T)$.

We want to show that $\mathscr{E}(T_\pi^*) \leq \mathscr{E}(T_{\pi'}^*)$ where $\pi = (d_0, ..., d_{n-1})$ and $\pi' = (d'_0, ..., d'_{n-1})$ such that $\pi \lhd \pi'$. By Proposition 3.12 we may assume that π and π' differ at only two entries, say d_j (d'_j) and d_k (d'_k) with $d'_j = d_j + 1, d'_k = d_k - 1$ for some $j < k$.

Let u and v be vertices of T_π^* such that the degrees of u and v are d_j and d_k respectively. Also let w be a child of v. We construct a new tree, $T_{\pi'}$, by moving w (and all its descendants) from its parent, v, to u (see Figure 3.7). In other words
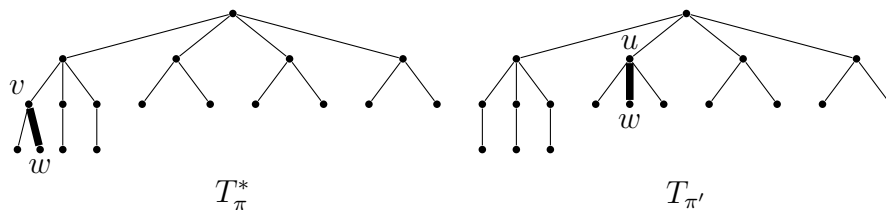
$$T_{\pi'} = T_\pi^* - vw + uw.$$

Figure 3.7: $\pi = (4, 4, 3, 3, 3, 3, 2, 2, 1, \ldots, 1)$ and $\pi' = (4, 4, 4, 3, 3, 2, 2, 2, 1, \ldots, 1)$.

By Theorem 3.10, $\mathscr{E}(T_{\pi'}^*) \geq \mathscr{E}(T_{\pi'})$. To prove $\mathscr{E}_{\nearrow}(T_\pi^*) \leq \mathscr{E}_{\nearrow}(T_{\pi'}^*)$ it suffices to show $\mathscr{E}_{\nearrow}(T_\pi^*) \leq \mathscr{E}_{\nearrow}(T_{\pi'})$. First note that

$$\varepsilon_{T_{\pi'}}(x) \leq \varepsilon_{T_\pi^*}(x) \text{ for all } x \in V(T_\pi^*).$$

Since $d_{T_{\pi'}}(x) = d_{T_\pi^*}(x)$ for any $x \in V(T_\pi^*) - \{u, v\}$, we have

$$\sigma_{T_{\pi'}}(x) \geq \sigma_{T_\pi^*}(x) \text{ for any } x \in V(T_\pi^*) - \{u, v\}.$$

Now we have

$$\mathscr{E}(T_{\pi'}) - \mathscr{E}(T_{\pi}^{*}) = (\sigma_{T_{\pi'}}(v) - \sigma_{T_{\pi}^{*}}(v)) + (\sigma_{T_{\pi'}}(u) - \sigma_{T_{\pi}^{*}}(u))$$

$$+ \left(\sum_{x \in V(T_{\pi}^{*}) - \{u,v\}} \sigma_{T_{\pi'}}(x) - \sum_{x \in V(T_{\pi}^{*}) - \{u,v\}} \sigma_{T_{\pi}^{*}}(x) \right)$$

$$\geq (\sigma_{T_{\pi'}}(v) - \sigma_{T_{\pi}^{*}}(v)) + (\sigma_{T_{\pi'}}(u) - \sigma_{T_{\pi}^{*}}(u))$$

Noting that $d_{T_{\pi'}}(v) = d_{T_{\pi}^{*}}(v) - 1$ and $d_{T_{\pi'}}(u) = d_{T_{\pi}^{*}}(u) + 1$, we have

$$\mathscr{E}(T_{\pi'}) - \mathscr{E}(T_{\pi}^{*}) \geq (\sigma_{T_{\pi'}}(v) - \sigma_{T_{\pi}^{*}}(v)) + (\sigma_{T_{\pi'}}(u) - \sigma_{T_{\pi}^{*}}(u))$$

$$= \frac{f(d_{T_{\pi'}}(v))}{g(\varepsilon_{T_{\pi'}}(v))} - \frac{f(d_{T_{\pi}^{*}}(v))}{g(\varepsilon_{T_{\pi}^{*}}(v))} + \frac{f(d_{T_{\pi'}}(u))}{g(\varepsilon_{T_{\pi'}}(u))} - \frac{f(d_{T_{\pi}^{*}}(u))}{g(\varepsilon_{T_{\pi}^{*}}(u))}$$

$$= \frac{f(d_{T_{\pi}^{*}}(v) - 1)}{g(\varepsilon_{T_{\pi}^{*}}(v))} - \frac{f(d_{T_{\pi}^{*}}(v))}{g(\varepsilon_{T_{\pi}^{*}}(v))} + \frac{f(d_{T_{\pi}^{*}}(u) + 1)}{g(\varepsilon_{T_{\pi}^{*}}(u))} - \frac{f(d_{T_{\pi}^{*}}(u))}{g(\varepsilon_{T_{\pi}^{*}}(u))}$$

$$= \frac{f(d_{T_{\pi}^{*}}(u) + 1) - f(d_{T_{\pi}^{*}}(u))}{g(\varepsilon_{T_{\pi}^{*}}(u))} - \frac{f(d_{T_{\pi}^{*}}(v)) - f(d_{T_{\pi}^{*}}(v) - 1)}{g(\varepsilon_{T_{\pi}^{*}}(v))}$$

$$\geq 0.$$

$\square$

3.5 Applications

In this section we briefly comment on potential applications of our results. Letting $f(x) = 1$ and $g(x) = \frac{1}{x}$, we have

$$\mathscr{E}_{\searrow}(T) = \sum_{v \in V(T)} \varepsilon_T(v)$$

being minimized by the greedy tree and maximized by the greedy caterpillar among all trees of a given degree sequence. This is consistent with the findings in [18].

Similarly, if $f(x) = 1$ and $g(x) = \frac{1}{x^2}$,

$$\mathscr{E}_{\searrow}(T) = \sum_{v \in V(T)} \varepsilon_T^2(v)$$

is known as the first Zagreb eccentricity index [10, 20].

And of course, when $f(x) = g(x) = x$ we have the original connective eccentricity index

$$\mathscr{E}_{\nearrow}(T) = \sum_{v \in V(T)} \frac{d_T(v)}{\varepsilon_T(v)}.$$

The importance of Theorem 3.10 and Theorem 3.13 lies in the fact that many extremal results on different classes of trees follow as immediate corollaries. These corollaries are the same as the ones found in Section 2.3. One may see [37] for an example of such applications.

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