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Extremal Trees with Respect to Functions on Adjacent Vertex Degrees*

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Abstract

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

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

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

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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 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 [3, 4, 7, 8, 11, 17] 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* [11]

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

This concept can be naturally generalized to

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

for $\alpha \neq 0$, also known as the *connectivity index* (see for example [5]). 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 [9], trees with restricted degrees [12] and trees with given *degree sequence* (the non-increasing sequence of degrees of internal vertices) [5, 14] have been characterized over the years.

Natural variations of $R(T)$ and $w_\alpha(T)$ were brought forward as the *sum-connectivity index* [25]

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

and the *general sum-connectivity index* [26]

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

Many interesting mathematical properties on these two indices, including some extremal results, can be found in [25, 26] and the studies that follow.

Another variant of $R(T)$ was proposed more recently, as the *harmonic index* [7]

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

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 [24].

Other examples of such graph invariants includes the *third Zagreb index* [13], defined as

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

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* [10], defined as

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

Last but certainly not the least, the *Atom-Bond connectivity index* [6], defined as

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

is a rather complicated example of such graph invariants that has recently received much attention (for example, see [23]).

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 1 (Greedy Tree) *[15] 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 $deg(v_{11}) \geq deg(v_{12}) \geq \ldots$;

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 $deg(v_{11}) \geq deg(v_{12}) \geq \ldots$, 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 1 shows an example of a greedy tree.

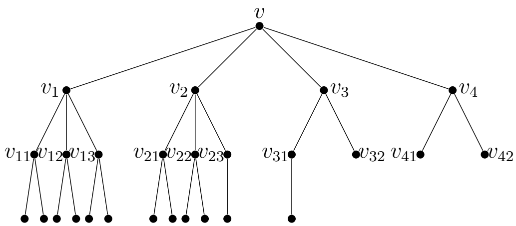

Figure 1. A greedy tree with degree sequence $(4, 4, 4, 3, 3, 3, 3, 3, 3, 3, 2, 2, 1, \ldots, 1)$.

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

$$f(a, b) + f(c, d) \geq f(c, b) + f(a, d) \text{ for any } a \geq c \text{ and } b \geq d. \tag{1}$$

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

$$R_f(T) = \sum_{uv \in E(T)} f(deg(u), deg(v)). \tag{2}$$

It is worth pointing out that (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 [15].

Theorem 1.1 *[15] For any escalating function f and $R_f(T)$ defined as in (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

$$f(a, b) + f(c, d) \leq f(c, b) + f(a, d) \text{ for any } a \geq c \text{ and } b \geq d. \tag{3}$$

Theorem 1.2 *[15] For any de-escalating function f and $R_f(T)$ defined as in (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 note. Majorization techniques is a fruitful method for localizing graph topological indicators and there is a wide literature (for example see [1, 2, 20–22] etc.) about this topic.

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

Definition 2 (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:*

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

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

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

For example: Let $\pi = (5, 5, 4, 4, 3, 3, 2, 1, ..., 1)$ 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 1.3 *[16] 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 note, 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 Main result

In this section we prove our main result, stated in Theorems 2.1 and 2.2.

Theorem 2.1 *Given two degree sequences* π *and* π' *with* $\pi \triangleleft \pi'$. *Let* T^*_π *and* $T^*_{\pi'}$ *be the greedy trees with degree sequences* π *and* π' *respectively. For an escalating function* f *with*

$$\frac{\partial f}{\partial x} \geq 0 \tag{4}$$

and

$$\frac{\partial^2 f}{(\partial x)^2} \geq 0, \tag{5}$$

we have

$$R_f(T^*_\pi) \leq R_f(T^*_{\pi'}).$$

Proof. Given the conditions (1), (4) and (5), we want to show

$$R_f(T^*_\pi) \leq R_f(T^*_{\pi'})$$

for

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

By Proposition 1.3 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. Note that $T_{\pi'}$ has degree sequence π' but is not necessarily a greedy tree.

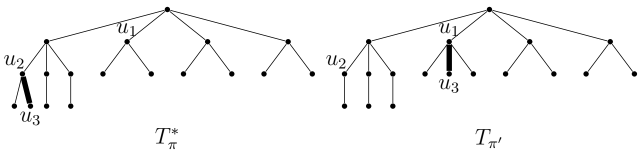

Figure 2. $\pi = (4,4,3,3,3,3,2,2,1,\ldots,1)$ and $\pi' = (4,4,4,3,3,2,2,2,1,\ldots,1)$.

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_2u_3 to u_1u_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

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

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

$$(f(\mathcal{A}+1,\mathcal{D}_1) - f(\mathcal{C},\mathcal{D}_1)) \tag{6}$$
$$+((f(\mathcal{A}+1,\mathcal{B}) - f(\mathcal{A},\mathcal{B})) - (f(\mathcal{C},\mathcal{D}) - f(\mathcal{C}-1,\mathcal{D}))) \tag{7}$$
$$+\left(\sum_{i=1}^{\mathcal{A}-1}(f(\mathcal{A}+1,\mathcal{B}_i) - f(\mathcal{A},\mathcal{B}_i)) - \sum_{j=2}^{\mathcal{C}-1}(f(\mathcal{C},\mathcal{D}_j) - f(\mathcal{C}-1,\mathcal{D}_j))\right). \tag{8}$$

Next we consider each of these three terms (6), (7), and (8).

- First note that

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

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

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 (6), (7) and (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 1.1. Therefore

$$R_f(T^*_\pi) \leq R_f(T_{\pi'}) \leq R_f(T^*_{\pi'}).$$

■

Remark 1 *Note that, as in condition* (1)*, the discrete version of the conditions* (4) *and* (5) *would be sufficient for our argument. We state Theorem 2.1 with* $\frac{\partial f}{\partial x}$ *and* $\frac{\partial^2 f}{(\partial x)^2}$ *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 2.2 *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*

$$\frac{\partial f}{\partial x} \leq 0 \tag{9}$$

and

$$\frac{\partial^2 f}{(\partial x)^2} \leq 0, \tag{10}$$

we have

$$R_f(T^*_\pi) \geq R_f(T^*_{\pi'}).$$

3 General extremal structures

First we assume the function f to be escalating and satisfies conditions (4), (5), and that $R_f(.)$ is defined as in (2). We now immediately have the following consequences. We include a brief proof for each of them for completeness.

Corollary 3.1 *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 1.1 and 2.1. ■

Corollary 3.2 *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 1.1 and 2.1. ■

Corollary 3.3 *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 1.1 and 2.1. ■

Corollary 3.4 *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 1.1 and 2.1.

■

Corollary 3.5 *Among all trees of order n with matching number β and degree sequence $(n - \beta, 2, \ldots, 2, 1, \ldots, 1)$ 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 1.1 and 2.1. ■

Remark 2 *Of course, it is easy to see the analogues of the above statements for de-escalating functions satisfying conditions* (9) *and* (10). *We omit the exact statements here.*

4 Applications

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

4.1 Connectivity index

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

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

is the connectivity index, a natrual 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 1.1 holds.

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

Theorem 4.1 ([12, 14]) *Among trees with given degree sequence, the connectivity index is maximized (minimized) by the greedy tree for* $\alpha > 0$ ($\alpha < 0$).

Remark 3 *Furthermore, if* $\alpha > 1$*, it is easy to verify* (4) *and* (5). *Consequently Theorem 2.1 holds and the corresponding corollaries in Section 3 hold.*

4.2 General Sum-connectivity index and the third Zagreb index

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

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

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 1.1.

Theorem 4.2 *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 4 *Furthermore, if* $\alpha \geq 0$*, it is easy to verify* (4) *and* (5) *for* $f(x,y) = (x+y)^{\alpha}$*. Therefore Theorem 2.1 applies (when* $\alpha \geq 1$ *and* $f(x,y)$ *is escalating) and the corresponding corollaries in Section 3 hold.*

Remark 5 *Noting that the third Zagreb index is a special case of the general sum-connectivity index with* $\alpha = 2$*. Both Theorems 1.1 and 2.1, and their consequences from Section 3 apply. We skip the exact statements.*

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

4.3 Reformulated Zagreb index

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

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

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 1.1 holds.

Theorem 4.3 *Among trees with given degree sequence, the reformulated Zagreb index is maximized by the greedy tree.*

Remark 6 *Furthermore, it is easy to verify (4) and (5) for* $f(x,y) = (x+y-2)^2$ *. Therefore Theorem 2.1 applies and the corresponding corollaries in Section 3 hold.*

4.4 Atom-Bond connectivity index

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

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

is perhaps one of the most complicated graph invariants defined on adjacent vertex degrees. In [18] 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 4.1 *For all positive integers c and d,*

$$f(c+1,d+1) + f(c,d) \leq f(c,d+1) + f(c+1,d). \tag{11}$$

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

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

Hence (11) holds. ∎

Lemma 4.2 *For any nonnegative integer k and positive integers c, d,*

$$f(c+k, d+1) + f(c, d) \leq f(c, d+1) + f(c+k, d). \tag{12}$$

Proof. Through repeated applications of (11), we have

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

So (12) holds. ■

Proposition 4.4 *The function $f(x, y) = \sqrt{\frac{x+y-2}{xy}}$ is de-escalating on $\mathbb{N} \times \mathbb{N}$.*

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

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

Let $a = c+k$ and $b = d+r$ with nonnegative integers k, r. Through repeated applications of (12), we have

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

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

By Proposition (4.4) and Theorem 1.1, we have the following statement.

Theorem 4.5 *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 (9) and (10) do not both hold in order to apply Theorem 2.2.

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.

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