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Functions on Adjacent Vertex Degrees of Trees with Given Degree Sequence

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Communication

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Abstract: In this note we consider a discrete symmetric function $f(x, y)$ where

$$f(x, a) + f(y, b) \geq f(y, a) + f(x, b) \qquad \text{for any } x \geq y \text{ and } a \geq b,$$

associated with the degrees of adjacent vertices in a tree. The extremal trees with respect to the corresponding graph invariant, defined as

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

are characterized by the "greedy tree" and "alternating greedy tree". This is achieved through simple generalizations of previously used ideas on similar questions. As special cases, the already known extremal structures of the Randić index follow as corollaries. The extremal structures for the relatively new sum-connectivity index and harmonic index also follow immediately, some of these extremal structures have not been identified in previous studies.

MSC: 05C05, 05C07, 05C35

Keywords: Degrees • Function • Index • Trees

1. Introduction

Graph invariants known as topological indices are frequently used in applied mathematics, biochemistry and other related fields to describe the structure of an object. The values of these indices often have close correlation with various properties (for example, the boiling point or surface pressure of a chemical compound) of the objects under consideration.See for instance [1, 2, 4, 5, 7, 12] for some of such applications. Among them, a group of indices defined

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in terms of the degrees of adjacent vertices have been studied extensively. The goal of this note is to provide a general characterization for the extremal structures with respect to such indices defined for a particular type of functions.

In this note we restrict our attention to trees with given *degree sequence* (the nonincreasing sequence of internal vertex degrees). For such a tree T, the most well known such index is probably the *Randić index* [7]

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

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 [3]). 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 these indices) for trees in general [6], trees with restricted degrees [8] and trees with given degree sequence [3, 10] have been characterized over the years.

A natural variation of $R(T)$ was named the *sum-connectivity index* [16]

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

and the *general sum-connectivity index* [17]

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

Many interesting mathematical properties of these two indices, including some extremal results, can be found in [16, 17].

Another variant of $R(T)$ is the *harmonic index* [4]

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

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 [15].

A fundamental question in the study of such invariants asks for the extremal structures under certain constraints that maximize or minimize a topological index. As mentioned above, some of such extremal structures have been characterized regarding the aforementioned indices. In this note, we point out that these indices can be described in a general way and the corresponding extremal structures can be characterized through a unified approach.

This is achieved by generalizing the approaches taken on previous related questions and considering a symmetric bivariate function $f(x, y)$ (defined on $\mathbb{N}\times\mathbb{N}$) such that

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

Furthermore, strict inequality is implied if both conditions are strict. For a tree T, let the *connectivity function* associated with f be

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

Noting 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 $H(T)$, $w_\alpha(T)$ for any α, and $\chi_\alpha(T)$ for $\alpha > 1$ or $\alpha < 0$. For $0 < \alpha < 1$, $\chi_\alpha(T)$ can be discussed in a similar way as in the rest of this note, only with reversed extremal structures (i.e., the extremal tree maximizing $\chi_\alpha(T)$ for $\alpha > 1$ or $\alpha < 0$ is a minimizing tree for $\chi_\alpha(T)$ for $0 < \alpha < 1$ and vice versa). We will show the following, that among trees of given degree sequence, $R_f(T)$ is maximized by the *greedy trees* (Definition 2.1) in Section 2 and minimized by the *alternating greedy trees* (Definition 3.1) in Section 3.

Theorem 1.1.

For any function f satisfying (1) and $R_f(T)$ defined as in (2), $R_f(T)$ is maximized by the greedy tree and minimized by an alternating greedy tree among trees with given degree sequence.

2. Greedy trees

Greedy trees have been shown to be extremal with respect to many other graph invariants among trees of a given degree sequence (see, for instance, [9, 11, 13, 14]). With respect to invariants based on adjacent degrees, some extremal structures were obtained before but surprisingly not all.

Definition 2.1 (Greedy trees).

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 $v_1, v_2, \ldots$, assign the largest degrees available to them such that $\deg(v_1) \geq \deg(v_2) \geq \cdots$;

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

(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.

For example, Figure 1 shows a greedy tree with degree sequence $(4, 4, 4, 3, 3, 3, 3, 3, 3, 3, 2, 2)$.

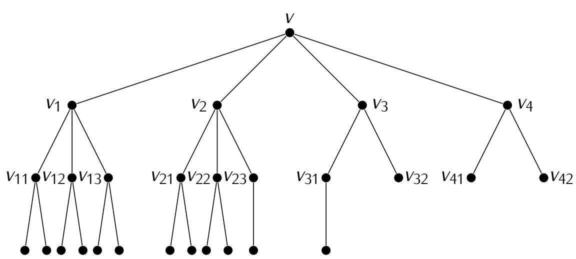

Figure 1. A greedy tree

Particularly interesting to our study, the weight $w_1(T)$ has been shown to be maximized by the greedy tree [3] and it was pointed out that the technique there can be easily modified to show that $R(T)$ or $w_\alpha(T)$ for negative α are maximized by the greedy trees among trees with a given degree sequence [10].

We provide a brief proof for the extremality of the greedy tree with respect to general $R_f(T)$. For this purpose we consider a longest path in the extremal tree T, labeled as $P(v_0, v_{t+1}) = v_0 v_1 \ldots v_t v_{t+1}$ with v_0 and v_{t+1} being leaves. Let

T_i $(i = 1, \dots, t)$ denote the connected components containing v_i in $T - E(P(v_0, v_{t+1}))$. Note that the order of T_i's does not affect the contribution of any edge (to $R_f(T)$) not on $P(v_0, v_{t+1})$. The following statement and its proof are rather similar to those in [11], we provide a slightly simplified argument.

Lemma 2.2.
For a tree with given degree sequence that maximizes $R_f(T)$ and $s \le (t+1)/2$, there is an extremal tree that satisfies

$$deg(v_s) \le deg(v_{t+1-s}) \le deg(v_k) \text{ for } s \le k \le t+1-s. \tag{3}$$

Proof. Let v_k be the vertex with the largest degree on this path, without loss of generality, one can assume that

$$deg(v_{k-1}) \le deg(v_{k+1}) \le deg(v_k).$$

First note that the establishment of

$$deg(v_{k-i}) \le deg(v_{k+i})$$

and

$$deg(v_{k+i}) \ge deg(v_{k+i+1})$$

will imply (3) and automatically place v_k as the middle vertex of the path $P(v_0, v_{t+1})$. Suppose (for contradiction) that (3) does not hold.

(1) Let i be the smallest value such that

$$deg(v_{k-i}) \le deg(v_{k+i})$$

does not hold. Then we have

$$deg(v_{k-i}) > deg(v_{k+i}) \text{ and } deg(v_{k-i+1}) \le deg(v_{k+i-1}).$$

Consider the tree

$$T' = T - \{v_{k-i}v_{k-i+1}\} - \{v_{k+i}v_{k+i-1}\} + \{v_{k+i}v_{k-i+1}\} + \{v_{k-i}v_{k+i-1}\}$$

as in Figure 2. From T to T', the value of $f(.,.)$ stay the same for all other pairs of adjacent vertex degrees except for the pairs $\{v_{k-i}, v_{k-i+1}\}, \{v_{k+i}, v_{k+i-1}\}$ in T and $\{v_{k+i}, v_{k-i+1}\}, \{v_{k-i}, v_{k+i-1}\}$ in T'. By the definition of $f(.,.)$, we have

$$\begin{aligned} &f(deg(v_{k-i+1}), deg(v_{k+i})) + f(deg(v_{k+i-1}), deg(v_{k-i})) \\ \ge &f(deg(v_{k-i+1}), deg(v_{k-i})) + f(deg(v_{k+i-1}), deg(v_{k+i})) \end{aligned}$$

and consequently

$$R_f(T') \ge R_f(T).$$

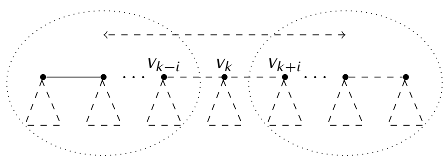

Figure 2. Case (1)

(2) Without loss of generality, let i be the smallest value such that

$$deg(v_{k+i}) \ge deg(v_{k+i+1})$$

does not hold. Note that $i \ge 1$.

(a) If $deg(v_{k+i+2}) < deg(v_{k+i+1})$, consider the tree

$$T' = T - \{v_{k+i}v_{k+i-1}\} - \{v_{k+i+2}v_{k+i+1}\} + \{v_{k+i}v_{k+i+2}\} + \{v_{k+i-1}v_{k+i+1}\}$$

as in Figure 3. Same argument as Case (1) shows that

$$R_f(T') > R_f(T).$$

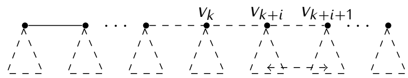

Figure 3. Case (2-a)

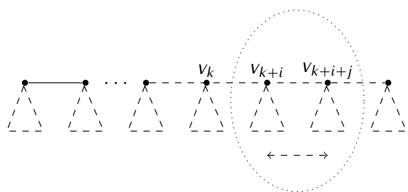

Figure 4. Case (2-b)

(b) More generally, if $deg(v_{k+i+2}) \geq deg(v_{k+i+1})$, let j be the largest value such that $deg(v_{k+i+j}) \geq deg(v_{k+i+j-1})$ (note that, since v_{t+1} is a leaf, we must have $deg(v_{t+1}) < deg(v_t)$). Then consider the tree

$$T' = T - \{v_{k+i}v_{k+i-1}\} - \{v_{k+i+j}v_{k+i+j+1}\} + \{v_{k+i}v_{k+i+j+1}\} + \{v_{k+i-1}v_{k+i+j}\}$$

as in Figure 4 and we have

$$R_f(T') \geq R_f(T).$$ □

Remark 2.3.
We did not need the strictness of inequalities as we only intend to show the extremality (but not unique extremality) of the greedy trees.

As established in the study of greedy trees for other graph invariants (see for instance [11]), Lemma 2.2 implies the extremality of the greedy tree among trees with given degree sequence.

3. Alternating greedy trees

Being much less known, the alternating greedy tree has only appeared (to our best knowledge) in the study of the Randić index [10] and was not formally defined. We repeat the definition here in the form of the algorithm to construct such a tree.

Definition 3.1 (Alternating greedy trees).
Given the nonincreasing degree sequence $(d_1, d_2, \ldots, d_m)$ of internal vertices, the alternating greedy tree is constructed through the following recursive algorithm:

(i) If $m-1 \le d_m$, then the alternating greedy tree is simply obtained by a tree rooted at r with d_m children, $d_m - m + 1$ of which are leaves and the rest with degrees $d_1, \ldots, d_{m-1}$;

(ii) Otherwise, $m-1 \ge d_m + 1$. We produce a subtree T_1 rooted at r with $d_m - 1$ children with degrees $d_1, \ldots, d_{d_{m-1}}$;

(iii) Consider the alternating greedy tree S with degree sequence $(d_{d_m}, \ldots, d_{m-1})$, let v be a leaf with the smallest neighbor degree. Identify the root of T_1 with v.

As an example (Figures 5, 6, 7), for the given degree sequence $(8, 7, 6, 6, 5, 5, 3, 3, 3, 2)$:

- T_1 is constructed with degrees $\{8, 2\}$ (as in (ii)), leaving the degree sequence $(7, 6, 6, 5, 5, 3, 3, 3)$ (as in (iii)) with the corresponding alternating greedy tree S_1;
- To construct S_1, T_2 is formed with degrees $\{7, 6, 3\}$, leaving the degree sequence $(6, 5, 5, 3, 3)$ with the corresponding alternating greedy tree S_2;
- To construct S_2, T_3 is formed with degrees $\{6, 5, 3\}$, leaving the degree sequence $(5, 3)$ to provide us the trivial S_3 (as in (i));
- Attaching T_3 to S_3 (i.e., identifying the root of T_3 with a leaf of S_3 whose neighbor has the smallest degree in S_3, as in (iii)) yields S_2;
- Then attaching T_2 to S_2 (i.e., identifying the root of T_2 with a leaf of S_2 whose neighbor has the smallest degree in S_2) yields S_1;
- In the final step, it is obvious that the two choices (two leaves of S_1 with the same neighbor degree) for attaching T_1 to S_1 yield two different such alternating greedy trees. Consequently, unlike the greedy trees, alternating greedy trees are not necessarily unique.

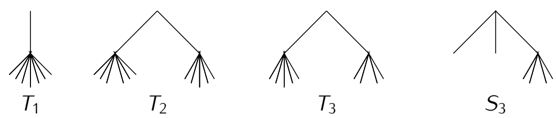

Figure 5. Construction of T_1, T_2, T_3, and S_3

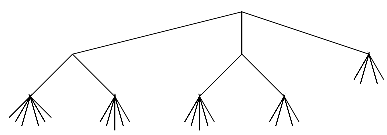

Figure 6. The alternating greedy tree S_1 from T_2, T_3 and S_3

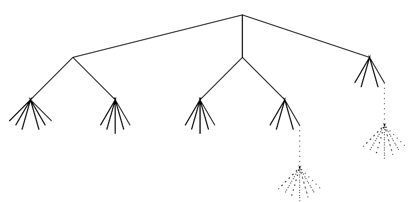

Figure 7. The alternating greedy trees T or T' from T_1 and S_1

To see that the alternating greedy trees minimize $R_f(T)$ among trees with given degree sequence, we again consider a longest path $P(v_0, v_{t+1}) = v_0 v_1 \ldots v_t v_{t+1}$ in an extremal tree and claim the following.

Lemma 3.2.
For the trees with given degree sequence that minimize $R_f(T)$ and $i \leq (t+1)/2$, there exists one such tree where

$$deg(v_i) \leq deg(v_{t+1-i}) \leq deg(v_k) \text{ for } i \leq k \leq t+1-i$$

if i is even; and

$$deg(v_i) \geq deg(v_{t+1-i}) \geq deg(v_k) \text{ for } i \leq k \leq t+1-i$$

if i is odd.

The proof follows from the same logic as that in [10] and details are similar to that of Lemma 2.2. We leave the proof out to keep this note short. It is not difficult to see that Lemma 3.2 implies the extremality of alternating greedy trees (not necessarily unique) [10].

4. Concluding remarks

We show the extremality of the greedy trees and alternating greedy trees with respect to the connectivity function $R_f(T)$ among trees with given degree sequence. This simple generalization, proved through similar techniques as before, answers the extremal questions with respect to a number of graph invariants. An interesting fact is that as long as the condition (1) is preserved, R_f is maximized by the greedy tree and minimized by the alternating greedy tree regardless of whether f is increasing or decreasing with respect to each variable.

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