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Extremal trees and their properties for Sigma index with fixed degree sequence

Fateme Movahedi
Department of Mathematics
Faculty of Sciences
Golestan University
Gorgan
Iran

Abstract

For a simple graph $\mathcal{A} = (V_{\mathcal{A}}, E_{\mathcal{A}})$ where $V_{\mathcal{A}}$ and $E_{\mathcal{A}}$ are the vertex set and the edge set, respectively, the Sigma index of $\mathcal{A}$ is defined as

$$\sigma(\mathcal{A}) = \sum_{xy \in E_{\mathcal{A}}} (\eta_x - \eta_y)^2,$$

where η_x denotes the degree of $x \in V_{\mathcal{A}}$.

In order to minimize and maximize the Sigma index among all trees, the extremal trees with fixed degree sequence are described in this study. The properties of the extremal trees are identified.

Subject Classification: *05C35, 05C09, 05C07.*

Keywords: *Extremal tree, Sigma index, Degree sequence.*

1. Introduction

Consider a simple, undirected graph $\mathcal{A} = (V_{\mathcal{A}}, E_{\mathcal{A}})$ with vertices $V_{\mathcal{A}} = \{v_1, \ldots, v_n\}$ and edges $E_{\mathcal{A}} = \{e_1, \ldots, e_m\}$. The neighborhood of a vertex $u \in V_{\mathcal{A}}$, symbolized by $N_{\mathcal{A}}(u)$, is the set comprising all vertices that share an edge with u. That is, $N_{\mathcal{A}}(u) = \{v \in v_{\mathcal{A}} | uv \in E_{\mathcal{A}}\}$.

The cardinality of the set of edges incident to a vertex u in graph $\mathcal{A}$ is represented by its degree, η_u. A vertex possessing a degree of one is termed a leaf. A vertex that is connected to a leaf is called a support vertex. The length of the shortest path between vertices u and v is the distance between them, represented by the symbol $d(u, v)$. We consider the tree obtained by deleting and

ORCID-ID: **0000-0001-7863-7915**

E-mail: **f.movahedi@gu.ac.ir**

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adding the edges $e_1, e_2, \dots, e_t$ as $T - \{e_1, e_2, \dots, e_t\}$ and $T + \{e_1, e_2, \dots, e_t\}$, respectively.

For a connected graph $\mathcal{A}$, an irregularity measure (IM) is a non-negative graph invariant. A graph $\mathcal{A}$ is regular if and only if its IM is zero. The Sigma index, one of the most well-known irregularity indicators, is described as [1, 2]

$$\sigma(\mathcal{A}) = \sum_{uv \in E_{\mathcal{A}}} (\eta_u - \eta_v)^2,$$

where η_x is the degree of the vertex $x \in E_{\mathcal{A}}$, respectively. For more literature, on the Sigma index, readers might refer to [2-8].

Recent research in graph theory is centered around extremal problems concerning topological indices. A recent work explored extremal trees with a prescribed degree sequence, focusing on the maximization (minimization) of the general Randic$'$ index for $\alpha < 0$ $(\alpha > 0)$.

In [9] the extremal trees for the first and second reformulated Zagreb indices are presented. In [10] a new algorithm is proposed to determine the extremal tree that maximizes the general Randic$'$ index for fixed degree sequence.

According to the minimizing and maximizing of the Sombor index, Movahedi [11] described the extremal trees with a specified degree sequence. The geometric-arithmetic index of trees was given an upper bound based on the order and domination number by Bermudo [12], who also categorized the extremal trees that reached this bound. For some most recent research on the extremal problems see [13-18].

Gutman et al. [2] studied connected graphs with a fixed order and maximum sigma index. [19] identifies the one graph with the highest sigma index out of all connected k-cyclic graphs. The following extreme problem with the Sigma index is examined in this work.

Problem: Determine the highest and lowest values of the sigma index by identifying and characterizing extremal trees with fixed degree sequences.

In a tree, a degree sequence $(\eta_1, \eta_2, \dots, \eta_k)$ is a decreasing sequence representing the degrees of the non-leaf vertices where $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_k \geq 2$. This paper focuses on trees that optimize the sigma index. We consider a tree to be extremal if it achieves the highest or lowest sigma index among all trees with the same vertex degrees.

2. Preliminaries

This section presents lemmas used to prove the main theorems. The following lemmas can be easily proved.

Lemma 2.1: *Suppose* $g(x, y) = (x - y)^2$ *where* $x, y \geq 1$. *If* $y \geq x$, *then* $g(x, 1) \leq g(y, 1)$.

Lemma 2.2: *Suppose* $f(x) = (x - \alpha)^2 - (x - \beta)^2$ *with* $x, \alpha, \beta \geq 1$. *Then the* $f(x)$ *is a decreasing function if* $\alpha \geq \beta$ *and an increasing function if* $\alpha \leq \beta$.

Lemma 2.3: *Suppose* $h(x) = (x-y)^2$ *with* $y \geq 1$. *Then, for every* $x \geq y$, $h(x)$ *is an increasing function, and for every* $x \leq y$, $h(x)$ *is a decreasing function.*

3. Properties of extremal trees for the Sigma index with fixed degree sequence

First, some properties of an extremal tree with the minimum Sigma index are stated.

Theorem 3.1: *Suppose* T *is a minimum optimal tree. Suppose* $P = v_1 v_2 \dots v_k$ *is a path in* T, *where* $k \geq 4$ *and* $\eta_{v_1} < \eta_{v_k}$. *Then* $\eta_{v_2} \leq \eta_{v_{k-1}}$.

Proof: We assume that, of the trees with the provided degree sequence $\mathcal{D}$, T has the lowest Sigma index. Assume for contradiction that $\eta_{v_2} > \eta_{v_{k-1}}$. We take $T' = T - \{v_1 v_2, v_{k-1} v_k\} + \{v_1 v_{k-1}, v_2 v_k\}$. Therefore, the degree sequence of T' and T is identical.

By applying Lemma 2.2 and since $\eta_{v_1} < \eta_{v_2}$, we have

$$\begin{aligned}\sigma(T') - \sigma(T) &= (\eta_{v_1} - \eta_{v_{k-1}})^2 + (\eta_{v_2} - \eta_{v_k})^2 - (\eta_{v_1} - \eta_{v_2})^2 - (\eta_{v_{k-1}} - \eta_{v_k})^2 \\ &= ((\eta_{v_2} - \eta_{v_k})^2 - (\eta_{v_{k-1}} - \eta_{v_k})^2) - ((\eta_{v_1} - \eta_{v_2})^2 - (\eta_{v_1} - \eta_{v_{k-1}})^2) \\ &= f(\eta_{v_k}) - f(\eta_{v_1}) < 0.\end{aligned}$$

This contradicts the minimality of T. Hence, $\eta_{v_2} \leq \eta_{v_{k-1}}$.

The following results are obtained by Theorem 3.1, as is in [10].

Corollary 3.2: *Suppose* T *is a minimum optimal tree. Then, no path* $P = v_1 v_2 \dots v_k$ *exists in the tree* T *for* $k \geq 3$, *in which* $\eta_{v_1}, \eta_{v_k} > \eta_{v_i}$ *for* $2 \leq i \leq k-1$.

Corollary 3.3: *Suppose* T *is a minimum optimal tree. No two non-adjacent edges* uv *and* $u'v'$ *in* T *such that* $\eta_u < \eta_{u'} \leq \eta_{v'} < \eta_v$.

We study properties of trees maximizing the sigma index for fixed degree sequence.

Theorem 3.4: *Consider* T *a maximum optimal tree. Let* $P = v_0 v_1 v_2 \cdots v_k v_{k+1}$ *be a path in* T, *where* v_0 *and* v_{k+1} *are leaves. For* $i+1 \leq j \leq k-i+1$ *and* $i \leq \frac{t+1}{2}$,

(i) $\eta_{v_i} \geq \eta_{v_{k-i+1}} \geq \eta_{v_j}$, for i odd,

(ii) $\eta_{v_i} \leq \eta_{v_{k-i+1}} \leq \eta_{v_j}$, for i even.

Proof: We assume that, of the trees with the provided degree sequence $\mathcal{D}$, T has the largest Sigma index. We use induction on i to demonstrate this result. Since $2 \leq j \leq k$, we demonstrate that $\eta_{v_1} \geq \eta_{v_k} \geq \eta_{v_j}$ for $i = 1$. For some $2 \leq j \leq$

k, assume for contradiction that $\eta_{v_1} < \eta_{v_j}$. We take $T' = T - \{v_0v_1, v_jv_{j+1}\} + \{v_0v_j, v_1v_{j+1}\}$. Clearly that T' has the degree sequence $\mathcal{D}$. By applying Lemmas 2.1, 2.2, 2.3, and $\eta_{v_{j+1}} > 1$,

$$\begin{aligned}\sigma(T') - \sigma(T) &= (\eta_{v_0} - \eta_{v_j})^2 + (\eta_{v_1} - \eta_{v_{j+1}})^2 - (\eta_{v_0} - \eta_{v_1})^2 - (\eta_{v_j} - \eta_{v_{j+1}})^2 \\ &= ((\eta_{v_j} - 1)^2 - (\eta_{v_1} - 1)^2) + ((\eta_{v_1} - \eta_{v_{j+1}})^2 - (\eta_{v_j} - \eta_{v_{j+1}})^2) \\ &= f(1) - f(\eta_{v_{j+1}}) > 0,\end{aligned}$$

This contradicts the minimality of T. Hence, $\eta_{v_1} \geq \eta_{v_j}$ for every $2 \leq j \leq k$. Analogously, we can deduce that $\eta_{v_1} \geq \eta_{v_k}$ and $\eta_{v_k} \geq \eta_{v_j}$. Consequently, $\eta_{v_1} \geq \eta_{v_k} \geq \eta_{v_j}$ where $2 \leq j \leq k$. We proceed by induction, assuming the claim holds for smaller values of i.

The induction hypothesis states that $\eta_{v_{i-1}} \geq \eta_{v_{k-i+1}} \geq \eta_{v_j}$ for $i+1 \leq j \leq k-i+1$ if $i \geq 2$ is even. Assume that for some $i+1 \leq j \leq k-i+1$, $\eta_{v_i} > \eta_{v_j}$ for contradiction. With the degree sequence $\mathcal{D}$, we choose $T'' = T - \{v_{i-1}v_i, v_jv_{j+1}\} + \{v_{i-1}v_j, v_iv_{j+1}\}$.

Using Lemma 2.2, since the induction hypothesis states that $d(v_{i-1}) \geq d(v_{j+1})$,

$$\begin{aligned}\sigma(T'') - \sigma(T) &= (\eta_{v_{i-1}} - \eta_{v_j})^2 + (\eta_{v_i} - \eta_{v_{j+1}})^2 - (\eta_{v_{i-1}} - \eta_{v_i})^2 - (\eta_{v_j} - \eta_{v_{j+1}})^2 \\ &= ((\eta_{v_{i-1}} - \eta_{v_j})^2 - (\eta_{v_{i-1}} - \eta_{v_i})^2) + ((\eta_{v_{j+1}} - \eta_{v_i})^2 - (\eta_{v_{j+1}} - \eta_{v_j})^2) \\ &= f(\eta_{v_{i-1}}) - f(\eta_{v_{j+1}}) > 0,\end{aligned}$$

This contradicts the minimality of T. Thus, $\eta_{v_i} \leq \eta_{v_j}$ for $i+1 \leq j \leq k-i+1$. Similarly, $\eta_{v_i} \leq \eta_{v_{k-i+1}}$ and $\eta_{v_{k-i+1}} \leq \eta_{v_j}$. Therefore, if i is even, then $\eta_{v_i} \leq \eta_{v_{k-i+1}} \leq \eta_{v_j}$ where $i+1 \leq j \leq k-i+1$. If $i > 2$ is odd, it follows from a similar technique, to obtain $\eta_{v_i} \geq \eta_{v_{k-i+1}} \geq \eta_{v_j}$.

Define L_i as the set of vertices neighboring a nearest leaf node, where the distance between them is i. Therefore, $L_0 = \{u \in V(T): \eta_u = 1\}$ and $L_1 = \{u \in V(T): u \text{ is a support vertex}\}$. Let d^m be the minimum degree of a support vertex, and L_1^m be the set of leaves adjacent to these minimum-degree support vertices. Let $\overline{L_1^m}$ be the remaining leaves. We construct a new tree T'_i by grafting the root of T_i onto a leaf in L_1^m.

Theorem 3.5: *If T'_1 and T'_2 are trees that were derived from T, then $\sigma(T'_1) \geq \sigma(T'_2)$ comes from finding the root v_i of T_i with $u' \in L_1^m$ and $v' \in \overline{L_1^m}$, respectively.*

Proof: Let u and v be respective next to u' and v'. Theorem 3.4 tells us that $d(u) \leq d(v)$. Consequently, we have

$$\begin{aligned}\sigma(T_1') - \sigma(T_2') &= ((n_{v_i}+1)-n_u)^2 + (n_u-1)^2 - ((n_{v_i}+1)-n_v)^2 + (n_v-1)^2 \\ &= (((n_{v_i}+1)-n_u)^2 - ((n_{v_i}+1)-n_v)^2) + ((n_u-1)^2 - (n_v-1)^2) \\ &= f(1) - f(n_{v_i}+1) > 0,\end{aligned}$$

Therefore, $\sigma(T'_1) \geq \sigma(T'_2)$. This completes the proof.

4. Characterizing the extremal trees for the Sigma index with fixed degree sequence

Wang [20] explored a more general form of topological index for a tree T, given by

$$R_f(T) = \sum_{uv \in E_T} f(\eta_u, \eta_v),$$

when f is a symmetric function that maps pairs of natural numbers to real numbers.

Theorem 4.1: [20] *Suppose* $f: \mathbb{N} \times \mathbb{N} \to \mathbb{R}$ *is a symmetric function and for* $y \leq x$ *and* $\alpha \geq \beta$,

$$f(x,\alpha) + f(y,\beta) \geq f(y,\alpha) + f(x,\beta). \quad (1)$$

Then Among trees with a fixed degree sequence, the greedy tree maximizes $R_f(T)$*, while the alternating greedy tree minimizes it.*

For the Sigma index with fixed degree sequence, we demonstrate that the trees produced by the Greedy algorithm are minimum optimal trees and the alternating greedy trees are the maximum optimal trees. First, we provide the greedy algorithm and the alternating greedy algorithm for constructing the optimal trees.

Greedy algorithm (Constructing a greedy tree)

Input In decreasing order, the non-leaf vertices' degree sequence is $\mathcal{D} = (\eta_1, \eta_2, \dots, \eta_m)$.

Output A tree having degree sequence $\mathcal{D}$.

1. Assign v to the root vertex with degree η_1.
2. Assign $v_1, v_2, \dots, v_{\eta_1}$ to the children of v such that $\eta_{v_i} = \eta_{i+1}$, for $1 \leq i \leq \eta_1$.
3. Assign $v_1^1, v_2^1, \dots, v_{\eta_2-1}^1$ to the children of v_1 (except v) such that $\eta_{v_i^1} = \eta_{\eta_1+i+1}$, for $1 \leq i \leq \eta_2 - 1$. Do the same for the vertices $v_2, v_3, \dots, v_{\eta_1}$, respectively.
4. For each newly labeled vertex, repeat step (3), always prioritizing the unlabeled neighbors of the vertex with the highest degree among the already labeled vertices.

Example 4.2: To illustrate the construction of a greedy tree with $\mathcal{D} = (5, 4, 3, 3, 2, 2, 2)$, we present an example. As shown in Figure 1, the greedy algorithm starts by choosing a root node of degree 5 and attaching child nodes with degrees 4, 3, 3, 2, and 2.

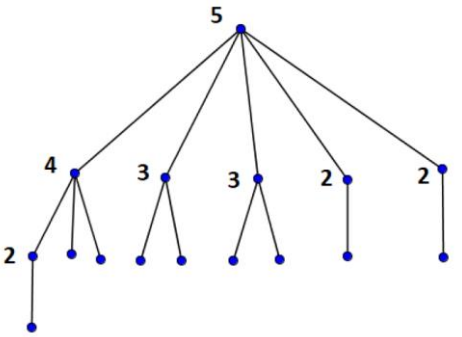

Figure 1
Optimal tree built using the greedy algorithm with $\mathcal{D} = (5, 4, 3, 3, 2, 2, 2)$.

In the following algorithm, the alternating greedy trees are constructed.

Alternating greedy algorithm. (Constructing an alternating greedy tree)
Input The degree sequence $D = (\eta_1, \eta_2, \dots, \eta_m)$ of the non-leaf vertices in descending order.
Output A tree having degree sequence $\mathcal{D}$.

1. Consider η_m.
   1.1 If $\eta_m \geq m - 1$, then tree T constructs by rooted at u with η_m children such that its children have degrees $\eta_1, \eta_2, \dots, \eta_{m-1}$ and $\eta_m - m + 1$ leaves adjacent to u.
   1.2 For $\eta_m \leq m - 2$, we construct subtree T_1 by rooted at u_1 with $\eta_m - 1$ children such that the degrees of its children are $\eta_1, \eta_2, \dots, \eta_{\eta_{m-1}}$ with $u_1 \in L_2$ and the children of u_1 are in L_1. Subtree T_2 is constructed by rooted at u_2 with $\eta_{m-1} - 1$ children whose their degrees are $\eta_{\eta_m}, \eta_{\eta_m+1}, \dots, \eta_{(\eta_m+\eta_{m-1}-2)}$. Similarly, we can get subtrees $T_3, T_4, \dots$ until T_k satisfies the condition of step (1.1). Therefore, we have $d(v_k) = \eta_{m-k+1}$.
2. Assign $i = k$ and $T = T_i$. Finding the root v_{i-1} with $v \in L_1^m$ creates a new tree T'_{i-1} from T and T_{i-1} rooted at v_{i-1}.
3. The tree T'_{i-1} is created from T and T_{i-1} using the same procedure as step (2) for $T = T_i$ and $i = k - 1, k - 2, \dots, 1$. Trees $T'_{k-2}, T'_{k-3}, \dots, T'_1$ are constructed.
4. Set $T = T'_1$ with $\mathcal{D} = (\eta_1, \eta_2, \dots, \eta_m)$.

Example 4.3: An alternating greedy tree with the degree sequence $\mathcal{D} = (5,4,3,3,2,2,2)$ is created in this example. Step (1.2) of the alternating greedy algorithm gives us the subset T_1, which has 1 child of degree 5. To create a new degree sequence $\mathcal{D} = (3,3,2)$ for the new degree sequence $\mathcal{D}_1 = (4,3,3,2,2)$, we build tree T_2 (Figure 2). The fact that $\mathcal{D}_2$ satisfies step (1.1) is readily apparent. In step (2), we attach subtrees T_1 to T'_2 to create the most optimal tree $T'_1 = T$ (Figure 4) and T_2 to T_3 to produce T'_2 (Figure 3).

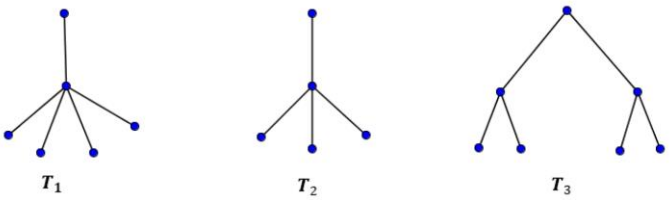

Figure 2
Construction of subtrees

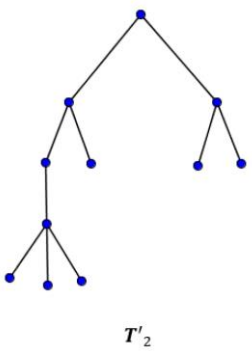

Figure 3
Attaching subtrees

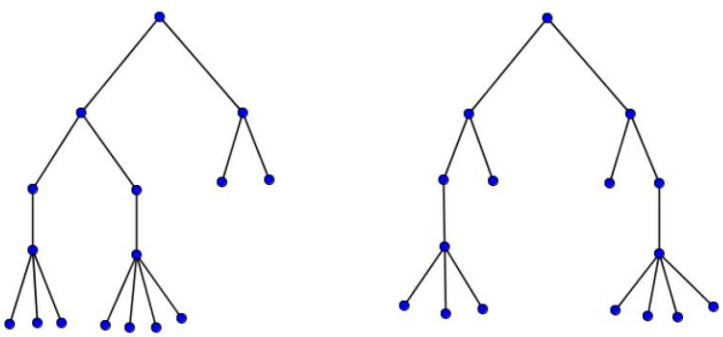

Figure 4
The alternating greedy trees with $\mathcal{D} = (5,4,3,3,2,2,2)$.

We show that the extremal trees with the provided degree sequence are constructed by the greedy algorithm and the alternating greedy algorithm.

Theorem 4.4: *For given degree sequence, the greedy tree and alternating greedy tree minimize and maximize, respectively, the Sigma index among trees.*

Proof: Consider T a tree with fixed degree sequence $\mathcal{D}$. Let $f(x,\alpha) = -(x-\alpha)^2$ and define $R_f(T) = -\sum_{uv\in E_T}(\eta_u - \eta_v)^2 = -\sigma(T)$. We show that the condition (1) holds for the function $f(x,\alpha)$.

We have that

$$\begin{aligned} & f(x,\alpha) + f(y,\beta) \geq f(y,\alpha) + f(x,\beta) \\ \Leftrightarrow \quad & -(x-\alpha)^2 - (y-\beta)^2 \geq -(y-\alpha)^2 - (x-\beta)^2 \\ \Leftrightarrow \quad & (x-\alpha)^2 + (y-\beta)^2 \leq (y-\alpha)^2 + (x-\beta)^2 \\ \Leftrightarrow \quad & 0 \leq \beta y - \alpha y + \alpha x - x\beta \\ \Leftrightarrow \quad & 0 \leq (y-x)(\beta-\alpha). \end{aligned}$$

The condition holds whenever $x \geq y$ and $\alpha \geq \beta$. Therefore, Theorem 4.1 holds for $R_f(T) = -\sigma(T)$ and consequently, the greedy tree minimizes $\sigma(T)$, but an alternating greedy tree among trees with a fixed degree sequence maximizes it.

Declaration of competing interest

The author declares no conflict of interest that could have influenced their research.

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