# Extremal trees with fixed degree sequence for $\sigma$-irregularity 

Darko Dimitrov ${ }^{1, *}$, Wei Gao ${ }^{2}$, Wenshui Lin ${ }^{3}$, Jinsong Chen ${ }^{4}$<br>${ }^{1}$ Faculty of Information Studies, Novo Mesto 8000, Slovenia<br>${ }^{2}$ School of Information Science and Technology, Yunnan Normal University, Kunming 650500, China<br>${ }^{3}$ School of Informatics, Xiamen University, Xiamen 361005, China<br>${ }^{4}$ School of Mathematics and Statistics, Fuzhou University, Fuzhou 350108, China

(Received: 28 May 2023. Received in revised form: 3 November 2023. Accepted: 6 November 2023. Published online: 27 November 2023.) © 2023 the authors. This is an open-access article under the CC BY (International 4.0) license (www.creativecommons.org/licenses/by/4.0/).


#### Abstract

A natural extension of the well-known Albertson irregularity of graphs is the so-called $\sigma$-irregularity. For a simple graph $G$, it is defined as $\sigma(G)=\sum_{u v \in E(G)}\left(d_{G}(u)-d_{G}(v)\right)^{2}$, where $d_{G}(v)$ denotes the degree of a vertex $v$ of $G$. In this study, we characterize trees with minimal and maximal $\sigma$-irregularity among trees with a given degree sequence. Specifically, we show that greedy trees minimize $\sigma$-irregularity, while adopting trees maximize it among trees with a prescribed degree sequence.


Keywords: irregularity (of graph); irregularity measures; $\sigma$-irregularity; extremal trees.
2020 Mathematics Subject Classification: 05C05, 05C07, 05C35, 05C75.

## 1. Introduction

Let $G$ be a simple undirected connected graph with $|V(G)|=n$ vertices and $|E(G)|=m$ edges. The degree of a vertex $v$ in $G$ is the number of edges incident with $v$ and it is denoted by $d_{G}(v)$. A graph $G$ is regular if all its vertices have the same degree, otherwise, it is irregular. Knowing how irregular a given graph is important in many applications and problems.

The imbalance of an edge $e=u v \in E$, defined as $\operatorname{imb}(e)=\left|d_{G}(u)-d_{G}(v)\right|$, appears implicitly in the context of Ramsey problems with repeat degrees [9], and later in the work of Chen, Erdős, Rousseau, and Schlep [12], where 2-colorings of edges of a complete graph were considered. In [8], Albertson defined the irregularity of $G$ as the sum of imbalances of all edges of a graph, i.e.,

$$
\operatorname{irr}(G)=\sum_{e \in E(G)} \operatorname{imb}(e)=\sum_{u v \in E(G)}\left|d_{G}(u)-d_{G}(v)\right| .
$$

For results on the Albertson irregularity, we refer the readers to [2, 4, 8, 18, 19].
To overcome certain shortcomings of the Albertson irregularity, as pointed out in [1], a new measure of irregularity of a graph, so-called the total irregularity of a graph, was defined as

$$
\operatorname{irr}_{\mathrm{t}}(G)=\frac{1}{2} \sum_{(u, v) \in V(G) \times V(G)}\left|d_{G}(u)-d_{G}(v)\right|
$$

Results of the total irregularity as well as a comparison between the irregularity and the total irregularity of a graph was studied in $[3,5,6,15,16,23]$. Trying to avoid the absolute value calculation in the Albertson irregularity, one naturally arrived at the irregularity measure $\sigma(G)$ introduced in [20] and defined as

$$
\sigma(G)=\sum_{u v \in E(G)}\left(d_{G}(u)-d_{G}(v)\right)^{2}
$$

In [7] graphs with maximal $\sigma$-irregularity were characterized. The inverse $\sigma$-irregularity problem was solved in [20]. $k$-cyclic graphs with maximal $\sigma$-irregularity were determined in [10]. For complete split-like graphs, which represent a broad subclass of bidegreed connected graphs, in [22] it was shown that for these graphs the equality $\sigma(G)=n^{2} \operatorname{Var}(G)$ holds. Here $\operatorname{Var}(G)$ is the variance of the vertex degrees of a graph $G$

$$
\begin{equation*}
\operatorname{Var}(G)=\frac{1}{n} \sum_{v \in V(G)} d_{G}(v)^{2}-\left(\frac{1}{n} \sum_{v \in V(G)} d_{G}(v)\right)^{2} \tag{1}
\end{equation*}
$$

[^0]another well-established irregularity measure also known as Bell's irregularity measure [11].
A sequence $\mathcal{D}=\left(d_{1}, d_{2}, \ldots, d_{n}\right)$ is graphical if there is a graph whose vertex degrees are $d_{i}, i=1, \ldots, n$. If in addition $d_{1} \geq d_{2} \geq \cdots \geq d_{n}$, then $\mathcal{D}$ is a degree sequence. In the rest of the paper we assume that the degrees of the pendent vertices are excluded from the degree sequence.

For a tree $T$ and $i=0,1, \ldots$, let $L_{i}=L_{i}(T)$ be the set of vertices in $T$, whose minimum distance from to the set of pendent vertices of $T$ is $i$. Clearly, $L_{0}$ is exactly the set of pendent vertices in $T$.

Lin, Gao, Chen, and Lin in [21], and Gan, Liu, and You in [17] introduced the so-called switching transformation when they studied the atom-bond connectivity index. Next, we present it in the context of $\sigma$-irregularity.

Proposition 1.1. Let $G=(V, E)$ be a connected graph with $u v, x y \in E(G)$ and $u y, x v \notin E(G)$. Let $H=G-u v-x y+u y+x v$. If $d(u) \geq d(x)$ and $d(v) \leq d(y)$, then $\sigma(H) \leq \sigma(G)$, with the equality if and only if $d(u)=d(x)$ or $d(v)=d(y)$.

Proof. The change of the $\sigma$-irregularity after the above transformation is

$$
\begin{aligned}
\Delta \sigma(H, G) & =\sigma(H)-\sigma(G) \\
& =(d(u)-d(y))^{2}+(d(x)-d(v))^{2}-(d(u)-d(v))^{2}-(d(x)-d(y))^{2} \\
& =2(d(u)-d(x))(d(v)-d(y)) \leq 0
\end{aligned}
$$

Observe that $H$ in the above proposition is not necessarily connected. As it was pointed out in [13], if $G$ is for example the path $v u w y x$, then $H$ is a disjoint union of $K_{3}$ and $K_{2} . H$ is disconnected only if in $G-u v-x y$ there is no $v-u, v-y$, $x-u$, or $x-y$ paths.

In the following two sections, we consider the trees with minimal and maximal $\sigma$-irregularity among trees with a given degree sequence. The results, and their corresponding proofs, presented there are close to those presented in [14], where trees of a given degree sequence that maximize the sum of the products of the degrees of adjacent vertices were determined. Related results concerning the Randić index, atom-bond connectivity index and Wiener index were presented in [24-26].

## 2. Trees with fixed degree sequence and minimal $\sigma$-irregularity

First, we prove some properties of the trees with minimum $\sigma$-irregularity. These lead to an algorithm that constructs a tree with minimum $\sigma$-irregularity, also known as a greedy tree.

Lemma 2.1. Let $T$ be a tree with minimum $\sigma$-irregularity among the trees with fixed degree sequence. Let $P=v_{1} v_{2} \ldots v_{t}$ be a path in $T$, where $t \geq 4$ and $d\left(v_{1}\right)<d\left(v_{t}\right)$. Then, $d\left(v_{2}\right) \leq d\left(v_{t-1}\right)$.

Proof. Assume that the claim of the proposition is not true and that $d\left(v_{2}\right)>d\left(v_{t-1}\right)$. Let $T^{\prime}$ be the tree obtained by deleting the edges $v_{1} v_{2}$ and $v_{t-1} v_{t}$, and adding the edges $v_{1} v_{t-1}$ and $v_{2} v_{t}$ to $T$. Notice that $T$ and $T^{\prime}$ have the same degree sequence. With the above relation of the degrees $d\left(v_{1}\right), d\left(v_{2}\right), d\left(v_{t-1}\right), d\left(v_{t}\right)$, applying Proposition 1.1, we get that $\sigma\left(T^{\prime}\right)-\sigma(T)<0$. This is a contradiction to the initial assumption that $T$ is a tree with minimum $\sigma$-irregularity.

As a consequence of Lemma 2.1, one can obtain the following three corollaries. The argument of the proof of the next corollary is adopted from [14].

Corollary 2.1. Let $T$ be a tree with minimum $\sigma$-irregularity among the trees with fixed degree sequence. Then there is no path $P=v_{1} v_{2} \ldots v_{t}$ in $T$ with $t \geq 3$ such that $d\left(v_{1}\right)>d\left(v_{i}\right)$ and $d\left(v_{t}\right)>d\left(v_{i}\right)$ for some $2 \leq i \leq t-1$.

Proof. We assume that the above claim is false and that there is a path $P=v_{1} v_{2} \ldots v_{t}$ in $T$ with $t \geq 3$, such that for some $2 \leq i \leq t-1$, the relations $d\left(v_{1}\right)>d\left(v_{i}\right)$ and $d\left(v_{t}\right)>d\left(v_{i}\right)$ hold. Also, it holds that $2 \leq d\left(v_{i}\right)$.

Firstly, consider the case when $d\left(v_{i}\right)<d\left(v_{i+1}\right)$. Let $P^{\prime}=v_{-k} v_{-k+1} \ldots v_{0} v_{1} \ldots v_{i} v_{i+1}$ be a path such that $d\left(v_{-k}\right)=1$. Note that $k \geq 0$, since $d\left(v_{1}\right)>d\left(v_{i}\right)$. By Lemma 2.1, $d\left(v_{-k}\right)<d\left(v_{i+1}\right)$ implies $d\left(v_{-k+1}\right) \leq d\left(v_{i}\right)$, and thus, $d\left(v_{-k+1}\right)<d\left(v_{i}\right)$. Again applying Lemma 2.1, $d\left(v_{-k+1}\right)<d\left(v_{i}\right)$ implies $d\left(v_{-k+2}\right) \leq d\left(v_{i}\right)$, and consequently $d\left(v_{-k+2}\right)<d\left(v_{i}\right)$. Repeating this argument, we obtain $d\left(v_{1}\right) \leq d\left(v_{i}\right)$, which is a contradiction to the initial assumption $d\left(v_{1}\right)>d\left(v_{i}\right)$.

Secondly, consider the case when $d\left(v_{i}\right)>d\left(v_{i+1}\right)$. Now, let $P^{\prime}=v_{i} v_{i+1} \ldots v_{t} v_{t+1} \ldots v_{t+k-1} v_{t+k}$ be a path such that $d\left(v_{t+k}\right)=1$. Applying repeatedly Lemma 2.1 as in the previous case, we obtain that $d\left(v_{i+1}\right) \geq d\left(v_{t+k-1}\right), \ldots, d\left(v_{i+1}\right) \geq d\left(v_{t}\right)$, and thus, $d\left(v_{i}\right)>d\left(v_{t}\right)$, a contradiction to the assumption $d\left(v_{i}\right)<d\left(v_{t}\right)$.

Finally, assume that $d\left(v_{i}\right)=d\left(v_{i+1}\right)$. Let $p$ be the smallest index larger than $i+1$ such that $d\left(v_{i}\right)>d\left(v_{p}\right)$ or $d\left(v_{i}\right)<d\left(v_{p}\right)$ is satisfied. Notice that if not before this is satisfied when $p=t$, namely then by the initial assumption $d\left(v_{i}\right)<d\left(v_{t}\right)$. Then, $d\left(v_{i}\right)=d\left(v_{p-1}\right)<d\left(v_{p}\right)$ or $d\left(v_{i}\right)=d\left(v_{p-1}\right)>d\left(v_{p}\right)$ and we can proceed as in one of the two previous cases, to obtain again a contradiction.

Corollary 2.2. Let $T$ be a tree with minimum $\sigma$-irregularity among the trees with fixed degree sequence. For every positive integer $d$, the vertices with degrees at least d induce a subtree of $T$.

Proof. Let $T^{\prime}$ be the graph induced by the vertices of degree at least $d$. Assume that $T^{\prime}$ is not a tree. Let $v_{i}$ and $v_{j}$ be two vertices that belong to different components of $T^{\prime}$. Consider the path $P$ between $v_{i}$ and $v_{j}$ in $T$. Since $v_{i}$ and $v_{j}$ belong to different components of $T^{\prime}$, there must exist a vertex $v_{k}$ in $P$ with $d\left(v_{k}\right)<d$. However, due to Corollary 2.1, it is not possible.

Corollary 2.3. Let $T$ be a tree with minimum $\sigma$-irregularity among the trees with fixed degree sequence. Then there are no two non-adjacent edges $v_{1} v_{2}$ and $v_{3} v_{4}$ such that $d\left(v_{1}\right)<d\left(v_{3}\right) \leq d\left(v_{4}\right)<d\left(v_{2}\right)$.

Proof. Having two edges $v_{1} v_{2}$ and $v_{3} v_{4}$, let consider the possible paths in $T$, which contain all vertices $v_{1}, v_{2}, v_{3}$, and $v_{4}$ and begin and end with one them. There are four such possibilities: $P_{1}=v_{1} v_{2} \ldots v_{3} v_{4}, P_{2}=v_{1} v_{2} \ldots v_{4} v_{3}, P_{3}=v_{2} v_{1} \ldots v_{3} v_{4}$, and $P_{4}=v_{2} v_{1} \ldots v_{4}, v_{3}$.

If there exist the path $P_{1}$, by the claim of the corollary, we have that $d\left(v_{1}\right)<d\left(v_{4}\right)$ and $d\left(v_{3}\right)<d\left(v_{2}\right)$. On the other hand, applying Lemma 2.1, it follows that $d\left(v_{2}\right) \leq d\left(v_{3}\right)$, which is a contradiction.

Similarly, contradictions can be shown if there exist paths $P_{2}, P_{3}$, and $P_{4}$.
By Corollary 2.2 the degrees of vertices of $T$ at level $L_{i}$ are not larger than the degrees of vertices at $L_{i+1}$ for all $i=0,1,2, \ldots$. Thus the vertices of larger degrees have farther distances from $L_{0}$ than the vertices of smaller degrees. It is not difficult to see that the tree $T$ with minimal $\sigma$-irregularity is not always uniquely determined up to isomorphism (see Figure 1 for an example). However, having the above properties one can efficiently construct a tree with minimal $\sigma$-irregularity, with the algorithm first proposed by Delorme et al. [10] and later generalized by Wang [24] and named the greedy algorithm. Now, by this algorithm, an extremal tree $T$ that achieves the minimum $\sigma$-irregularity among the trees with fixed degree sequence $\mathcal{D}=\left\{d_{1}, d_{2}, \ldots, d_{m}\right\}$ can be constructed as:

1. Label the vertex with the largest degree as $v$ (the root).
2. Label the neighbors of $v$ as $v_{1}, v_{2}, \ldots$, assign the largest degree available to them such that $d\left(v_{1}\right) \geq d\left(v_{2}\right) \geq \ldots$.
3. 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 $d\left(v_{11}\right) \geq d\left(v_{12}\right) \geq \ldots$, then do the same for $v_{2}, v_{3}, \ldots$.
4. Repeat 3 . for all newly labeled vertices, always starting with the neighbors of the labeled vertex with the largest degree whose neighbors are not labeled yet.

Theorem 2.1. Given the degree sequence, the greedy tree minimizes the $\sigma$-irregularity.
Proof. The greedy tree obviously satisfies Lemma 2.1 and Corollaries 2.1-2.3. However, there could be other trees for which these conditions hold (see Example 2.1). Now, we only show that the $\sigma$-irregularity of the greedy tree achieves the minimum among these trees. Let denote the greedy tree by $T$. Assume that $T$ does not minimize the $\sigma$-irregularity. Let $T^{\prime}$ be a rooted tree that has minimum $\sigma$-irregularity. Since $T^{\prime}$ is not a greedy tree, there are two vertices $v_{i}$ and $v_{k}$, with $d\left(v_{i}\right) \geq d\left(v_{k}\right)$ and $i>k$, such that $v_{i}$ has a child $v_{j}$ and $v_{k}$ has a child $v_{l}$, with $d\left(v_{k}\right) \leq d\left(v_{l}\right)$. We apply the switching transformation from Proposition 1.1 by deleting edges $v_{i} v_{j}$ and $v_{k} v_{l}$ and adding edges $v_{i} v_{l}$ and $v_{k} v_{i}$. Observe that after this transformation, the resulting tree remains connected since there is a path between $v_{i}$ and $v_{k}$. After this transformation, the $\sigma$-irregularity does not increases. We apply as many times the switching transformation as above until we obtain a greedy tree $T$. After all this transformations the $\sigma$-irregularity does not increase. Since $T^{\prime}$ is a tree with minimum $\sigma$-irregularity and the obtained greedy tree $T$ does not have larger $\sigma$-irregularity, it follows that the greedy tree has also minimum $\sigma$-irregularity.

Example 2.1. In Figure 1 two trees, which have maximum $\sigma$-irregularity among all trees with degree sequence $\mathcal{D}=$ $(5,5,5,4,3,3,3,2,2)$, are presented. The tree $T$ is obtained by the "greedy algorithm".

We would like to note that for a given degree sequence, the greedy tree, which achieves the minimum $\sigma$-irregularity also archived the minimum (general) Randić index for $\alpha<0$ [24], the minimum atom-bond connectivity index [17, 21, 25] and the minimum Wiener index [26].


Figure 1: Two extremal trees of degree sequence $\mathcal{D}=(5,5,5,4,3,3,3,2,2)$ with the minimum $\sigma$-irregularity. Observe that only $T$ is obtained by the "greedy algorithm".

## 3. Trees with fixed degree sequence and maximal $\boldsymbol{\sigma}$-irregularity

As in the previous section, here also several results and definition will be adapted from [17,21,24,25]. The next result is crucial for characterizing and constructing trees with maximum $\sigma$-irregularity and a given degree sequence.

Lemma 3.1. Let $T$ be a tree with maximum $\sigma$-irregularity. Then, every path with end-vertices of degree 1 , can be enumerated as $v_{0} v_{1} \ldots v_{t} v_{t+1}$ in $T$, where $d\left(v_{0}\right)=d\left(v_{t+1}\right)=1$ and $1 \leq i \leq(t+1) / 2$, such that the following properties hold:
(a) if is odd, then $d\left(v_{i}\right) \geq d\left(v_{t+1-i}\right) \geq d\left(v_{k}\right) \quad$ for $i<k<t+1-i$;
(b) if i is even, then $d\left(v_{i}\right) \leq d\left(v_{t+1-i}\right) \leq d\left(v_{k}\right)$ for $i<k<t+1-i$.

Proof. We prove the above claims by induction on $i$.
For $i=1$, we have to show that $d\left(v_{1}\right) \geq d\left(v_{t}\right) \geq d\left(v_{k}\right)$, for $2 \leq k \leq t-1$.
Firstly, if $d\left(v_{1}\right) \geq d\left(v_{t}\right)$ does not hold, then we enumerate the vertices in the considered path in the reversed order. Then, we stay by this enumeration.

Secondly, we show that $d\left(v_{1}\right) \geq d\left(v_{k}\right)$. We assume that it is not true and that $d\left(v_{1}\right)<d\left(v_{k}\right)$. We obtain a tree $T^{\prime}$ from $T$ by deleting the edges $v_{0} v_{1}$ and $v_{k} v_{k+1}$ and adding edges $v_{0} v_{k}$ and $v_{1} v_{k+1}$. With the constraints, $d\left(v_{k+1}\right)>d\left(v_{0}\right)=1$ and $d\left(v_{k}\right)>d\left(v_{1}\right)$, by Proposition 1.1, we have that $\sigma\left(T^{\prime}\right)-\sigma(T)>0$. This contradicts the claim that $T$ is a tree with maximum $\sigma$-irregularity, and thus, $d\left(v_{1}\right) \geq d\left(v_{k}\right), 2 \leq k \leq t-1$, holds.

The relation $d\left(v_{t}\right) \geq d\left(v_{k}\right), 2 \leq k \leq t-1$, we prove similarly. Now, we delete the edges $v_{t} v_{t+1}$ and $v_{k-1} v_{k}$ and add edges $v_{t} v_{k-1}$ and $v_{t+1} v_{k}$ from $T$ obtaining the tree $T^{\prime}$. With the assumption $d\left(v_{t}\right)<d\left(v_{k}\right)$ and the relation $d\left(v_{k-1}\right)>d\left(v_{0}\right)=1$, by Proposition 1.1, we obtain that $\sigma\left(T^{\prime}\right)-\sigma(T)>0$. This is again a contradiction. It follows that $d\left(v_{t}\right) \geq d\left(v_{k}\right)$, for $2 \leq k \leq t$ and thereby the case $i=1$ is proven.

Now assume that $i \geq 2$ is even. Then $i-1$ is odd, and by the induction hypothesis, we may assume that $d\left(v_{i-1}\right) \geq$ $d\left(v_{t-i+2}\right) \geq d\left(v_{k}\right)$, for $i-1<k<t+2-i$. We want to show that $d\left(v_{i}\right) \geq d\left(v_{t+1-i}\right) \geq d\left(v_{k}\right)$, for $i<k<t+1-i$. Assume that this is not true and that $d\left(v_{i}\right)>d\left(v_{t+1-i}\right)>d\left(v_{k}\right)$. Here, we delete the edges $v_{i-1} v_{i}$ and $v_{k} v_{k+1}$ and add the edges $v_{i-1} v_{k}$ and $v_{i} v_{k+1}$ to $T$ obtaining a tree $T^{\prime}$ with same degree sequence as $T$. For $i<k<t+1-i$, it holds that $d\left(v_{i-1}\right)>d\left(v_{k+1}\right)$ and $d\left(v_{i}\right)>d\left(v_{k}\right)$. Thus, $\sigma\left(T^{\prime}\right)-\sigma(T)>0$, which is a contradiction to the maximum optimality of $T$, and we may conclude that $d\left(v_{i}\right) \geq d\left(v_{k}\right)$, for $i \leq k \leq t+1-i$. In the same way, we can prove $d\left(v_{i}\right) \geq d\left(v_{t+1-i}\right)$.

When $i \geq 2$ is odd, we can similarly show $d\left(v_{i}\right) \geq d\left(v_{t+1-i}\right) \geq d\left(v_{k}\right)$ by the same argument as we use above for even $i$.
Lemma 3.1 implies the following weaker statement:
Corollary 3.1. In a tree with maximum $\sigma$-irregularity, let $v_{i} \in L_{i}$ for $i=0,1, \ldots$, then we may assume, for $j>i \geq 1$, that

- $d\left(v_{i}\right) \geq d\left(v_{j}\right)$ if is odd;
- $d\left(v_{i}\right) \leq d\left(v_{j}\right)$ if is even.

For a tree $T$, let $d^{*}$ be the minimum degree of vertices in the set $L_{1}(T)$. Let $V_{p}^{*}(T)$ represent the set of pendant vertices whose adjacent vertices have a degree of $d^{*}$ in tree $T$. Let $\overline{V_{p}^{*}(T)}$ be the set of pendant vertices in tree $T$ that are not part of $V_{p}^{*}(T)$.

Lemma 3.2. Let $v^{\prime}$ and $v^{\prime \prime}$ be two vertices of a tree $T$ such that $v^{\prime} \in V_{p}^{*}(T)$ and $v^{\prime \prime} \in \overline{V_{p}^{*}(T)}$. We obtain trees $T_{1}^{*}$ and $T_{2}^{*}$ by identifying the roots $r_{i}$ of an arbitrary tree $T_{i}$ with $v^{\prime}$ and $v^{\prime \prime}$, respectively. Then, $\sigma\left(T_{1}^{*}\right)>\sigma\left(T_{2}^{*}\right)$.

Proof. Suppose $v_{1}$ and $v_{2}$ are adjacent to $v^{\prime}$ and $v^{\prime \prime}$, respectively. Obviously, $d\left(v_{1}\right)<d\left(v_{2}\right)$. It holds

$$
\begin{aligned}
\sigma\left(T_{1}^{*}\right)-\sigma\left(T_{2}^{*}\right) & =\left(d\left(v_{1}\right)-\left(d\left(r_{i}\right)+1\right)\right)^{2}+\left(1-d\left(v_{2}\right)\right)^{2}-\left(1-d\left(v_{1}\right)\right)^{2}-\left(d\left(v_{2}\right)-\left(d\left(r_{i}\right)+1\right)\right)^{2} \\
& =\left(d\left(v_{1}\right)-\left(d\left(r_{i}\right)+1\right)\right)^{2}+\left(1-d\left(v_{2}\right)\right)^{2} \\
& =-2 d\left(r_{i}\right)\left(d\left(v_{1}\right)-d\left(v_{2}\right)\right)>0
\end{aligned}
$$

By Lemma 3.2, a tree with maximum $\sigma$-irregularity is obtained by attaching a tree $T_{i}$ to a vertex in $T$. We now construct an extremal tree with a given degree sequence using the following adopting algorithm [17]. The obtained tree will be referred to as an adopting tree.

Let $\mathcal{D}=\left(d_{1}, d_{2}, \ldots, d_{m}\right)$ represent the degree sequence corresponding to the non-pendant vertices $v_{1}, v_{2}, \ldots, v_{m}$. Recall that, as per the definition of a degree sequence given in the introduction, it is assumed that $d_{1} \geq d_{2} \geq \cdots \geq d_{m}$

1. We create subtrees $T_{i}$ as follows:

- $T_{1}$ is rooted at $r_{1}$ and is assigned $d_{m}-1$ children whose degrees are $d_{1}, d_{2}, \ldots, d_{d_{m}-1}$. These $d_{m}-1$ children are exclusively adjacent to pendant vertices, in addition to being adjacent to a non-pendant root vertex.
- $T_{2}$ is rooted at $r_{2}$ and is assigned $d_{d_{m}-1}-1$ children whose degrees are $d_{d_{m}}, d_{d_{m}+1}, \ldots, d_{d_{m}+d_{d_{m}-1}-2}$. Similarly, except to the root $r_{2}$, these $d_{d_{m}-1}-1$ children are solely adjacent to pendant vertices.
- We continue similarly to create trees $T_{3}, T_{4}, \ldots$ rooted at $r_{3}, r_{4}, \ldots$, each of which is assigned $d_{m-2}-1, d_{m-3}-1, \ldots$ children, respectively.

2. We terminate this process by the tree $T_{l}$ rooted at $r_{l}$ when one of the following conditions is met: either there are fewer than $d_{m-l+1}-1$ children available for assignment, or there are no remaining degrees to choose from for $T_{l+1}$. As a result, we obtain subtrees $T_{1}, T_{2}, \ldots, T_{l}$ with $d\left(r_{l}\right)=d_{m-l+1}$.
3. Let $r=r_{l}$ and $T=T_{l}$. We obtain $T^{(l-1)}$ from $T$ and $T_{l-1}$ rooted at $r_{l-1}$ by identifying a pendant vertex from $T$ with $r_{l-1}$. Next, we let $T=T^{(l-1)}$. We obtain $T^{(l-2)}$ from $T$ and $T_{l-2}$ rooted at $r_{l-2}$. This process continues similarly for $T_{l-3}, \ldots, T_{1}$.
4. We terminate the construction by setting $T=T^{1}$.

The tree $T$ obtained by the above algorithm is not necessarily unique, since a subtree $T_{l}$ may be rooted in several ways, as shown below in Example 3.1.

Theorem 3.1. Given a degree sequence, an adopting tree $T$ obtained by the adopting algorithm has the maximum $\sigma$-irregularity.

Proof. It is easy to check that $T$ satisfies Lemma 3.1 and Corollary 3.1. Next, we show that $T$ indeed has the maximum $\sigma$-irregularity among the trees with the same degree sequence. Assume that it is not true and that another tree $T^{\prime}$, with the same degree sequence as $T$, not obtained by the adopting algorithm, has the maximum $\sigma$-irregularity, larger than $\sigma(T)$.

Next, we show that $T^{\prime}$ must contain the subtree $T_{1}$, as described in the adopting algorithm, otherwise, it cannot have maximum $\sigma$-irregularity. Recall that the subtree $T_{1}$ has a radius 2 , and it is rooted at $r_{1}\left(v_{m}\right)$. Its children are vertices with degrees $d_{1}, d_{2}, \ldots, d_{d_{m}-1}$ and its grandchildren all have a degree 1. A vertex of degree $d_{1}$ in $T$ is adjacent to a vertex of degree $d_{m}$ and $d_{1}-1$ vertices of degree 1. Assume that in $T^{\prime}$ this is not true and a vertex of degree $d_{1}$ is adjacent to a nonpendent vertex of degree $d_{j}$ different from $d_{m}$. Observe that $d_{j}>d_{m}$, since $d_{m}$ is the smallest degree of the non-pendent vertices. Let $d_{k}$ be a degree of a non-pendent vertex in $T^{\prime}$ adjacent to a vertex of degree $d_{m}$. It holds that $d_{k} \geq d_{m}$. Also $d_{k} \neq d_{1}$, due to the above assumption that a vertex of degree $d_{1}$ is not adjacent to a non-pendent vertex of degree $d_{m}$. Thus, $d_{1}>d_{k}$, since $d_{1}$ is the largest degree. Denote by $v_{j}, v_{k}$, and $v_{m}$, the vertices with degrees $d_{j}, d_{k}$, and $d_{m}$, respectively. Let $T^{\prime \prime}=T^{\prime}-v_{1} v_{j}-v_{m} v_{k}+v_{1} v_{m}+v_{j} v_{k}$. Then,

$$
\sigma\left(T^{\prime \prime}\right)-\sigma\left(T^{\prime}\right)=-\left(d_{1}-d_{j}\right)^{2}-\left(d_{m}-d_{k}\right)^{2}+\left(d_{1}-d_{m}\right)^{2}+\left(d_{j}+d_{k}\right)^{2}=2\left(d_{1}-d_{k}\right)\left(d_{j}-d_{m}\right)>0
$$

This is a contradiction on the assumption that $T^{\prime}$ has maximum $\sigma$-irregularity. It follows that $T^{\prime}$ has a maximum $\sigma$-irregularity if in $T^{\prime} v_{1}$ is adjacent to a vertex with degree $d_{m}$. With this conclusion, applying the same argument we can show that if $T^{\prime}$ has a maximum $\sigma$-irregularity then $v_{2}$ is adjacent to a vertex with degree $d_{m}$. We may continue with
the same argumentation for $v_{3}, v_{4}, \ldots, v_{m-1}$. Thus, we may conclude that $T^{\prime}$ has a maximum $\sigma$-irregularity if it contains $T_{1}$ as subtree.

Similarly, we may conclude that the rest of the subtrees $T_{i}, i=2, \ldots, l$, must be subtrees of $T^{\prime}$ if $T^{\prime}$ has maximum $\sigma$-irregularity.

Lemma 3.2 guarantees the way of connecting the subtrees $T_{i}, i=1, \ldots l$ such that the resulting tree has maximum $\sigma$-irregularity. Observe that in this way, the subtrees $T_{i}, i=1, \ldots l$ are connected by the adopting algorithm. Therefore, $T^{\prime}$ must be isomorphic to one of the trees, if there is more than one, obtained by the adopting algorithm. Thus, we may conclude that $T^{\prime}$ and $T$ have the maximum $\sigma$-irregularity.

Example 3.1. In Figure 2 four trees, which have maximum $\sigma$-irregularity among all trees with degree sequence $\mathcal{D}=$ (5, 5, 5, 4, 3, 3, 3, 2, 2), are presented. All trees $T, T^{\prime}, T^{\prime \prime}$, and $T^{\prime \prime \prime}$ can be obtained by the "adopting algorithm".


Figure 2: The subgraphs $T_{1}, T_{2}, T_{3}$, and $T_{4}$ generated from the degree sequence $\mathcal{D}=(5,5,5,4,3,3,3,2,2)$ as described in the first step of the "adopting algorithm". Based on these subtrees, the four trees $T, T^{\prime}, T^{\prime \prime}$, and $T^{\prime \prime \prime}$ with maximum $\sigma$-irregularity are obtained.

Notice also here that for a given degree sequence, the adopting tree, which achieves the maximum $\sigma$-irregularity also achieved the maximum (general) Randić index for $\alpha>0$ [24], and the minimum atom-bond connectivity index [17, 25].

## 4. Conclusion and further work

In this work, we characterize the trees with minimum and maximum $\sigma$-irregularity of given order and fixed degree sequence. The trees, which have minimal (respectively maximal) values for several graph topological invariants (including the (general) Randić index, the atom-bond connectivity index, the Albertson irregularity) also minimize/maximize the $\sigma$-irregularity.

It is easy to see that the greedy tree is always unique. The tree generated by the adopting algorithm is unique when all degrees larger than one occur only once in the degree sequence. However, in general, it is not unique.

Problem 4.1. Find the sufficient and necessary conditions for the extremal tree with respect to $\sigma$-irregularity to be unique.
When the tree with extremal $\sigma$-irregularity is not unique it will be of interest to find a way to enumerate all of them.
Problem 4.2. Modify the greedy and adopting algorithms such that they generate all trees with minimal, respectively maximal, $\sigma$-irregularity.

## Acknowledgements

This work was partially supported by the Slovenian research agency ARRS (Program No. P1-0383 and Project No. J1-3002) and the National Natural Science Foundation of China (Grant No. 12271182 and Grant No. 11771362).

## References

[1] H. Abdo, S. Brandt, D. Dimitrov, The total irregularity of a graph, Discrete Math. Theor. Comput. Sci. 16 (2014) 201-206.
[2] H. Abdo, N. Cohen, D. Dimitrov, Graphs with maximal irregularity, Filomat 28 (2014) 1315-1322.
[3] H. Abdo, D. Dimitrov, The total irregularity of graphs under graph operations, Miskolc Math. Notes 15 (2014) 3-17.
[4] H. Abdo, D. Dimitrov, The irregularity of graphs under graph operations, Discuss. Math. Graph Theory 34 (2014) 263-278.
[5] H. Abdo, D. Dimitrov, The total irregularity of some composite graphs, Int. J. Comput. Appl. 122 (2015) 1-9.
[6] H. Abdo, D. Dimitrov, Non-regular graphs with minimal total irregularity, Bull. Aust. Math. Soc. 92 (2015) 1-10.
[7] H. Abdo, D. Dimitrov, I. Gutman, Graphs with maximal $\sigma$-irregularity, Discrete Appl. Math. 250 (2018) 57-64.
[8] M. O. Albertson, The irregularity of a graph, Ars Combin. 46 (1997) 219-225.
[9] M. O. Albertson, D. Berman, Ramsey graphs without repeated degrees, Congr. Numer. 83 (1991) 91-96.
[10] A. Ali, A. M. Albalahi, A. M. Alanazi, A. A Bhatti, A. E. Hamza, On the maximum sigma index of k-cyclic graphs, Discrete Appl. Math. 352 (2023) $58-62$.
[11] F. K. Bell, A note on the irregularity of graphs, Linear Algebra Appl. 161 (1992) 45-54.
[12] G. Chen, P. Erdős, C Rousseau, R. Schelp, Ramsey problems involving degrees in edge-colored complete graphs of vertices belonging to monochromatic subgraphs, European J. Combin. 14 (1993) 183-189.
[13] X. Chen, X. Li, W. Lin, On connected graphs and trees with maximal inverse sum indeg index, Appl. Math. Comput. 392 (2021) \#125731.
[14] C. Delorme, O. Favaron, D. Rautenbach, Closed formulas for the numbers of small independent sets and matchings and an extremal problem for trees, Discrete Appl. Math. 130 (2003) 503-512.
[15] D. Dimitrov, T. Réti, Graphs with equal irregularity indices, Acta Polytech. Hung. 11 (2014) 41-57.
[16] D. Dimitrov, R. Škrekovski, Comparing the irregularity and the total irregularity of graphs, Ars Math. Contemp. 9 (2015) 25-30.
[17] L. Gan, B. Liu, Z. You, The ABC index of trees with given degree sequence, MATCH Commun. Math. Comput. Chem. 68 (2012) 137-145.
[18] I. Gutman, P. Hansen, H. Mélot, Variable neighborhood search for extremal graphs. 10. Comparison of irregularity indices for chemical trees, J. Chem. Inf. Model. 45 (2005) 222-230.
[19] P. Hansen, H. Mélot, Variable neighborhood search for extremal graphs. 9. Bounding the irregularity of a graph, DIMACS Ser. Discrete Math. Theoret. Comput. Sci. 69 (2005) 253-264.
[20] I. Gutman, M. Togan, A. Yurttas, A. S. Cevik, I. N. Cangul, Inverse problem for sigma index, MATCH Commun. Math. Comput. Chem. 79 (2018) $491-508$.
[21] W. Lin, T. Gao, Q. Chen, X. Lin, On the minimal ABC index of connected graphs with given degree sequence, MATCH Commun. Math. Comput. Chem. 69 (2013) $571-578$.
[22] T. Reti, On some properties of graph irregularity indices with a particular regard to the $\sigma$-index, Appl. Math. Comput. 344 (2019) 107-115.
[23] T. Réti, D. Dimitrov, On irregularities of bidegreed graphs, Acta Polytech. Hung. 10 (2013) 117-134.
[24] H. Wang, Extremal trees with given degree sequence for the Randić index, Discrete Math. 308 (2008) 3407-3411.
[25] R. Xing, B. Zhou, Extremal trees with fixed degree sequence for atom-bond connectivity index, Filomat 26 (2012) 683-688.
[26] X.-D. Zhang, Q.-Y. Xiang, L.-Q. Xu, R.-Y. Pan, The Wiener index of trees with given degree sequences, MATCH Commun. Math. Comput. Chem. 60 (2008) 623-644.


[^0]:    *Corresponding author (darko.dimitrov11@gmail.com).

