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The σ-irregularity of trees with maximum degree 5

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ABSTRACT

The σ-irregularity, a variant of the well-established Albertson irregularity, is a topological invariant defined for a graph $G = (V, E)$ as $\sigma(G) = \sum_{uv \in E}(d(u) - d(v))^2$, where $d(u)$ and $d(v)$ denote the degrees of vertices u and v, respectively. Recent research has successfully characterized chemical trees with the maximum σ-irregularity. In this paper, we expand upon this research by establishing several structural properties of maximal trees with prescribed maximum degree Δ. Application of these properties enables us to characterize maximal trees with $\Delta = 5$. We establish that extremal trees contain only vertices of degrees 1, 2 and Δ. Moreover, the number of edges with both end-vertices having the degree 2 or Δ is very small, so almost all edges have the (second) maximum possible contribution to σ-irregularity. We believe this property or similar should extend to maximal trees for any value of Δ, so this is an interesting direction for further research.

1. Introduction

Let $G = (V, E)$ be a graph with the vertex set $V = V(G)$ and the edge set $E = E(G)$. Unless explicitly stated otherwise, all graphs in this paper are assumed to be simple and finite. The *degree* $d_G(v)$ of a vertex $v \in V(G)$ is defined to be the number of neighbors of v in G. For a pair of vertices $u, v \in V(G)$, by $d_G(u, v)$ we denote the *distance* of these two vertices, i.e. the length of a shortest path connecting them. If the graph G is clear from context, we omit the subscript G. A graph G is *regular* if all its vertices have a same degree, otherwise it is said to be *irregular*. The concept of irregularity has been widely researched within various scientific fields such as chemistry and network theory [6,8–10,12,17,18].

One of the well-known irregularity measures of a graph G is the *Albertson irregularity* [4] denoted by $\mathrm{irr}(G)$ and defined as follows

$$\mathrm{irr}(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|.$$

This index received considerable attention from the scientific community, we refer here to a selection of relevant studies [1,2,4,5,12,14].

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A downside of the Albertson irregularity is the inherent need to calculate absolute values, hence it is natural to propose a similar index, the so-called *σ-irregularity*, defined for a graph G by

$$\sigma(G) = \sum_{uv \in E(G)} (d_G(u) - d_G(v))^2.$$

Some fundamental properties of the σ-irregularity were given by Gutman et al. in [13], such as the following basic relation

$$\sigma(G) = F(G) - 2M_2(G), \tag{1}$$

where $F(G)$ denotes the *forgotten index* defined by

$$F(G) = \sum_{u \in V(G)} d(u)^3,$$

while $M_2(G)$ denotes the *second Zagreb index* defined by

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

In [3], a characterization of graphs with the maximum value of σ-irregularity is provided, and also some lower bounds on the σ-irregularity. In [3,13], the inverse problem for σ-irregularity is solved, i.e., the problem of establishing the existence of a graph with the σ-irregularity equal to a given non-negative integer. The research of the relation of σ-irregularity with some other well-known irregularity measures is conducted by Réti in [16]. Also, in a recent paper [7] the characterization of graphs with a prescribed degree sequence having extremal σ-irregularity is given. The so called total σ-irregularity, which is a variant of σ-irregularity, has also recently been studied [11,15].

A graph G is said to be *chemical* if the maximum vertex degree in G is 4. A *tree* is a connected acyclic graph. Among the (chemical) trees explored in [3], the path graph is shown to have the smallest σ-irregularity. In [19], the characterization of chemical trees with maximal σ-irregularity was provided. Here, we extend this outcome by giving several properties of trees with prescribed maximum degree Δ exhibiting maximal σ-irregularity. The application of these properties to the case $\Delta = 5$ yields a characterization of maximal trees.

Before delving into properties of maximal trees with respect to σ-irregularity, we introduce the necessary additional notation and preliminaries. In a tree T, a *k-vertex* is a vertex of degree k. Particularly, a *leaf* is a vertex of degree 1. A vertex of a tree T is an *internal leaf* if it has precisely one neighbor with a degree greater than 1. Notice that an internal leaf of T is a leaf in the tree T' obtained from T by removing all leaves, hence the name. A vertex with degree at least 3 will be called a *big vertex*. The number of vertices in T of degree i is denoted by n_i, where i ranges from 1 to Δ. Similarly, the number of edges in T with end-vertices of degrees i and j, for $1 \le i \le j \le \Delta$, is denoted by $m_{i,j}$. If T is a tree with maximal σ-irregularity on a given number of vertices n, we refer to it as a *maximal tree*.

The present paper is organized as follows. In the next section we give several properties of maximal trees with prescribed maximum degree Δ, for any $\Delta \ge 3$. In the third section, these properties are applied to the case $\Delta = 5$ for which the characterization of maximal trees is obtained.

2. Properties of maximal trees for general Δ

In this section we will establish several properties of maximal trees with the maximum degree Δ, which hold for any $\Delta \ge 3$. We start with the following proposition which will be a useful tool in proving further properties of maximal trees and it stems from a simple tree transformation.

Proposition 1. *Let T be a maximal tree with the maximum degree Δ, and $P = ux \cdots yv$ a path in T. If $d(u) > d(v)$, then $d(x) \le d(y)$. Also, if $d(x) > d(y)$, then $d(u) \le d(v)$.*

Proof. To prove the first claim of the proposition, suppose that $d(u) > d(v)$. If $d(u, v) = 1$, then $x = v$ and $y = u$, so $d(x) = d(v) < d(u) = d(y)$, and the claim holds. Next, if $d(u, v) = 2$, then $x = y$ which implies $d(x) = d(y)$, so the claim also holds. Hence, let us assume that $d(u, v) \ge 3$. Assume to the contrary that $d(x) > d(y)$. Let T' be the tree obtained from T by removing edges ux and yv, and adding edges uy and xv instead. Notice that

$$\begin{aligned}\sigma(T') - \sigma(T) &= (d(u) - d(y))^2 - (d(u) - d(x))^2 + (d(v) - d(x))^2 - (d(v) - d(y))^2 \\ &= 2(d(u) - d(v))(d(x) - d(y)) > 0,\end{aligned}$$

which contradicts to T being maximal.

Now, let us prove the second claim of the proposition. Suppose that $d(x) > d(y)$, which is only possible if $x \ne y$. Assume to the contrary that $d(u) > d(v)$. Then again for the tree $T' = T - ux - yv + yu + xv$ we have

$$\sigma(T') - \sigma(T) = 2(d(u) - d(v))(d(x) - d(y)) > 0,$$

a contradiction. ∎

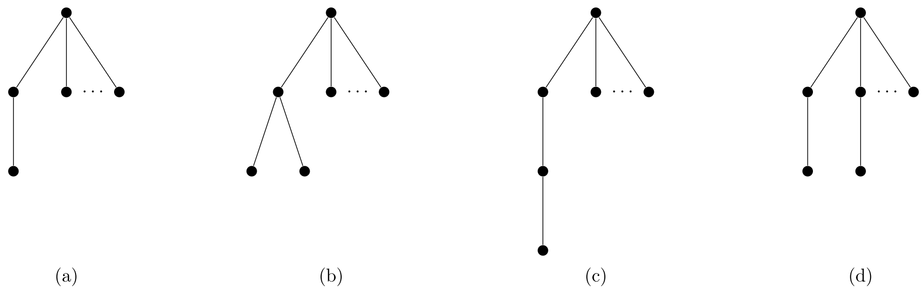

Fig. 1. Trees T of maximal-degree Δ on $n = \Delta + 2$ and $n = \Delta + 3$ vertices.

The next property we wish to establish is that all internal leaves of maximal trees have maximum degree Δ. The property holds provided that the number of vertices in a tree is sufficiently large, and it will be extensively used in the next section where we will establish maximal trees for $\Delta = 5$.

To arrive at this result, we need the following three lemmas.

Lemma 2. *Let T be a maximal tree with maximum degree $\Delta \geq 3$. If T contains at least two big vertices, then $m_{2,1} = 0$.*

Proof. Assume to the contrary, that T does contain an edge uv with $d(u) = 2$ and $d(v) = 1$. Let x be the big vertex closest to u, and let y be the neighbor of x which is not a leaf, such that the path P connecting y and v contains x, i.e., $P = yx \cdots uv$. Notice that such a vertex y must exist, since T contains at least two big vertices, and there is no big vertex on the path connecting x and v. Since $d(v) < d(y)$, Proposition 1 implies $d(u) \geq d(x)$, a contradiction. ■

There is only one tree T of maximum degree Δ with $n = \Delta + 1$ vertices, obviously the star; and also one such T on $n = \Delta + 2$ vertices, see Fig. 1(a). If $n = \Delta + 3$, we have three non-isomorphic trees, shown in Fig. 1(b)–(d), and the maximum of $\sigma(\cdot)$ is attained by the tree in (c).

Let us show that a maximal tree T with the sufficiently many vertices does have at least two big vertices. This is established by the following lemma.

Lemma 3. *Let T be a maximal tree on n vertices with maximum degree $\Delta \geq 3$. If $n \geq \Delta + 4$, then T contains at least two big vertices.*

Proof. Assume to the contrary that T does not contain two big vertices. Then T has precisely one vertex u of degree Δ, and so it consists of Δ pending paths attached to u.

First suppose that one of these pending paths has length at least 4, say

$$P = u \cdots v_3 v_2 v_1 v_0, \quad d(v_0) = 1,\ d(v_1) = d(v_2) = d(v_3) = 2.$$

If we modify T by deleting the edge $v_0 v_1$ and adding $v_0 v_2$, we obtain a new tree

$$T' = T - v_0 v_1 + v_0 v_2.$$

In T', the degree of v_2 increases from 2 to 3, while v_1 decreases from 2 to 1. Thus, $\sigma(T') > \sigma(T)$, contradicting the maximality of T. Hence no pending path may have length at least 4.

Next, suppose there are two distinct pending paths, each of length 2 or 3, say

$$v_0 v_1 \cdots u, \quad u v_2 \cdots v_3,$$

with $d(v_1) = d(v_2) = 2$ and $d(v_0) = d(v_3) = 1$. Applying Proposition 1 on the subpath $v_0 v_1 \cdots u v_2$ we obtain that vertex v_1 has to be big, a contradiction.

From the above, it follows that T has at most one pending path of length 3 and all others are of length 1, and consequently

$$n \leq \Delta + 3.$$

This contradicts the assumption $n \geq \Delta + 4$, which establishes the claim. ■

An immediate consequence of Lemmas 2 and 3 is the following corollary.

Corollary 4. *Let T be a maximal tree on n vertices with maximum degree $\Delta \geq 3$. If $n \geq \Delta + 4$, then $m_{1,2} = 0$.*

The next important step towards the result we aim at, is the following lemma in which we establish that almost all internal vertices of a maximal tree have the degree Δ.

Lemma 5. *Let T be a maximal tree on n vertices with maximum degree $\Delta \geq 3$. If $n \geq \Delta + 4$, then at most one internal leaf of T has the degree smaller than Δ.*

Proof. The assumption $n \geq \Delta + 4$ implies that T contains at least two distinct internal leaves. Assume to the contrary, that at least two internal leaves have the degree less than Δ. Let u and v be two such internal leaves at the maximum possible distance, and we may assume $d(u) \geq d(v)$. If u and v are neighbors, then u and v are the only non-leaf vertices of T. Since the maximum degree of T is Δ, at least one of u and v must have the degree Δ, say u. So, v is the only internal leaf of T which may have the degree smaller than Δ, which proves the claim in this case.

Assume next that u and v are not neighbors, i.e., $d(u, v) \geq 2$. Denote the neighbors of u by u_i, for $i = 1, \ldots, d(u)$, so that u_i is a leaf for $i \geq 2$. Similarly, let the neighbors of v be denoted by v_i, for $i = 1, \ldots, d(v)$, so that v_i is a leaf for $i \geq 2$. Since $n \geq \Delta + 4$, Lemma 3 implies that T contains at least two big vertices. Lemma 2 further implies that every leaf of T is a neighbor of a vertex of degree at least three. This means that $d(u) \geq 3$ and $d(v) \geq 3$. Recall that we assumed $d(u) \geq d(v)$. If $d(u) > d(v)$, then Proposition 1 implies $d(u_1) \leq d(v_1)$. If $d(u) = d(v)$ and $d(u_1) > d(v_1)$, then we swap labels of u and v, and also u_i and v_i for every i. Either way, we obtain $d(u) \geq d(v)$ and $d(u_1) \leq d(v_1)$. Let $T' = T - vv_2 + uv_2$, and notice that $\sigma(T') - \sigma(T) = \sigma_1 + \sigma_2 + \sigma_3$ where

$$\begin{aligned}\sigma_1 &= (d(v) - 2)((d(v) - 1 - 1)^2 - (d(v) - 1)^2) \\ &\quad + (d(u) - 1)((d(u) + 1 - 1)^2 - (d(u) - 1)^2), \\ \sigma_2 &= (d(u) + 1 - 1)^2 - (d(v) - 1)^2, \\ \sigma_3 &= (d(v) - 1 - d(v_1))^2 - (d(v) - d(v_1))^2 \\ &\quad + (d(u) + 1 - d(u_1))^2 - (d(u) - d(u_1))^2.\end{aligned}$$

Notice that $\sigma_1 = (d(u) - d(v) + 1)\,(2d(u) + 2d(v) - 5)$, so $d(u) \geq d(v) \geq 3$ implies $\sigma_1 > 0$. Notice further that due to $d(u) \geq d(v)$ it holds that $\sigma_2 > 0$. Finally, it holds that $\sigma_3 = 2d(u) - 2d(v) + 2d(v_1) - 2d(u_1) + 2$, where $d(u) \geq d(v)$ and $d(v_1) \geq d(u_1)$ implies $\sigma_3 > 0$. This amounts to $\sigma(T') - \sigma(T) > 0$, a contradiction with T being maximal. ■

A tree T with only one internal leaf has $n = \Delta + 1$ vertices, so a tree T on $n \geq \Delta + 4$ vertices must have at least two internal leaves. On the other hand, a tree T on $n \leq 2\Delta - 1$ vertices cannot have two vertices of degree Δ. Hence, the result of Lemma 5 is the best possible for maximal trees on n vertices, where $\Delta + 4 \leq n \leq 2\Delta - 1$. In the next theorem we show that the presence of this one internal leaf with the degree less than Δ is only due to the small number of vertices, i.e. that for $n \geq 2\Delta$ all internal leaves in a maximal tree are of degree Δ.

Theorem 6. *Let T be a maximal tree with maximum degree Δ. If $n \geq 7$, for $\Delta = 3$ and $n \geq 2\Delta$, for $\Delta \geq 4$, then all internal leaves of T are of degree Δ.*

Proof. Notice that $n \geq \Delta + 4$ for each $\Delta \geq 3$.

Assume to the contrary that there exists an internal leaf u of T with $d(u) < \Delta$. Lemma 5 implies that all other internal leaves of T are of degree Δ. A vertex of T which is neither a leaf nor an internal leaf will be called a *core* vertex of T. Notice that $n \geq 2\Delta$ and $d(u) < \Delta$ imply that T contains at least one core vertex.

Let us show that the degree of each core vertex of T is at most $d(u)$. For that purpose, let v be a core vertex of T, and let w be a neighbor of v such that $d(w, u) > d(v, u)$ and w is not a leaf. Such a vertex w must exist in T, since v is not an internal leaf. If $d(v) > d(u)$, due to Proposition 1, we would have $d(w) \leq 1$, a contradiction. Hence, it must hold that $d(v) \leq d(u)$.

We now distinguish the following two cases.

Case 1: *All core vertices in T have precisely two neighbors with degrees greater than* 1. Here, we distinguish two subcases regarding the degrees of core vertices in T.

Subcase 1.a: *All core vertices have the degree* 2. Since all core vertices are of degree 2, the tree T contains precisely two internal leaves u and v, and one of the two internal leaves must have the degree Δ, say v. Let P be the path in T connecting u and v, then the core vertices of T are the interior vertices of P.

If T contains precisely one core vertex w, then from $n \geq 2\Delta$ and $d(w) = 2$ we conclude $d(u) = \Delta - 1$. Let $T' = T - vw + vu$, and notice that the contribution of the edges vw and uv taken together to $\sigma(T') - \sigma(T)$ is $0 - (\Delta - 2)^2$, the contribution of the edge uw is $(\Delta - 1)^2 - (\Delta - 3)^2$, and the contribution of $\Delta - 2$ leaves of T attached to u is $(\Delta - 1)^2 - (\Delta - 2)^2$. Hence, we have

$$\begin{aligned}\sigma(T') - \sigma(T) &= -(\Delta - 2)^2 + (\Delta - 1)^2 - (\Delta - 3)^2 + (\Delta - 2)((\Delta - 1)^2 - (\Delta - 2)^2) \\ &= \Delta^2 + \Delta - 6 > 0\end{aligned}$$

for $\Delta \geq 3$, a contradiction.

So, let us assume T contains more than one core vertex. This implies that u and v are connected by a path P of the length ≥ 3, and all internal vertices of P are core vertices which are of degree 2. Let $P' = zwu$ be the subpath of the path connecting u and v. Consider the tree $T' = T - zw + zu$, and notice that the contribution of the edges zw and zu to $\sigma(T') - \sigma(T)$ is $(d(u)-2)^2 - 0$, the contribution of the edge wu is $(d(u)-1)^2 - (d(u)-2)^2$, and the contribution of $d(u)-1$ leaves of T attached to u is $d(u)^2 - (d(u)-1)^2$. We obtain

$$\begin{aligned}\sigma(T') - \sigma(T) &= (d(u)-2)^2 + (d(u)-1)^2 - (d(u)-2)^2 + (d(u)-1)(d(u)^2 - (d(u)-1)^2)\\ &= 3d(u)^2 - 5d(u) + 2 > 0\end{aligned}$$

for $d(u) \geq 2$, a contradiction.

Subcase 1.b: *There exists a core vertex v of T with $d(v) \geq 3$.* We may assume that v is the core vertex of the degree ≥ 3 closest to u. This implies that every internal vertex of the path P connecting u and v is of degree 2 in T. Due to $d(v) \geq 3$ and the assumption that v contains at most two non-leaf vertices, we conclude that there exists a leaf v_1 of T attached to v. Let $T' = T - v_1v + v_1u$ and let us consider the difference $\sigma(T') - \sigma(T)$.

Since v is a core vertex of T, recall that $d(v) \leq d(u)$. This implies that the contribution of the edges v_1v and v_1u to $\sigma(T') - \sigma(T)$ is strictly positive. This also implies that the sum of the contributions of edges of P to $\sigma(T') - \sigma(T)$ is strictly positive.

Let v_2 be the non-leaf neighbor of v not contained on P, and u_1 a leaf of T attached to u. If $d(v_2) \geq d(v)$ then the contribution of v_2v to $\sigma(T') - \sigma(T)$ is positive, otherwise if $d(v_2) < d(v)$ then the contribution of v_2v may be negative, but it is $\geq (d(v)-2)^2 - (d(v)-1)^2$. Hence, the sum σ_1 of contributions of edges v_2v and u_1u is

$$\begin{aligned}\sigma_1 &\geq (d(v)-2)^2 - (d(v)-1)^2 + d(u)^2 - (d(u)-1)^2\\ &= 2d(u) - 2d(v) + 2 > 0,\end{aligned}$$

since $d(u) \geq d(v)$.

Let E_v be the set of all leaves of T incident to v distinct from v_1v and E_u the set of all leaves incident to u except u_1u. Since $d(v) \leq d(u)$ and v_2v is not a leaf, we conclude $|E_v| < |E_u|$. We conclude that

$$\begin{aligned}\sigma(T') - \sigma(T) &> |E_v|\,((d(v)-2)^2 - (d(v)-1)^2) - |E_u|\,(d(u)^2 - (d(u)-1)^2)\\ &> |E_v|\,(2d(u) - 2d(v) + 2) > 0,\end{aligned}$$

a contradiction.

Case 2: *There exists a core vertex in T with at least three neighbors with degrees greater than* 1. Let v be a core vertex of T with at least three non-leaf neighbors closest to u. Let P be the subpath of T connecting u and v, and notice that the choice of v implies that all the internal vertices of P have the degree 2 in T.

Subcase 2.a: *All non-leaf neighbors of v are internal leaves of T.* This implies that v is the only core vertex of T and uv is an edge of T, i.e., u and v are neighbors.

Suppose first that there exists a leaf w attached to v in T. Let $T' = T - wv + wu$ and let us consider the difference $\sigma(T') - \sigma(T)$. Since $d(v) \leq d(u)$, the sum of contributions of edges wv and wu to $\sigma(T') - \sigma(T)$ is strictly positive. For the same reason, the contribution of the edge uv is also strictly positive. A non-leaf neighbor z of v is an internal leaf of T, so $d(z) = \Delta$. This implies that for every such z the contribution of the edge vz to $\sigma(T') - \sigma(T)$ is strictly positive. It remains to consider leaves of T incident to v which are distinct from wv, denote the set of such edges by E_v. Notice that edges of E_v are the only edges in T with negative contribution to $\sigma(T') - \sigma(T)$. Denote by E_u the set of leaves incident to u. Since $d(v) \leq d(u)$ and v has more non-leaf neighbors than u, we conclude $|E_v| < |E_u|$. Hence, we obtain

$$\begin{aligned}\sigma(T') - \sigma(T) &\geq |E_v|\,((d(v)-2)^2 - (d(v)-1)^2) - |E_u|\,(d(u)^2 - (d(u)-1)^2)\\ &> |E_v|\,(2d(u) - 2d(v) + 2) > 0,\end{aligned}$$

a contradiction.

Suppose now that there are no leaves attached to v in T. Denote by z a leaf of T which is not attached to u. Let $T' = T - uv + uz$, and notice that $d(v) \leq d(u)$ implies that the sum of contributions of edges uv and uz to $\sigma(T') - \sigma(T)$ is strictly positive. Hence, we have

$$\begin{aligned}\sigma(T') - \sigma(T) &> (d(v)-1)((\Delta - (d(v)-1))^2 - (\Delta - d(v))^2) + (\Delta - 2)^2 - (\Delta - 1)^2\\ &= (d(v)-2)\,(2\Delta - 2d(v) - 1) > 0,\end{aligned}$$

a contradiction.

Subcase 2.b: *There exists a non-leaf neighbor of v which is a core vertex of T.* Let P be the path connecting u and v in T. Let u_1 (resp. v_1) be the neighbor of u (resp. v) which belongs to P. If v_1 is the only neighbor of v which is a core vertex of T, then v has a non-leaf neighbor v_2 which is an internal leaf of T. Lemma 5 implies $d(v_2) = \Delta$. Now, since $d(u) < \Delta = d(v_2)$, Proposition 1 implies $d(u_1) \geq d(v)$, a contradiction since $d(u_1) = 2$ and $d(v) > 2$.

Hence, there exists a core vertex $v_2 \neq v_1$ which is a neighbor of v. We may assume that among neighbors of v distinct from v_1 which are core vertices, v_2 has the smallest degree. Also, since v_2 is a core vertex, we have $d(v_2) \leq d(u)$. Let

$v_3 \neq v_1$ be the third non-leaf neighbor of v, and the choice of v_2 implies $d(v_2) \leq d(v_3)$. Let $T' = T - v_2v + v_2u$, and notice that the sum of the contributions of edges of the path P to $\sigma(T') - \sigma(T)$ is strictly positive due to $d(v) \leq d(u)$.

Denote by u_2 and u_3 a pair of leaves attached to u in T. Also, let σ_1 be the sum of contributions to $\sigma(T') - \sigma(T)$ of the edges v_2v, v_2u, v_3v, u_2u, u_3u. It holds that

$$\begin{aligned}\sigma_1 &= (d(v_3) - (d(v) - 1))^2 - (d(v_3) - d(v))^2 + (d(v_2) - (d(u) + 1))^2 - (d(v_2) - d(v)^2) \\ &\quad + 2(d(u)^2 - (d(u) - 1)^2) \\ &= (d(u) - d(v_2))^2 + 3d(u) + d(v)(d(v) - 2) + 3(d(u) - d(v_2)) + 2d(v_3).\end{aligned}$$

Since $d(u) \geq d(v_2)$, it follows that $\sigma_1 > 0$. Now, let E_v (resp. E_u) be the set of edges incident to v (resp. u) in T distinct from v_iv (resp. u_iu), for $1 \leq i \leq 3$. Obviously, $|E_v| = d(v) - 3$ and $|E_u| = d(u) - 3$, so $d(v) \leq d(u)$ implies $|E_v| \leq |E_u|$. The contribution of each edge e from E_v to $\sigma(T') - \sigma(T)$ is $\geq (d(v) - 2)^2 - (d(v) - 1)^2$, and notice that this contribution may be negative. On the other hand, the contribution of each edge e of $|E_u|$ to $\sigma(T') - \sigma(T)$ is $\geq d(u)^2 - (d(u) - 1)^2 > 0$. Since $\sigma_1 > 0$ and the contribution of edges of P to $\sigma(T') - \sigma(T)$ is also strictly positive, we conclude that

$$\begin{aligned}\sigma(T') - \sigma(T) &> |E_v|\,((d(v) - 2)^2 - (d(v) - 1)^2) + |E_u|\,(d(u)^2 - (d(u) - 1)^2) \\ &\geq |E_v|\,((d(v) - 2)^2 - (d(v) - 1)^2 + d(u)^2 - (d(u) - 1)^2) \\ &= |E_v|\,(2d(u) - 2d(v) + 2) > 0,\end{aligned}$$

a contradiction.

To summarize, in each of the two possible cases we have proved that the assumption that there exists an internal leaf u of T with $d(u) < \Delta$ leads to contradiction. We conclude that all internal leaves of T must be of the degree Δ, and we are done. ■

Let us next prove one additional property of maximal trees.

Proposition 7. *Let T be a maximal tree with maximum degree $\Delta \geq 3$ and $n \geq \Delta + 4$. Then $m_{2,2} \leq 2$.*

Proof. Assume to the contrary that $m_{2,2} \geq 3$. Let $e_i = u_iv_i$, for $i \in \{1, 2, 3\}$, be three edges of T with $d(u_i) = d(v_i) = 2$. If all three edges e_i are pairwise vertex disjoint, denote by w_i the other neighbor of v_i, for $i = 1, 2, 3$. Let

$$\begin{aligned}T' &= T - u_3v_3 - v_3w_3 + u_3w_3 - u_2v_2 - v_2w_2 + u_2w_2 \\ &\quad - v_1w_1 + v_1v_2 + v_2w_1 + v_3v_1,\end{aligned}$$

and notice that the contribution of edges v_iw_i and u_iw_i to the difference $\sigma(T') - \sigma(T)$ cancels out for $i \in \{1, 2\}$, while the contribution of edges u_iv_i equals zero. The contribution of edges v_1w_1 and v_2w_1 to the difference also cancels out, so we have

$$\sigma(T') - \sigma(T) = (3 - 2)^2 + (3 - 1)^2 > 0,$$

a contradiction.

Assume next that two of the edges e_i share an end-vertex, say $v_1 = u_2$, and the third edge e_3 is vertex disjoint with e_1 and e_2. Let $T' = T - u_3v_3 - v_3w_3 + u_3w_3 + v_3v_1$, and let us consider again the difference $\sigma(T') - \sigma(T)$. Notice that the contribution of edges v_3w_3 and u_3w_3 to the difference cancels out, the contribution of u_3v_3 equals zero, the contribution of edges u_1v_1 and u_2v_2 equals $(3 - 2)^2 - 0$, so we have

$$\sigma(T') - \sigma(T) = 2(3 - 2)^2 + (3 - 1)^2 > 0,$$

a contradiction.

Assume finally that two pairs of edges e_i share an end-vertex, say $v_1 = u_2$ and $v_2 = u_3$. Let $T' = T - u_3v_3 - v_3w_3 + u_3w_3 + v_3v_1$, and notice that the contribution of the edges v_3w_3 and u_3w_3 to $\sigma(T') - \sigma(T)$ cancels out, the contribution of the edge u_3v_3 is zero, the contribution of edges u_1v_1 and u_2v_2 is $(3 - 2)^2 - 0$, and the contribution of v_3v_1 is $(3 - 1)^2$. Hence, summing all this we again obtain $\sigma(T') - \sigma(T) > 0$, a contradiction. ■

3. Case $\Delta = 5$

In this section we will characterize extremal trees with $\Delta = 5$. In order to do so, we will heavily rely on the property of maximal trees stated in Theorem 6. For Theorem 6 to apply, we will assume throughout the section that considered trees have at least $2\Delta = 10$ vertices. We first wish to show that an extremal tree with $\Delta = 5$ does not contain vertices of degree 3. To arrive to this result, we first need the following two lemmas regarding the edges incident to vertices of degree 3.

Lemma 8. *Let T be a maximal tree on $n \geq 10$ vertices with $\Delta = 5$. Then, $m_{3,3} = 0$.*

Proof. Assume to the contrary that T does contain an edge uv with $d(u) = d(v) = 3$. Denote by u_1 and u_2 (resp. v_1 and v_2) the two remaining neighbors of u (resp. v). Let $T' = T - u_1u - u_2u + u_1v + u_2v$. Notice that

$$\begin{aligned}\sigma(T') - \sigma(T) &\geq (d(u_1) - 5)^2 - (d(u_1) - 3)^2 + (d(u_2) - 5)^2 - (d(u_2) - 3)^2 \\ &\quad + (d(v_1) - 5)^2 - (d(v_1) - 3)^2 + (d(v_2) - 5)^2 - (d(v_2) - 3)^2 \\ &\quad + (5 - 1)^2 - (3 - 3)^2 \\ &= 32 - 4d(u_1) - 4d(u_2) + 32 - 4d(v_1) - 4d(v_2) + 16 \\ &\geq 32 - 4 \cdot 5 - 4 \cdot 5 + 32 - 4 \cdot 5 - 4 \cdot 5 + 16 = 0\end{aligned}$$

with equality if and only if each of the vertices u_1, u_2, v_1 and v_2 has the degree 5. If at least one of the vertices u_1, u_2, v_1, v_2 has a degree distinct from 5, we have a contradiction with T being maximal. So, let us assume each of the vertices u_1, u_2, v_1, v_2 is of degree 5.

Let $T_{u_2v_2}$ be the connected component of $T - u_1u - v_1v$ which contains the edge uv. Since $d(u_2) = 5 > 1$, $T_{u_2v_2}$ must contain an internal leaf z of T, so Theorem 6 implies that $d(z) = 5$. Denote by z_1 and z_2 the two neighbors of z in T which are leaves. Let $T' = T - u_1u - v_1v + u_1z_1 + v_1z_2$. Notice that the contribution of the pair of edges u_1u and u_1z_1, just as the pair v_1v and v_1z_2, to the difference $\sigma(T') - \sigma(T)$ equals $(9 - 4)$. The contribution of each of the edges u_2u and v_2v also equals $(9 - 4)$, and the contribution each of the edges z_1z and z_2z equals $(9 - 16)$. Finally, the contribution of the edge uv is zero, so we have

$$\sigma(T') - \sigma(T) \geq 4(9 - 4) + 2(9 - 16) = 6 > 0,$$

a contradiction with T being maximal. ■

After we have eliminated edges with both end-vertices of degree 3, next we wish to do the same with edges such that one end-vertex is of degree 1 and the other of degree 3.

Lemma 9. *Let T be a maximal tree on $n \geq 10$ vertices with $\Delta = 5$. Then, $m_{1,3} = 0$.*

Proof. Assume to the contrary that T contains an edge uv with $d(u) = 1$ and $d(v) = 3$. Let v_1 and v_2 denote the other two neighbors of v, where we may assume $d(v_1) \leq d(v_2)$. If $d(v_1) = 1$, then v would be an internal leaf of T with $d(v) = 3$, which contradicts Theorem 6. Hence, we may assume $d(v_1) \geq 2$. Lemma 8 implies $3 \notin \{d(v_1), d(v_2)\}$.

If $d(v_1) = 2$, let x denote the neighbor of v_1 distinct from v. Let $T' = T - xv_1 + xv$, and notice that the contribution of the edge uv to $\sigma(T') - \sigma(T)$ is $(9 - 4)$, the contribution of the edge v_1v is $(9 - 1)$, so we have

$$\begin{aligned}\sigma(T') - \sigma(T) &= (9 - 4) + (9 - 1) + (d(x) - 4)^2 - (d(x) - 2)^2 + (d(v_2) - 4)^2 - (d(v_2) - 3)^2 \\ &= 32 - 4d(x) - 2d(v_2) \geq 2 > 0,\end{aligned}$$

a contradiction with T being maximal.

If $d(v_1) \geq 4$, let us consider internal leaves of T. If v_1 and v_2 are the only two internal leaves of T, then $d(v_1) = d(v_2) = 5$. Let $T' = T - v_1v + v_1u$, and notice that the sum of contributions of edges v_1v and v_1u to $\sigma(T') - \sigma(T)$ is $(9 - 4)$, the contribution of the edge uv is $(0 - 4)$, and of v_2v is $(9 - 4)$. Hence, we obtain

$$\sigma(T') - \sigma(T) = 2(9 - 4) + (0 - 4) = 6 > 0$$

a contradiction. So, we may assume that there exists an internal leaf z in T distinct from v_1 and v_2.

Let w be the only neighbor of z which is not a leaf. Let $T' = T - uv - zw + wu + uz$. Notice that each of the edges v_1v and v_2v contributes to $\sigma(T') - \sigma(T)$ with at least $(4 - 1)$, and the edges uv and uz taken together contribute at least $(9 - 4)$. Hence, it holds that

$$\begin{aligned}\sigma(T') - \sigma(T) &\geq ((d(w) - 2)^2 - (d(w) - 5)^2) + (9 - 4) + 2(4 - 1) \\ &= 6d(w) - 10 \geq 2 > 0,\end{aligned}$$

a contradiction with T being maximal, so we are done. ■

We are now in a position to prove that a maximal tree with $\Delta = 5$ does not contain vertices of degree 3.

Lemma 10. *Let T be a maximal tree on $n \geq 10$ vertices with $\Delta = 5$. Then, $n_3 = 0$.*

Proof. Assume to the contrary that T does contain a vertex u with $d(u) = 3$. Denote by u_1, u_2 and u_3 the three neighbors of u, and we may assume that $d(u_1) \leq d(u_2) \leq d(u_3)$. Lemmas 8 and 9 imply that the degrees of u_1, u_2 and u_3 take their values from the set $\{2, 4, 5\}$.

Assume first that $d(u_1) = d(u_2) = d(u_3) = 2$. Denote by x the neighbor of u_1 distinct from u, and let $T' = T - xu_1 + xu$. Notice that the contribution of each of the edges u_2u and u_3u to $\sigma(T') - \sigma(T)$ is $(4 - 1)$, and the contribution of u_1u is

$(9-1)$. We obtain

$$\begin{aligned}\sigma(T')-\sigma(T) &= 2(4-1)+(9-1)+(d(x)-4)^2-(d(x)-2)^2\\ &= 26-4d(x)\geq 6>0,\end{aligned}$$

a contradiction.

Assume next that $d(u_1)=d(u_2)=2$ and $d(u_3)\geq 4$. Denote by x and y the neighbor of u_1 and u_2, respectively, distinct from u. Let $T'=T-xu_1-yu_2+xu+yu$ and consider the difference $\sigma(T')-\sigma(T)$. Notice that the contribution of each of the edges u_1u and u_2u to the difference is $(16-1)$, and since $d(u_3)\in\{4,5\}$ the contribution of the edge u_3u is at least $(0-4)$, so we have

$$\begin{aligned}\sigma(T')-\sigma(T) &\geq ((d(x)-5)^2-(d(x)-2)^2)+((d(y)-5)^2-(d(y)-2)^2)\\ &\quad +\ 2(16-1)+(0-4)\\ &= 68-6d(y)-6d(x)\geq 8>0,\end{aligned}$$

a contradiction.

Assume further that $d(u_1)=2$ and $d(u_2)\geq 4$, which implies $d(u_3)\geq 4$ also. If $d(u_2)=4$, let $T'=T-u_1u+u_1u_2$ and consider the difference $\sigma(T')-\sigma(T)$. The edges u_1u and u_1u_2 taken together contribute $(9-1)$ to the difference, the edge u_2u contributes $(9-1)$, and the edge u_3u contributes at least $(4-1)$. Also, each of the three edges incident to u_2 distinct from u_2u contributes at least $(0-1)$. We conclude that

$$\sigma(T')-\sigma(T)\geq 2(9-1)+(4-1)+3(0-1)=16>0,$$

a contradiction. On the other hand, if $d(u_2)=5$, then $d(u_3)=5$ also. Let z be a leaf of T contained in the same component of $T-u_1u$ as u. Let $T'=T-u_1u+u_1z$, and notice that each of the edges u_2u and u_3u contributes to $\sigma(T')-\sigma(T)$ by $(9-4)$. The pair of edges u_1u and u_1z taken together contributes $(0-1)$, and the edge incident to z in T contributes no less than $(9-16)$. We obtain

$$\sigma(T')-\sigma(T)\geq 2(9-4)+(0-1)+(9-16)=2>0,$$

a contradiction.

Assume finally that $d(u_1)\geq 4$. Let z be a leaf of T contained in the same component of $T-u_1u$ as u. Let $T'=T-u_1u+u_1z$ and notice that each of the edges u_iu, given that $d(u_i)\in\{4,5\}$ contributes to $\sigma(T')-\sigma(T)$ either $(4-1)$ or $(9-4)$. Similarly, the edge incident to z in T contributes no less than $(9-16)$. Assuming the smallest possible contribution of edges u_iu, which is the worst case, we still have

$$\sigma(T')-\sigma(T)\geq 3(4-1)+(9-16)=2>0,$$

a contradiction, so we are done. ■

Next, we wish to establish that a maximal tree T with Δ does not contain a vertex of degree 4 either. Again, we will arrive to this result through the following two lemmas regarding the edges incident to a vertex of degree 4.

Lemma 11. *Let T be a maximal tree on $n\geq 10$ vertices with $\Delta=5$. Then, $m_{2,4}=0$.*

Proof. Assume to the contrary that T contains an edge uv with $d(u)=2$ and $d(v)=4$. Denote by u_1 the only neighbor of u distinct from v. Also, denote by v_1, v_2 and v_3 the three neighbors of v distinct from u. Let $T'=T-u_1u+u_1v$, and notice that the contribution of the edge uv to $\sigma(T')-\sigma(T)$ is $16-4$. Also, considering all the possible degrees of u_1, the contribution of the edges u_1u and u_1v taken together is no less than $(0-9)$. Similarly, considering all the possible degrees of v_i, the contribution of each edge v_iv is no less than $(0-1)$. We obtain

$$\sigma(T')-\sigma(T)\geq(16-4)+(0-9)+3(0-1)=0$$

with equality if and only if $d(u_1)=d(v_1)=d(v_2)=d(v_3)=\Delta$. If at least one of these degrees is not equal to Δ, then we have a contradiction with T being maximal. So, let us assume that all these degrees are indeed equal to Δ.

Let T_v be the connected component of $T-v_1v-v_2v$ which contains v. Since $d(v_3)=\Delta$, there exists an internal leaf z in the connected component of $T-v_1v-v_2v$ which contains v_3. By Theorem 6 we know $d(z)=\Delta$. Let z_1 and z_2 be two leaves attached to z in T. Now, let $T'=T-v_1v-v_2v+v_1z_1+v_2z_2$ and notice that the contribution to $\sigma(T')-\sigma(T)$ of the pair of edges v_iv and v_iz_i taken together is $(9-1)$, for $i\in\{1,2\}$, since $d(v_i)=5$. The contribution of the edge uv is $(0-4)$, the contribution of the edge v_3v is $(9-1)$, and the contribution of each of the edges z_iz, for $i\in\{1,2\}$, is $(9-16)$. Therefore, it holds that

$$\sigma(T')-\sigma(T)=2(9-1)+(0-4)+(9-1)+2(9-16)=6>0,$$

so we again have a contradiction. ■

We next wish to show that a maximal tree cannot contain an edge with one end-vertex of degree 1 and the other 4.

Lemma 12. *Let T be a maximal tree on $n \geq 14$ vertices with $\Delta = 5$. Then, $m_{1,4} = 0$.*

Proof. Assume to the contrary that T contains an edge uv with $d(u) = 1$ and $d(v) = 4$. Denote by v_1, v_2 and v_3 the three neighbors of v distinct from u, where we may assume $d(v_1) \leq d(v_2) \leq d(v_3)$. Notice that $d(v_2) = 1$ would imply $d(v_1) = 1$ also, so v would be an internal leaf of T with $d(v) = 4 < \Delta$, a contradiction with Theorem 6. Hence, we may assume $d(v_2) \geq 2$. Lemmas 10 and 11 imply $4 \leq d(v_2) \leq d(v_3)$. The same two lemmas imply that $d(v_1) = 1$ or $d(v_1) \geq 4$.

Assume first that $d(v_1) = 1$. If $d(v_2) = d(v_3) = 4$, let $T' = T - uv - v_1v + uv_2 + v_1v_3$, and notice that the contribution of the pair uv and uv_2 taken together to $\sigma(T') - \sigma(T)$ is $(16 - 9)$. The same holds for the pair v_1v and v_1v_3. Each of the edges v_iv, for $i \in \{2, 3\}$, contributes to the difference by $(9 - 0)$. Finally, each of the remaining six edges incident to v_2 and v_3 contributes no less than $(0 - 1)$. We conclude that

$$\sigma(T') - \sigma(T) \geq 2(16 - 9) + 2(9 - 0) + 6(0 - 1) = 26 > 0,$$

a contradiction.

If $d(v_2) = 4$ and $d(v_3) = 5$, then let $T' = T - v_1v + v_1v_2$. The contribution to $\sigma(T') - \sigma(T)$ of the pair $v_1v + v_1v_2$ taken together is $(16 - 9)$, of uv is $(4 - 9)$, of v_2v is $(4 - 0)$ and of v_3v is $(4 - 1)$. Also, the contribution of the remaining three edges incident to v_2 is no less than $(0 - 1)$, which yields

$$\sigma(T') - \sigma(T) \geq (16 - 9) + (4 - 9) + (4 - 0) + (4 - 1) + 3(0 - 1) = 6 > 0,$$

again a contradiction.

Finally, if $d(v_2) = d(v_3) = 5$, notice that $n \geq 14$ implies that T contains an internal leaf w distinct from v_2 and v_3. Denote by z the non-leaf neighbor of w. Lemma 10 implies $d(z) \neq 3$.

Let us first assume $d(z) \geq 4$. Let $T' = T - uv - wz + wu + uz$, and notice that the contribution to $\sigma(T') - \sigma(T)$ of the pair uv and uw taken together is 0. Considering all the possible values of z, the contribution of the pair wz and uz is no less than $(4 - 1)$. The contribution of v_1v is $(4 - 9)$, and the contribution of each of v_2 and v_3 is $(4 - 1)$. We obtain

$$\sigma(T') - \sigma(T) \geq (4 - 1) + (4 - 9) + 2(4 - 1) = 4 > 0,$$

a contradiction. So, we may assume $d(z) \leq 3$.

If $d(z) = 3$, let $T' = T - uv - v_1v + uz + v_1z$, and notice that the pair uv and uz taken together contributes to $\sigma(T') - \sigma(T)$ by $(16 - 9)$. The same holds for the pair v_1v and v_1z. Each of the edges v_2v and v_3v contributes $(9 - 1)$. The edge zw contributes $(0 - 4)$, and the two remaining edges incident to z contribute no less than $(0 - 4)$. Hence, we have

$$\sigma(T') - \sigma(T) \geq 2(16 - 9) + 2(9 - 1) + (0 - 4) + 2(0 - 4) = 18 > 0,$$

a contradiction.

If $d(z) = 2$, let $T' = T - uv - v_1v - v_2v - v_3v + v_2v_3 + uz + vz + v_1z$. Let x be the neighbor of z distinct from w, and notice that the edge zx contributes to $\sigma(T)$ by no less than $(1 - 9)$. As for the other edges, notice that all edges incident to v in T contribute to $\sigma(T)$ by $1 + 1 + 9 + 9$, also zw contributes to $\sigma(T)$ by 9. In T', all edges incident to z except xz contribute to $\sigma(T')$ by $16 + 16 + 16 + 0$, and the edge v_2v_3 contributes to $\sigma(T')$ by 0. We conclude

$$\sigma(T') - \sigma(T) \geq (1 - 9) + (16 + 16 + 16 + 0) - (1 + 1 + 9 + 9) = 20 > 0,$$

a contradiction.

Assume now that $d(v_1) \geq 4$. Denote by z an internal leaf of T distinct from v_1, v_2 and v_3, if such a vertex z exists. Let x be the only neighbor of z which is not a leaf and by y a neighbor of z which is a leaf. Let $T' = T - uv - xz - uv_1 + xu + uz + v_1y$ and notice that

$$\sigma(T') - \sigma(T) \geq (9 - 0) + (0 - 0) + (4 - 0) + (9 - 16) + 2(4 - 0) = 14 > 0,$$

so we have a contradiction.

It remains to consider the case of $d(v_1) \geq 4$ when v_1, v_2 and v_3 are the only internal leaves of T. If $d(v_1) = 4$, let $T' = T - uv + uv_1$. Notice that the contribution of the edges uv and uv_1 considered together to $\sigma(T') - \sigma(T)$ is $16 - 9$, the contribution of all the remaining edges is non-negative, so $\sigma(T') - \sigma(T) > 0$. If $d(v_1) = 5$, let $T' = T - v_1v + uv_1$. The contribution to $\sigma(T') - \sigma(T)$ of the edges v_1v and uv_1 taken together is $9 - 1$, of the edge uv is $1 - 9$, and for each of the edges v_2v and v_3v is $4 - 1$. We conclude

$$\sigma(T') - \sigma(T) \geq (9 - 1) + (1 - 9) + 2(4 - 1) = 6 > 0,$$

a contradiction. ■

Using the above two lemmas we can now establish that a maximal tree T does not contain a vertex of degree 4 either.

Lemma 13. *Let T be a maximal tree on $n \geq 14$ vertices with $\Delta = 5$. Then, $n_4 = 0$.*

Proof. Assume to the contrary that T does contain a vertex u with $d(u) = 4$. Denote by u_i, for $i = 1, \dots, 4$, the four neighbors of u. We may assume that $d(u_1) \le d(u_2) \le d(u_3) \le d(u_4)$. Lemmas 10–12 imply $d(u_1) \ge 4$. Since all internal leaves of T are of degree 5 and a vertex of degree 4 can only be neighbor to vertices of degree 4 or 5, we may assume $d(u_4) = 5$. Let z be an internal leaf of T contained in the same connected component of $T - u_1u - u_2u$ as u. Theorem 6 implies that $d(z) = 5$. Denote by x and y two leaves attached to z. Let $T' = T - u_1u - u_2u + u_1x + u_2y$ and notice that

$$\sigma(T') - \sigma(T) \ge (4-0) + (9-1) + 2(4-0) + 2(9-16) = 6 > 0,$$

so we obtain a contradiction with T being maximal. ■

Lemmas 10 and 13 imply the following corollary.

Corollary 14. *Let T be a maximal tree on $n \ge 14$ vertices with $\Delta = 5$. Then T contains only vertices of degrees 1, 2 and Δ.*

In order to fully characterize extremal trees with $\Delta = 5$, we need the following lemmas regarding the number and the position of vertices of the degree 2 in extremal trees.

Lemma 15. *Let T be a maximal tree on $n \ge 14$ vertices with $\Delta = 5$. Then, $m_{2,2} \le 1$. Moreover, if $m_{2,2} = 1$, then $m_{\Delta,\Delta} = 0$.*

Proof. Assume to the contrary that $m_{2,2} \ge 2$. Suppose first that all edges with both end-vertices of degree two are vertex disjoint. Denote by uv and ab a pair of edges with $d(u) = d(v) = d(a) = d(b) = 2$. Let u_1, v_1, a_1 and b_1 be the neighbors of u, v, a and b, respectively, which is not contained in $\{u, v, a, b\}$. Since all edges with both end-vertices of degree two are vertex disjoint, we conclude that $d(u_1) = d(v_1) = d(a_1) = d(b_1) = 5$. Let z be an internal leaf in T, and z_1 a leaf attached to z. Theorem 6 implies $d(z) = 5$. Denote by T' the tree obtained from T by removing all edges incident to vertices u, v, a and b, and then adding edges u_1v_1, a_1b_1, uz_1, vz_1, az_1 and bz_1. Notice that

$$\sigma(T') - \sigma(T) \ge 4(16-9) + (0-16) = 12 > 0,$$

and we have a contradiction.

Suppose next that not all such edges are vertex disjoint, i.e. that there exist two edges uv and vw in T with $d(u) = d(v) = d(w) = 2$. Denote by u_1 and w_1 the neighbor of u and w, respectively, which is not contained in $\{u, v, w\}$.

Assume first that there exists a vertex $z \notin \{u, v, w\}$ in T of degree 2. Denote by z_1 and z_2 its two neighbors, and let x be a leaf in T. Let T' be the tree obtained from T by removing all edges incident to vertices u, v, w, z and then adding edges u_1w_1, z_1z_2, xu, xv, xz and xw. Notice that

$$\sigma(T') - \sigma(T) \ge (0-9) + (16-9) + (0-0) + (16-0) + 2(16-9) = 28 > 0,$$

a contradiction.

Assume next that $\{u, v, w\}$ are all vertices of T of degree 2. Since $n \ge 14$, there exists a non-leaf vertex in T not contained in $\{u, v, w, u_1, w_1\}$. Hence, Corollary 14 implies that T contains an edge xy with $d(x) = d(y) = 5$. Let $T' = T - uv - vw - xy + uw + xv + yv$ and notice that

$$\sigma(T') - \sigma(T) \ge 2(9-0) > 0,$$

a contradiction. Hence, we have established that T contains at most one edge with both end-vertices of degree 2.

Finally, let us assume that T contains an edge with both end-vertices of the degree 2, denote them by u and v. We wish to establish that in such a case T does not contain an edge with both end-vertices of degree Δ. Assume to the contrary that T does contain such an edge xy. Denote by u_1 the neighbor of u distinct from v, and let $T' = T - u_1u - uv - xy + u_1v + xu + uv$. Notice that edges u_1u and u_1v contribute to $\sigma(T') - \sigma(T)$ by $(9-9)$, the edges uv and ux by $(9-0)$, and the edges xy and xu by $(9-0)$, so we have

$$\sigma(T') - \sigma(T) \ge (9-9) + 2(9-0) > 0,$$

a contradiction. ■

Lemma 16. *Let T be a maximal tree on $n \ge 14$ vertices with $\Delta = 5$. Then, $m_{\Delta,\Delta} \le 3$.*

Proof. Assume to the contrary that $m_{\Delta,\Delta} \ge 4$. Suppose first that every internal leaf of T is adjacent to a vertex of degree 2. Let u be an internal vertex of T, v its neighbor of degree 2 and w the other neighbor of v. Let xy be an edge of T with $d(x) = d(y) = \Delta$. For the tree $T' = T - uv - vw - xy + uw + xv + vy$ it obviously holds that $\sigma(T') = \sigma(T)$. Hence, we may consider only trees T in which at least one internal leaf is adjacent to a vertex of degree Δ.

Let u be an internal leaf of T and v its neighbor of degree Δ. Denote by u_i, for $i = 1, 2, 3, 4$, a leaf attached to u. Assume first that T contains precisely four edges with both end-vertices of the degree Δ. Denote by a_i and b_i, for $i = 1, 2, 3$, the six vertices of T distinct from u such that $d(a_i) = d(b_i) = \Delta$ and a_ib_i is the edge of T. We define the following two sets of edges

$$E^- = \{u_iu : i = 1, \dots, 4\} \cup \{a_ib_i : i = 1, 2, 3\};$$
$$E^+ = \{a_iu_i, u_ib_i : i = 1, 2\} \cup \{a_3u_3, u_3u_4, u_4b_3\}.$$

Let $T' = T - E^- + E^+$ and notice that T' must be a tree, since the removed edges u_iu are incident to leaves, and the removed edges a_ib_i are replaced by subpaths connecting a_i and b_i which contain vertices u_i. Now, each of the edges u_iu contributes to $\sigma(T') - \sigma(T)$ by -16, the fifth edge incident to u by 16, each of the edges a_ib_i by 0, each of the edges a_iu_i and u_ib_i by 9, and the edge u_3u_4 by 0. So, we obtain

$$\sigma(T') - \sigma(T) = 4 \cdot (-16) + 16 + 6 \cdot 9 = 6 > 0,$$

a contradiction.

Assume next that T contains at least five edges with both end-vertices of the degree Δ. We assume that one of them is incident to an internal leaf u, and let u_i be a leaf attached to u for $i = 1, \dots, 4$. Denote by a_i and b_i, for $i = 1, \dots, 4$, the vertices of T with $d(a_i) = d(b_i) = \Delta$ such that a_ib_i is an edge of T. We again define sets

$$E^- = \{u_iu : i = 1, \dots, 4\} \cup \{a_ib_i : i = 1, \dots, 4\};$$
$$E^+ = \{a_iu_i, u_ib_i : i = 1, \dots, 4\}.$$

Let $T' = T - E^- + E^+$ and notice that each of the edges u_iu contributes to $\sigma(T') - \sigma(T)$ by -16, the fifth edge incident to u by 16, each of the edges a_ib_i by 0, and each of the edges a_iu_i and u_ib_i by 9. Hence,

$$\sigma(T') - \sigma(T) = 4 \cdot (-16) + 16 + 8 \cdot 9 = 24 > 0,$$

a contradiction. ■

All the above lemmas yield that a maximal tree T with $\Delta = 5$ and $n \geq 14$ has the following properties:

(P_1) T contains only vertices of degrees 1, 2 and Δ;
(P_2) all internal leaves of T are of degree Δ;
(P_3) $m_{\Delta,\Delta} \leq 3$ and $m_{2,2} \leq 1$;
(P_4) if $m_{2,2} = 1$, then $m_{\Delta,\Delta} = 0$.

Denote by $\mathcal{T}_{n,\Delta}$ the family of all trees on $n \geq 8$ vertices with maximum degree $\Delta = 5$ which satisfy the properties (P_1)-(P_4). In the next theorem we establish that all trees of $\mathcal{T}_{n,\Delta}$ are maximal.

Theorem 17. *Let T be a tree with $\Delta = 5$ and $n \geq 14$. The tree T is maximal if and only if T belongs to $\mathcal{T}_{n,\Delta}$.*

Proof. If T is maximal, then T has all the properties (P_1)-(P_4), so T belongs to $\mathcal{T}_{n,\Delta}$. Conversely, if T belongs to $\mathcal{T}_{n,\Delta}$ we wish to prove that T is maximal. It is sufficient to show that all trees from $\mathcal{T}_{n,\Delta}$ have the same value of σ-irregularity. Let T be a tree from $\mathcal{T}_{n,\Delta}$. Denote by n_i the number of vertices of degree i in T. Property (P_1) implies $n_1 + n_2 + n_5 = n$. Due to Handshaking lemma, we also have $5n_5 + 2n_2 + n_1 = 2(n - 1)$. Next, consider the tree T' obtained from T by consecutive suppressions of vertices of degree 2 until there are no such vertices left. Notice that $m_{\Delta,\Delta}(T') - 3 \leq n_2(T) \leq m_{\Delta,\Delta}(T') + 1$, which implies that in T we have $n_2 = n_5 - 4 + j$ for $0 \leq j \leq 4 = \Delta - 1$.

Taking all the equations together, we have obtained a system of three linear equations in terms of n_1, n_2 and n_5 with the solution

$$n_1 = \frac{1}{5}(3n - 3j + 16), \quad n_2 = \frac{1}{5}(n + 4j - 18), \quad n_5 = \frac{1}{5}(n - j + 2).$$

In order for n_1, n_2 and n_5 to be integers, it must hold $j \equiv (n - 2) \bmod 5$. Since $0 \leq j \leq 4 = \Delta - 1$, we conclude that the value of j is determined by the value of n. This further implies that n_1, n_2 and n_3 are also determined by the value of n, i.e. the values of n_1, n_2 and n_3 do not depend on a tree T. Further, for a tree T it holds that $m_{1,\Delta} = n_1$ and

$$m_{2,\Delta} = \begin{cases} 2n_2 & \text{if } m_{2,2} = 0; \\ 2n_2 - 1 & \text{if } m_{2,2} = 1. \end{cases}$$

Since $m_{2,2} = 1$ if and only if $j = 4$, this implies that $m_{1,\Delta}$ and $m_{2,\Delta}$ are determined by the value of n. Notice that the property (P_2) implies $m_{1,2} = 0$, while $m_{\Delta,\Delta}$ may be greater than zero, but the contribution of such edges to $\sigma(T)$ equals zero. We conclude that $\sigma(T) = m_{1,\Delta}(\Delta - 1)^2 + m_{2,\Delta}(\Delta - 2)^2$, which implies that the value of $\sigma(T)$ is determined by n and it does not depend on T. ■

The above theorem yields the following corollary (see Fig. 2).

Corollary 18. *Let T be a maximal tree with $\Delta = 5$ and $n = \Delta k - 2 + j \geq 14$, where $0 \leq j \leq \Delta - 1$. Then,*

$$\sigma(T) = \begin{cases} \frac{1}{5}(3n - 3j + 16)(\Delta - 1)^2 + \frac{2}{5}(n + 4j - 18)(\Delta - 2)^2 & \text{if } j \neq 4, \\ \frac{1}{5}(3n - 3j + 16)(\Delta - 1)^2 + \frac{1}{5}(8j + 2n - 41)(\Delta - 2)^2 & \text{if } j = 4. \end{cases}$$

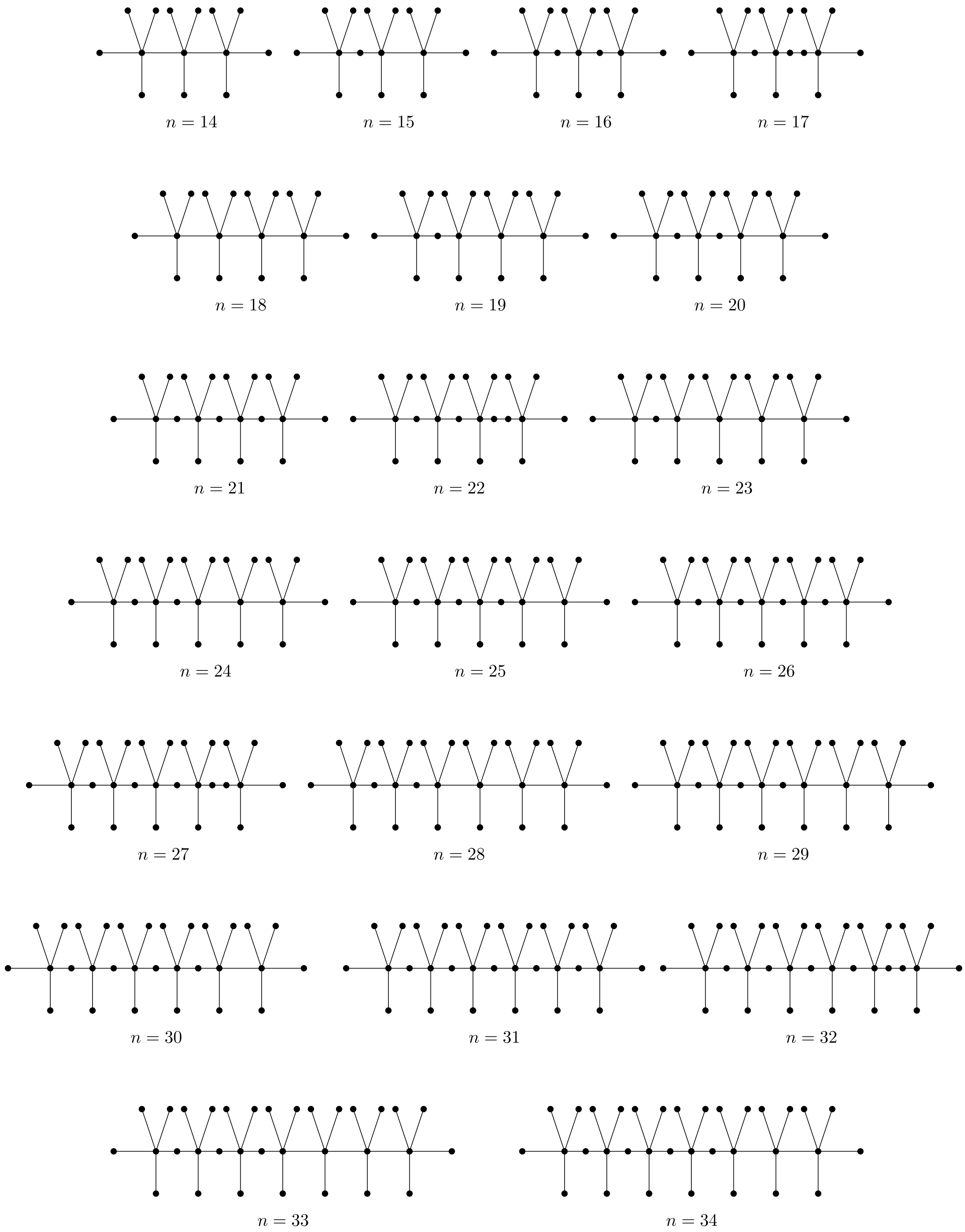

Fig. 2. Maximal trees T on n vertices with $\Delta = 5$, for $14 \leq n \leq 34$. (Mind that the list is not complete.).

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Data availability

No data was used for the research described in the article.

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