Discrete Mathematics and Theoretical Computer Science DMTCS vol. **14:1**, 2012, 159–174

α-Labelings and the Structure of Trees with Nonzero α-Deficit

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received 4th April 2011, *revised 4th May 2012*, *accepted 4th June 2012*.

We present theoretical and computational results on α-labelings of trees. The theorems proved in this paper were inspired by the results of a computer investigation of α-labelings of all trees with up to 26 vertices, all trees with maximum degree 3 and up to 36 vertices, all trees with maximum degree 4 and up to 32 vertices and all trees with maximum degree 5 and up to 31 vertices. We generalise a criterion for trees to have nonzero α-deficit, and prove an unexpected result on the α-deficit of trees with a vertex of large degree compared to the order of the tree.

Keywords: α-labeling, α-deficit, Graceful Tree Conjecture

1 Introduction

Let $G = (V, E)$ be a graph such that $n = |V|$. A *labeling* of G is an injective function f from V to the set of integers $\{0, 1, \ldots, |E|\}$. The induced label of each edge xy is $|f(x) - f(y)|$. If the resulting edge labels are distinct, then the labeling is said to be *graceful*. This notion was introduced by Rosa (1967) and many other graph labeling schemes have been proposed since (see Gallian (2009) for a regularly updated survey with more than one thousand references).

If T is a tree, then the function f is bijective and the set of possible vertex labels is $\{0, 1, \ldots, n-1\}$. A labeling of T is thus graceful if each integer from 1 to $n-1$ is assigned to an edge. The well known *Graceful Tree Conjecture*[(i)] states that every tree has a graceful labeling. Despite much effort, this conjecture is still open. However, some specific classes of trees are known to have a graceful labeling. Among them are: trees with at most 27 vertices (Aldred and McKay); trees with diameter at most 5 (Hrnčiar and Haviar (2001); Zhao (1989)); caterpillars (trees where the deletion of pendant vertices leaves a path, Rosa (1967));

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(i) This conjecture is also known as the Ringel-Kotzig or Rosa conjecture.

symmetrical trees (rooted trees in which all the vertices at the same level have the same degree, Poljak and Sûra (1982); Bermond and Sotteau (1976)) and olive trees (rooted trees constructed from k branches such that the ith branch is a path of length i, Abhyankar and Bhat-Nayak (2000); Pastel and Raynaud (1978)). We refer to Alfalayleh et al. (2004) for a survey on known results towards proving the Graceful Tree Conjecture.

A labeling f is *bipartite* if there exists an integer k such that for each edge xy either $f(x) \leq k < f(y)$ or $f(y) \leq k < f(x)$. A graceful labeling that is bipartite is an α-*labeling* (Rosa and Širáň (1995)). Unlike graceful labelings, there are several examples of trees that do not have an α-*labeling*. The α-size $\alpha(T)$ of a tree T is defined as the maximum number of distinct edge labels over all bipartite labelings of T.

Let $\alpha(n)$ be the smallest α-size among all trees with n vertices and $\alpha_3(n)$ be the smallest α-size among all trees with maximum degree 3 and n vertices. Rosa and Širáň (1995) proved that $5n/7 \leq \alpha(n) \leq (5n+4)/6$ for all $n \geq 4$. Bonnington and Širáň (1999) showed that $\alpha_3(n) \geq 5n/6$ for all $n \geq 12$. This last bound was improved by Brankovic et al. (2005b) to $\alpha_3(n) \geq \lfloor 6n/7 \rfloor - 1$. In the case of trees with maximum degree 3 which have a perfect matching, Brankovic et al. (2005a) further improved the bound to $\alpha_3(n) \geq \lceil ((k-1)n)/k \rceil - 1$ where $2k$ is the lower bound on the number of vertices of a tree with maximum degree 3 having a perfect matching that does not admit an α-labeling.

In order to emphasize the fact that we are mainly interested in how close we can come to an α-labeling, instead of using the α-size of a tree T, we use the α-deficit α_{def} defined as $n - 1 - \alpha(T)$.

The parameter α_{def} measures how far a tree is from having an α-labeling as it counts the minimum number of errors, that is, the minimum number of edge labels that are missing from the set of all possible labels. Trees with an α-labeling have deficit 0.

The main contributions of this paper are the two theorems stated here and the results of extensive computations which are presented in Section 2 and in Appendix A.

Let $T = (V, E)$ be a tree with bipartition classes V_1 and V_2 and a bipartite labeling $l : V \to \{0, \ldots, |V| - 1\}$. Define the edge parity of T to be $(\sum_{i=1}^{|E|} i) \mod 2 = \frac{1}{2}(|V| - 1)|V| \mod 2$. So if l is an α-labeling this is the sum of all edge labels modulo 2; it is 0 if $|V| \equiv 0, 1 \mod 4$ and 1 if $|V| \equiv 2, 3 \mod 4$.

Define the vertex parity of T to be $(\sum_{v \in V} \deg(v) l(v)) \mod 2$, or equivalently, to be the parity of the number of vertices of odd degree with odd label.

Theorem 1.1. *In a tree T with α-deficit 0 the edge parity and the vertex parities are equal.*

This theorem provides an explanation for the existence of trees with positive α-deficit, and moreover, as a consequence we can construct infinitely many such trees. The second theorem is very different to the results mentioned earlier in this section; it implies that under certain conditions, if there is a tree with n vertices and α-deficit d, then for all integers $n' > n$ there will also be a tree of the same deficit.

Theorem 1.2. *For all $k, d \in \mathbb{N}$ and $n \geq k^2 + k$, the number of trees T with n vertices, $\alpha_{def}(T) = d$ and maximum degree $n - k$ is the same.*

These theorems were suggested by computations of the α-deficit of all trees with up to 26 vertices and of trees with up to 36 vertices for several classes. These computations go far beyond anything that has been done before. To the best of our knowledge, until now only data on the α-deficit of trees up to 17 vertices was known; this appears in Van Bussel (2000). The results of our computations, presented in Appendix A, shed new light on the α-deficit; they support conjectures in the literature and also give rise to some surprising new conjectures about the α-deficit of general trees and trees with bounded degree.

The two theorems above are proved in Sections 4 and 5, a new proof of a theorem on m-comets is given in Section 3.1 and new conjectures are presented in the final section.

2 Computational results

Appendix A contains the numbers of trees with nonzero α-deficit for each vertex number up to 26.

The smallest trees for a given deficit d were stars with the central vertex of degree $3 \cdot d$ and each edge subdivided. These trees were called *comets* by Rosa and Širáň (1995). Note that comets are not necessarily the trees that have the smallest maximum degree for a given deficit.

In the tables in Appendix A the following things catch the eye:

- At the end of the lines with α-deficit one and two some series of numbers seem to grow that are repeated in every table for larger vertex numbers.
- While for small vertex numbers it looks like trees with maximum degree 3 and deficit are not unusual, they become sparse later.
- For maximum degree 3 and 4 no trees with α-deficit larger than one occur.

In order to better understand the first observation we investigated the trees with nonzero deficit and a given maximum degree depending on the number of vertices. For $|V| \in \{7, \dots, 26\}$ there is always exactly one tree with maximum degree $|V| - 4$ and nonzero deficit. We tested the conjecture that this tree is in fact always the smallest tree in the series – that is the 3-comet depicted in Figure 1 – with the center of a star with $|V| - 6$ vertices identified with the (unique) vertex of degree 3. As far as the list goes this turned out to be the case.

In fact a similar statement is true for all $k \in \{4, \dots, 10\}$: for each of these k there is a smallest number $m_+(k)$ such that the number of trees with $n \geq m_+(k)$ vertices, nonzero deficit and maximum degree $n - k$ stays constant (within the reach of these tables). In fact we have $m_+(4) = 7$, $m_+(5) = 9$, $m_+(6) = 11$, $m_+(7) = 13$, $m_+(8) = 15$, $m_+(9) = 18$ and $m_+(10) = 19$. In all cases the trees with $m_+(k), m_+(k) + 1, \dots, 26$ vertices were just the trees with $m_+(k)$ vertices plus the center of a star identified with a vertex of maximum degree of the original tree. Nevertheless there are examples when adding edges to a vertex of maximum degree in a tree can increase or decrease the deficit. In Section 5 we will prove that if you add enough pendant edges to the same vertex, the deficit will stay constant after some time. This gives an upper bound for the function $m(k)$ defined there which is similar to $m_+(k)$ but without the restriction to numbers in the table and trees with positive deficit.

For $k > 10$ no conclusions based on the computed results are possible, but the step from $m_+(10)$ to $m_+(11)$ seems to be astonishingly large.

The last two observations were a motivation to run more tests on trees with the maximum degree restricted to 3 and 4. The results are given in Tables 1 and 2.

$\lvert V\rvert$	7	8	9	10	12	15	23	31
	1	1	1	2	1	1	2	6

Tab. 1: The number of trees with maximum degree 3 and α-deficit 1. For vertex numbers $n \leq 36$ that are not mentioned, no trees with deficit exist. Trees with maximum degree 3 and α-deficit larger than 1 do not exist within this range.

Note that although trees with maximum degree 3 and α-deficit seem to get sparse for $|V| > 15$, in steps of 8 vertices deficitary trees seem to exist. Most (though not all) of the trees on 37 vertices have been tested without finding a tree with deficit.

Figures 1, 2 and 3 give all deficitary trees with maximum degree 3 that were found in this computation. Note that from 15 vertices on all deficitary maximum degree 3 trees that were found in this search come

$\lvert V\rvert$	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
	1	3	5	11	15	22	24	27	25	28	19	23	6	15	2	15	2

$\lvert V\rvert$	25	26	27	28	29	30	31	32
	26	0	63	0	152	0	271	0

Tab. 2: The number of trees with maximum degree 4 and α-deficit 1. Trees with maximum degree 4 and α-deficit larger than 1 do not exist within this range.

$\alpha_{\text{def}}\backslash\lvert V\rvert$	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	1	3	7	17	30	58	85	133	187	260	338	393	430	461	488	495
2	0	0	0	0	0	0	0	1	1	1	1	1	2	2	2	2

$\alpha_{\text{def}}\backslash\lvert V\rvert$	25	26	27	28	29	30	31
1	540	513	607	473	660	398	680
2	1	1	0	0	0	0	0

Tab. 3: The number of trees with maximum degree 5 and positive α-deficit. Trees with maximum degree 5 and α-deficit larger than 2 do not exist within this range.

from subdividing all edges of smaller trees. It would be interesting to know whether this is true also for $|V| > 36$.

The most striking property of Table 2 seems to be that for $n \in \{26, 28, 30, 32\}$ no deficitary trees exist, while for odd vertex numbers (and smaller even vertex numbers) a lot of deficitary trees exist. A possible explanation is given in Section 4.

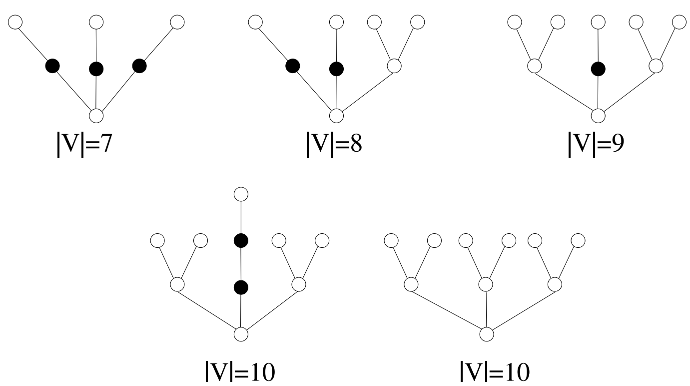

Fig. 1: Deficitary trees with maximum degree 3 up to 10 vertices. They were first given in Bonnington and Širáň (1999).

Inside the range of our computations maximum degree 5 is the smallest value that also allows deficit 2. Nevertheless up to 26 vertices only a small number of trees T with $\Delta(T) = 5$ have deficit 2 – at most 2 per vertex number. This motivated us to test trees with maximum degree 5 and more than 26 vertices. The results are given in Table 3. So it seems possible that α-deficit equal to two is only a local phenomenon for small trees with maximum degree 5 and that for more than 26 vertices the maximum deficit is also at most 1. All known trees T with $\Delta(T) = 5$ and $\alpha_{\text{def}}(T) = 2$ are given in Figure 4.

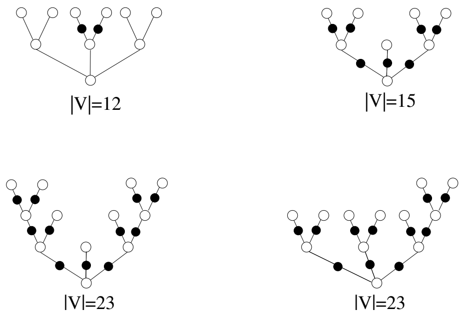

Fig. 2: Deficitary trees with maximum degree 3 and 12 to 23 vertices. The trees with up to 15 vertices were first given in Bonnington and Širáň (1999).

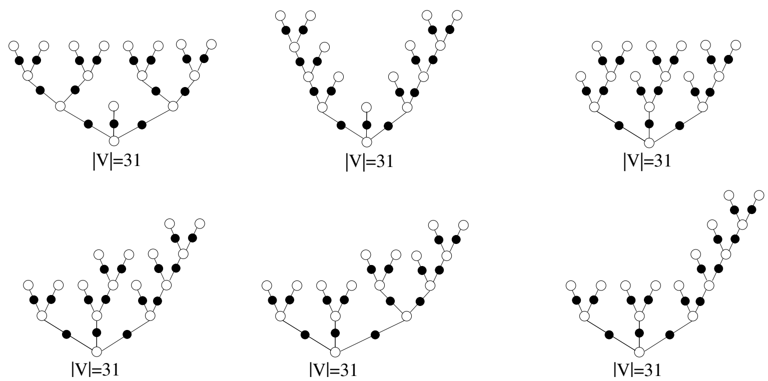

Fig. 3: Deficitary trees with maximum degree 3 and 31 vertices.

3 The α-deficit of comets

Rosa and Širáň (1995) defined an m-*comet*, $\mathcal{C}_m$, as a tree with $2m+1$ vertices: a central vertex w_0 and two sets of m vertices $\{w_1, w_2, \ldots, w_m\}$ and $\{w_{m+1}, w_{m+2}, \ldots, w_{2m}\}$ such that $E = \{w_0 w_i, w_i w_{m+i}; 1 \leq i \leq m\}$. The first tree in Figure 1 is for example an m-comet for $m = 3$. In our lists the smallest trees with a given α-deficit α are unique – they are the $(3 \cdot \alpha)$-comets. Theorem 3.1, which is a reformulation of Corollary 9 of Rosa and Širáň (1995), determines the α-deficit of m-comets.

Theorem 3.1. *Rosa and Širáň (1995) For every $m \geq 1$ and comet $\mathcal{C}_m$ we have $\alpha_{def}(\mathcal{C}_m) = \lfloor \frac{m}{3} \rfloor$.*

We give a new proof by applying the following theorem on nonattacking queens on a triangle.

Theorem 3.2. *Navisch and Lev (2005) For $n \geq 0$, let q_n be the maximum number of non-zero elements in a triangular $(0,1)$-matrix of side length n with at most one non-zero element in each row, in each column and in each diagonal. Then $q_n = \lfloor \frac{2n+1}{3} \rfloor$.*

Proof of Theorem 3.1: It is easy to check that the statement is true for $m \leq 5$. Let $\mathcal{C}_m$ be an m-comet with vertex set V, central vertex w_0 and bipartition (A, B) with $A = \{w_0, w_1, \ldots, w_m\}$ and $B = \{w_{m+1}, \ldots, w_{2m}\}$. Let f be a bipartite labeling. By Remark B.1, we can assume without loss of generality that $f(w_i) = i$, for $m+1 \leq i \leq 2m$. Note that no two edge labels of edges adjacent to the central vertex can

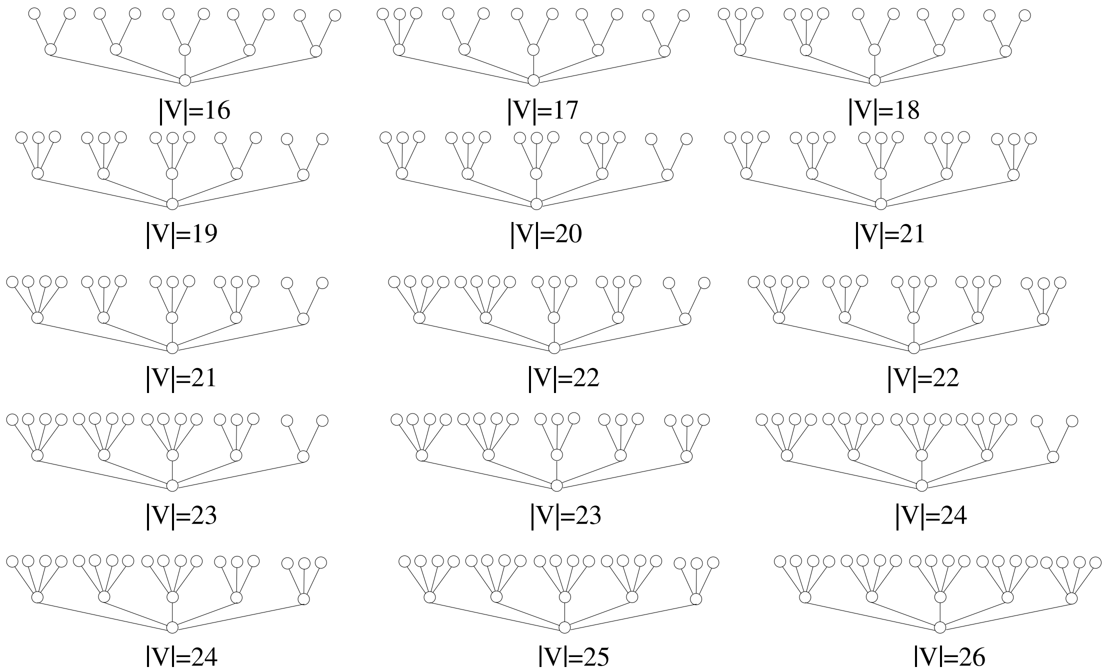

Fig. 4: All trees T with $\Delta(T) = 5$, $\alpha_{\text{def}}(T) = 2$ and at most 31 vertices.

be the same, so by removing vertex labels of leaves, we can obtain a partial labeling with the same deficit, but all existing edge labels being unique.

Let $M = (a_{i,j})_{0 \le i \le m, m+1 \le j \le 2m}$ be a matrix and $a_{i,j} = |j - i|$. The j-th column contains the possible labels of the two edges which are incident to w_j.

We have to label the vertices of A. Let $f(w_0) = k$, then the k-th row contains all m pairwise different labels of the edges $w_0 w_j$, $(m+1 \le j \le 2m)$. That is $a_{k,j} = |j - k|$, for $m+1 \le j \le 2m$, and let L be the set of these edge-labels. The remaining edges have to get induced labels with values in $\{0, 1, \dots, 2m\} - L$. Removing all entries $a_{r,s} \in L$ from M corresponds to removing diagonals in the matrix and we obtain an upper triangular matrix M_u of side length $m_u = k$ and a lower one M_l of side length $m_l = m - k$ (see Figure 5).

Marking an element $a_{i,j}$ in these triangular matrices if and only if the neighbour (different from w_0) of w_j is labeled i, we get a set of marks with the property that on every diagonal, in every column and in every row we have at most one mark (because every edge label and vertex label occurs at most once here).

Thus it follows with Theorem 3.2 that M_u^* (M_l^*) contains at most $q_u = \lfloor \frac{2m_u+1}{3} \rfloor$ ($q_l = \lfloor \frac{2m_l+1}{3} \rfloor$) non-zero elements.

Therefore we can label at most $m + 1 + q_u + q_l$ vertices, without creating a repetition of edge labels. We have that

$$q_u + q_l = \left\lfloor \frac{2k+1}{3} \right\rfloor + \left\lfloor \frac{2(m-k)+1}{3} \right\rfloor \le \left\lfloor \frac{2k+1}{3} + \frac{2(m-k)+1}{3} \right\rfloor = \left\lfloor \frac{2m+2}{3} \right\rfloor.$$

Observe that this upper bound on $q_u + q_l$ can be reached for any value of m. Indeed, if $m \equiv 0$ mod 3 or $m \equiv 1$ mod 3, it is the case when $k = 0$ and if $m \equiv 2$ mod 3 when $k = 1$.

Now it follows that $\alpha_{def}(\mathcal{C}_m) = 2m + 1 - (m + 1 + \lfloor \frac{2m+2}{3} \rfloor) = m - \lfloor \frac{2m+2}{3} \rfloor = \lfloor \frac{m}{3} \rfloor$.

Note that this construction can also be reversed – that is: a solution to the nonattacking queens problem also gives a labeling – and thus the statement is proved. □

$$
\begin{array}{cc}
 & \begin{array}{cccccc} m+1 & m+2 & m+3 & \dots & 2m-1 & 2m \end{array} \\
\begin{array}{r} 0 \\ 1 \\ k \longrightarrow \quad 2 \\ 3 \\ \vdots \\ m-1 \\ m \end{array} &
\left[\begin{array}{cccccc}
m+1 & m+2 & m+3 & & 2m-1 & 2m \\
m & m+1 & m+2 & & 2m-2 & 2m-1 \\
m-1 & m & m+1 & & 2m-3 & 2m-2 \\
m-2 & m-1 & m & & 2m-4 & 2m-3 \\
 & & & & & \\
2 & 3 & 4 & & m & m+1 \\
1 & 2 & 3 & & m-1 & m
\end{array}\right]
\end{array}
$$

Fig. 5: The matrix M used in the proof of Theorem 3.1. The two triangular matrices M_u and M_l are depicted for $k = 2$.

4 A criterion for non-zero α-deficit

In this section we prove Theorem 1.1, which states that a tree with an α-labeling l must have the same edge and vertex parities modulo 2. This theorem can be considered to be a generalisation of the criterion in Theorem 3.3 in Huang et al. (1982).

Proof of Theorem 1.1: Since l is an α-labeling, the sum of the edge labels, modulo 2, gives the edge parity. The edge parity is therefore $(\sum_{e\in E}(l(v_2) - l(v_1))) \mod 2 = (\sum_{e\in E}(l(v_2) + l(v_1))) \mod 2$ where $v_i \in V_i$ and $e = \{v_1, v_2\}$. This gives

$$(\sum_{v_1\in V_1} \deg(v_1)l(v_1) + \sum_{v_2\in V_2} \deg(v_2)l(v_2)) \mod 2,$$

which is in fact the vertex parity. □

Note that while the edge parity is a property of the tree that does not depend on the labeling, the vertex parity in general does.

Remark 4.1. *If T is a tree with bipartition classes V_1 and V_2 so that the parity of the vertex degrees is the same for all vertices inside a bipartition class, then the vertex parity does not depend on the labeling. In this case we will speak about the vertex parity of the tree.*

The proof is immediate because if all degrees are odd, the vertex parity is always the parity of the number of odd integers in $\{0, \ldots, |V| - 1\}$. If one class contains vertices of even degree, w.l.o.g. V_1, the vertex parity is either the parity of the number of odd integers in $\{0, \ldots, |V_1| - 1\}$ or in $\{|V_2|, \ldots, |V_2| + |V_1| - 1\}$, which are the same because $|V_2|$ is necessarily even.

We say that a tree T has the *parity property* if the parity of the vertex degrees is the same for all vertices inside a bipartition class and the vertex parity and edge parity differ.

Corollary 4.2. *Trees that have the parity property*

1. *do not have an α-labeling.*
2. *have a bipartition class of even degrees.*
3. *have an odd number of vertices.*

Proof: 1. is trivial

2. Assume that T does not contain a vertex of even degree. Then the vertex parity is $(\sum_{v \in V} \deg(v) l(v)) \mod 2 = (\sum_{v \in V} l(v)) \mod 2$ which is equal to $(\sum_{i=0}^{|V|-1} i) \mod 2 = (\sum_{i=1}^{|V|} i) \mod 2$ because $|V|$ is even. As this is the edge parity, T does not have the parity property.

3. Since one of the bipartition classes, w.l.o.g V_1, contains only vertices of even degree, the number of edges $\sum_{v \in V_1} \deg(v)$ is also even. Therefore the number of vertices, which is $|E| + 1$, is odd. $\square$

Figures 1, 2 and 3 show the deficitary trees with maximum degree 3 that have fewer than 37 vertices. In fact all but 5 trees are subdivisions of smaller trees with $4k$ vertices. The following explains why these trees have an α-deficit.

Corollary 4.3. *A tree with only vertices of odd degree and degree 2 has the parity property if and only if T can be obtained from a tree S with $4k$ vertices, all of odd degree, by replacing each edge by a path of length 2.*

Proof: Assume that T can be obtained by this construction. By construction the parities of the vertex degrees are the same in each of the bipartition classes. Since $|V| = 8k - 1$ the edge parity of T is 1. On the other hand a simple computation shows that the vertex parity is 0. So T has the parity property.

The fact that a tree with only vertices of odd degree and degree 2 that has the parity property is a subdivision of a smaller tree S with only odd degrees follows immediately because one bipartition class must have only vertices of degree 2 and the other only odd degrees. Suppose that the number v_S of vertices of S is not a multiple of 4. Then $v_S = 4k - 2$ for some k, and T has $8k - 5$ vertices and $8k - 6$ edges. Hence the edge parity is 1 and the vertex parity, $(\sum_{i=0}^{4k-3} i)$, is also 1. This is a contradiction. $\square$

As a corollary we obtain the following result, already presented in Huang et al. (1982):

Corollary 4.4. *Subdivisions of trees with $4k$ vertices – all of odd degree – have positive α-deficit.*

Note 4.5. *The infinite series of subdivided trees shown in Figure 6 all satisfy the parity property. These trees have $8j - 1$ vertices ($j \geq 1$). If the vertex labelled 0 is removed then the remaining $8j - 2$ edges have labels $1, 2, \ldots, 8j - 3$; with the vertex 0 included the label $4j + 1$ appears twice. Hence there are infinitely many trees with maximum degree 3 and α-deficit 1.*

In Figures 1, 2 and 3 it is easily seen that the known deficitary trees with maximum degree 3 and at least 15 vertices are exactly the trees with the parity property. For maximum degree 4 there are too many trees to present in detail or to check by hand. We checked the deficitary trees by computer and the result was that

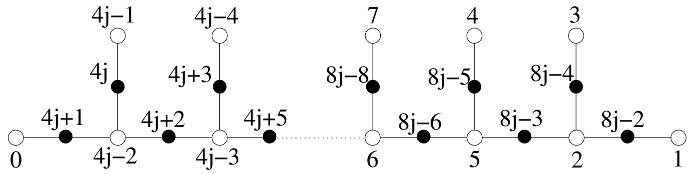

Fig. 6: For each $j \geq 1$ the tree shown has α-deficit 1.

while in the beginning only a small ratio of the deficitary trees had the parity property, this ratio increased with the number of vertices and for more than 25 vertices the known deficitary trees with maximum degree 4 all have the parity property. For maximum degree 5 something similar happens from 26 vertices on: within the range of the tables the number of deficitary trees with an even number of vertices (which cannot have the parity property) seems to decrease and for odd vertex numbers the ratio of deficitary graphs with the parity property increases from 17% for 27 vertices to 57% for 31 vertices. So also for $\Delta(T) = 5$ the parity property seems to gain importance as the number of vertices increases.

We discovered the parity property as a consequence of the computational results and at that time did not know about Theorem 3.3 in Huang et al. (1982). The program did not use the parity property. Now the algorithm could be improved by using the parity property in the beginning and also as a bounding criterion in the recursion when all vertices inside a partition class that still need to be labeled have the same parity.

5 The α-deficit of trees with a vertex of large degree compared to the number of vertices

The computational results in Section 2 and in Appendix A suggest that for every $k \in \mathbb{N}$ there exists some smallest $m(k)$ so that for every $n \geq m(k)$ and every $d \in \mathbb{N}$ the number of trees T with n vertices, $\alpha_{\text{def}}(T) = d$ and maximum degree $n - k$ is the same. In this section we will prove that such a value $m(k)$ does exist for every k.

To this end we will first prove that after adding a certain number of pendant vertices to a fixed vertex in a tree the α-deficit does not change.

Lemma 5.1. *Let T be a tree with bipartition classes V_1 and V_2 and a vertex $v \in V_1$. Let T_p denote the tree obtained from T by adding p pendant vertices to v.*

For all $p, p' \geq (|V_1| - 1)(|V_2| + 1)$ we have $\alpha_{def}(T_p) = \alpha_{def}(T_{p'})$.

Proof: We will prove that any bipartite labeling of T_p implies a bipartite labeling of T_{p+1} with the same deficit and vice versa. Assume $|V_1| > 1$. (Otherwise T_p is a star and so has deficit 0.)

We will denote the set of pendant vertices adjacent to v in T_p by P, and in T_{p+1} by P_{+1}. The bipartition classes of T_p and T_{p+1} are V_1 and $V_2 \cup P$, respectively V_1 and $V_2 \cup P_{+1}$.

Assume that l is a labeling of T_p which maps V_1 onto $\{0, \ldots, |V_1| - 1\}$. The Pigeonhole Principle implies that there are at least $|V_1| - 1$ vertices in P with consecutive labels. Assume that u is the largest of these consecutive labels. For $w \in T_{p+1}$ define

$$l_{+1}(w) = \begin{cases} l(w) & \text{if } w \in T_p \text{ and } l(w) \leq u \\ l(w) + 1 & \text{if } w \in T_p \text{ and } l(w) > u \\ u + 1 & \text{if } w \in T_{p+1} \setminus T_p \end{cases} .$$

With $d(l_{+1})$ the number of different edge labels induced by l_{+1} and $d(l)$ the number of different edge labels induced by l we will prove that $d(l_{+1}) = d(l) + 1$, which implies that the deficits induced by the labelings are the same.

Define the sets of edge labels

$$\begin{aligned} S &= \{l(v_2) - l(v_1) \mid \{v_1, v_2\} \in T_p, v_1 \in V_1, v_2 \in (V_2 \cup P), l(v_2) \leq u\}, \\ S_{+1} &= \{l_{+1}(v_2) - l_{+1}(v_1) \mid \{v_1, v_2\} \in T_{p+1}, v_1 \in V_1, v_2 \in (V_2 \cup P_{+1}), l_{+1}(v_2) \leq u\}, \\ L &= \{l(v_2) - l(v_1) \mid \{v_1, v_2\} \in T_p, v_1 \in V_1, v_2 \in (V_2 \cup P), l(v_2) > u\} \text{ and} \\ L_{+1} &= \{l_{+1}(v_2) - l_{+1}(v_1) \mid \{v_1, v_2\} \in T_{p+1}, v_1 \in V_1, v_2 \in (V_2 \cup P_{+1}), l_{+1}(v_2) > u\}. \end{aligned}$$

Then $d(l) = |L \cup S| = |L| + |S| - |L \cap S|$ and $d(l_{+1}) = |L_{+1} \cup S_{+1}| = |L_{+1}| + |S_{+1}| - |L_{+1} \cap S_{+1}|$. Note that $S = S_{+1}$ and that $L_{+1} = \{x + 1 \mid x \in L\} \cup \{u + 1 - l(v)\}$.

Let M be the set of edge labels of pendant vertices with consecutive labels $u - l(v), u - l(v) - 1, \ldots$. Then M contains $\{u - l(v), u - l(v) - 1, \ldots, u - l(v) - |V_1| + 2\}$. The smallest possible element in L and L_{+1} is $u + 1 - (|V_1| - 1) = u - |V_1| + 2$, which implies that $L \cap S = L \cap M$ and $L_{+1} \cap S_{+1} = L_{+1} \cap M$.

Now we will distinguish between two cases: $(u - l(v)) \notin L$ and $(u - l(v)) \in L$.

Assume first that $(u - l(v)) \notin L$. Then $|L_{+1}| = |L| + 1$ and $L_{+1} \cap M = \{x + 1 \mid x \in L \cap M\}$ and therefore $|L \cap M| = |L_{+1} \cap M|$.

If $(u - l(v)) \in L$ then $u + 1 - l(v) \in \{x + 1 \mid x \in L\}$. This implies that $|L_{+1}| = |L|$ and $L_{+1} \cap M = \{x + 1 \mid x \in L \cap M\} \setminus \{u + 1 - l(v)\}$ and therefore $|L \cap M| - 1 = |L_{+1} \cap M|$.

In both cases $d(l_{+1}) = d(l) + 1$.

Conversely, assume that a labeling l_{+1} of T_{p+1} is given. Then there is a sequence of at least $|V_1|$ vertices in P with consecutive labels. Let u be the largest label of these vertices and assume that the vertex labeled u is removed. Define

$$l(v) = \begin{cases} l_{+1}(v) & \text{if } v \in T_p \text{ and } l_{+1}(v) < u \\ l_{+1}(v) - 1 & \text{if } v \in T_p \text{ and } l_{+1}(v) > u \end{cases}.$$

It is easy to see that applying the previously discussed extension to this reduced labeling l produces l_{+1}, so the two labelings have in fact the same deficit. $\square$

We restate Theorem 1.2 here and give a proof. It enables us to present a function $m(k)$ as described in the beginning of the section.

Theorem. For all $k, d \in \mathbb{N}$, the number of trees T with

$$n \geq k^2 + k$$

vertices, $\alpha_{\text{def}}(T) = d$ and maximum degree $n - k$ is the same.

This implies that $m(k) \leq k^2 + k$.

Proof: Assume that $k \geq 3$. Otherwise all trees are stars or stars with one edge subdivided and it can easily be seen that these have deficit 0.

As $k \geq 3$ we have $n - k \geq n/2 + 1$. It follows that there can be only one vertex v of maximum degree $n - k$ in T. There are exactly $k - 1$ vertices different from v and not adjacent to v. This implies that at most $k - 1$ of the neighbours of v have another neighbour, so there are at least $n - 2k + 1$ pendant vertices.

Let $M(n, k, d)$ denote the set of all trees with n vertices, α-deficit d and maximum degree $n - k$. We claim that adding a new pendant vertex to the unique vertex of maximum degree defines a bijection between

$M(n,k,d)$ and $M(n{+}1,k,d)$. It is easy to see that the maximum degree and the number of vertices increase by one. What remains to be shown is that the α-deficit does not change.

Let T_0 be the tree obtained from T by removing $n-2k+1$ pendant vertices adjacent to v. Then T_0 has $2k-1$ vertices separated into bipartition classes of cardinality $|V_1|$ and $2k-1-|V_1|$.

By Lemma 5.1 the theorem is proved if the number of pendant vertices adjacent to v in T is at least $f(|V_1|) = (|V_1|-1)(2k-|V_1|)$. The maximum integer value for $f(|V_1|)$ can easily be determined to be k^2-k. Since $n \geq k^2+k$ we have $n-2k+1 \geq k^2+k-(2k-1) = k^2-k+1$. □

Together with the tables and the numbers of trees with given maximum degree obtained by *freetree* (Li and Ruskey (1999)), Theorem 1.2 implies the following corollary. Note that the values $m_+(k)$ obtained from the tables were only for nonzero deficit and that it also has to be taken into account from when on the number of trees with n vertices and maximum degree $n-k$ stays constant.

Corollary 5.2. *The function m, as described at the beginning of this section, must take values $m(1)=1$, $m(2)=4$, $m(3)=6$ and $m(4)=8$.*

6 Conclusions, questions, conjectures

The computational results in this paper suggest the following conjectures:

Conjecture 6.1.

1. *The smallest trees T with $\alpha_{def}(T)=k$ are the $3k$-comets.*
2. *The maximum α-deficit of a tree with maximum degree 3 or 4 is 1.*

Furthermore we have the following questions:

Question 6.2.

1. *Let T be a tree of maximum degree 3 and at least 15 vertices, or maximum degree 4 and at least 26 vertices. Is the parity property for T equivalent to T having positive α-deficit? Note that by Lemma 1 from Rosa and Širáň (1995) this would imply that the α-deficit of trees with maximum degree 3, resp. 4 is at most 1.*
2. *Are there trees with maximum degree 5, α-deficit 2 and more than 26 vertices?*
3. *Is there a function of the maximum degree d of a tree that gives an upper bound on the α-deficit (that is, a function which is independent from the number of vertices)?*
4. *Theorem 1.2 gives a quadratic upper bound for the function $m(k)$. The tables suggest a linear growth of the function, maybe even with a small constant. What is the exact asymptotic behaviour of this function?*

Acknowledgements

We want to thank Ljiljana Brankovic for introducing us to α-labelings and for helpful discussions during the development of the algorithms and Kris Coolsaet for his hint on the independent queens problem.

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Appendix A: Results

The number of trees with nonzero α-deficit for each vertex number up to 26 is given here. There are no trees with nonzero deficit and less than 7 vertices. On 7 vertices there is exactly one tree with α-deficit 1. It has maximum degree 3.

$\alpha_{def} \setminus \Delta$	3	4
1	1	1

Trees with 8 vertices

$\alpha_{def} \setminus \Delta$	3	4	5
1	1	3	1

Trees with 9 vertices

$\alpha_{def} \setminus \Delta$	3	4	5	6
1	2	5	3	1

Trees with 10 vertices

$\alpha_{def} \setminus \Delta$	4	5	6	7
1	11	7	3	1

Trees with 11 vertices

$\alpha_{def} \setminus \Delta$	3	4	5	6	7	8
1	1	15	17	7	3	1

Trees with 12 vertices

$\alpha_{def} \setminus \Delta$	4	5	6	7	8	9
1	22	30	18	7	3	1
2			1			

Trees with 13 vertices

$\alpha_{def} \setminus \Delta$	4	5	6	7	8	9	10
1	24	58	34	18	7	3	1
2			1	1			

Trees with 14 vertices

$\alpha_{def} \setminus \Delta$	3	4	5	6	7	8	9	10	11
1	1	27	85	73	35	18	7	3	1
2				1	2	1			

Trees with 15 vertices

$\alpha_{def} \setminus \Delta$	4	5	6	7	8	9	10	11	12
1	25	133	124	78	35	18	7	3	1
2		1	1	3	2	1			

Trees with 16 vertices

$\alpha_{def} \setminus \Delta$	4	5	6	7	8	9	10	11	12	13
1	28	187	232	140	79	35	18	7	3	1
2		1	2	4	4	2	1			

Trees with 17 vertices

$\alpha_{def} \setminus \Delta$	4	5	6	7	8	9	10	11	12	13	14
1	19	260	387	275	142	80	35	18	7	3	1
2		1	3	7	6	4	2	1			

Trees with 18 vertices

$\alpha_{def} \setminus \Delta$	4	5	6	7	8	9	10	11	12	13	14	15
1	23	338	623	484	284	144	80	35	18	7	3	1
2		1	4	8	13	6	4	2	1			
3						1						

Trees with 19 vertices

$\alpha_{def} \setminus \Delta$	4	5	6	7	8	9	10	11	12	13	14	15	16
1	6	393	943	868	521	291	144	80	35	18	7	3	1
2		1	5	10	19	14	6	4	2	1			
3						1	1						

Trees with 20 vertices

$\alpha_{def} \setminus \Delta$	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	15	430	1447	1497	971	535	291	144	80	35	18	7	3	1
2		2	8	15	27	26	14	6	4	2	1			
3							2	1						

Trees with 21 vertices

$\alpha_{def} \setminus \Delta$	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	2	461	1988	2475	1749	998	540	292	144	80	35	18	7	3	1
2		2	11	23	39	45	26	14	6	4	2	1			
3							2	2	1						

Trees with 22 vertices

$\alpha_{def} \setminus \Delta$	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
1	2	15	488	2687	3835	3187	1831	1010	542	292	144	80	35	18	7	3	1
2			2	15	33	49	74	49	26	14	6	4	2	1			
3								3	3	2	1						

Trees with 23 vertices

$\alpha_{def} \setminus \Delta$	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	2	495	3356	5807	5439	3400	1855	1020	544	293	144	80	35	18	7	3	1
2		2	16	46	62	105	90	49	26	14	6	4	2	1			
3					1	1	5	5	3	2	1						

Trees with 24 vertices

$\alpha_{def} \setminus \Delta$	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
1	26	540	4290	8737	9036	6090	3472	1863	1022	546	293	144	80	35	18	7	3	1
2		1	20	59	86	152	159	92	49	26	14	6	4	2	1			
3					2	2	3	10	5	3	2	1						
4									1									

Trees with 25 vertices

$\alpha_{\text{def}} \setminus \Delta$	5	6	7	8	9	10	11	12	13	14	15	16
1	513	5079	12403	14575	10812	6258	3466	1864	1028	546	293	144
2	1	21	82	125	221	257	171	92	49	26	14	6
3				1	4	4	11	11	5	3	2	1
4								1	1			

$\alpha_{\text{def}} \setminus \Delta$	17	18	19	20	21	22
1	80	35	18	7	3	1
2	4	2	1			
3						
4						

Trees with 26 vertices

Appendix B: The algorithm

In this section we will give a description of the branch and bound algorithm used to obtain the results. We implemented two independent algorithms in order to make the chance of an error in the algorithm and the results as small as possible. The second algorithm is much slower though, so that not all numbers could be checked independently.

Already in advance it was clear that the program had to be a compromise that had to perform well under two completely different circumstances. For trees that allow an α-labeling, this had to be found **very** fast because a huge number of trees had to be processed. So complicated look-ahead procedures that determine whether a partial labeling can be completed or not would slow down the computation for the large number of trees that have α-deficit 0. For trees with a large α-deficit (where such a look-ahead would be helpful) the cost of the search had to be in acceptable limits.

We use the following two well known properties of bipartite labelings (Rosa and Širáň (1995)):

Remark B.1. *Let $T = (V, E)$ be a tree with bipartition classes V_1 and V_2 and a bipartite labeling $l : V \to \{0, \ldots, |V| - 1\}$. Then there is a labeling with the same α-deficit as l that maps V_1 onto $\{0, \ldots, |V_1| - 1\}$.*

Proof: If l itself does not have this property we can replace it by $l'(v) = |V| - 1 - l(v)$. This labeling has the property and in fact the induced labels of the edges stay the same. $\square$

This result is used for restricting the search space by choosing a fixed bipartition class V_1 in the beginning of the algorithm and assigning only labels in the range $0, \ldots, |V_1| - 1$ to vertices in this class.

Remark B.2. *Given a tree $T = (V, E)$ with $V = \{1, \ldots, |V|\}$ and a bipartite labeling $l : V \to \{0 \ldots, |V| - 1\}$ using labels $0, \ldots, |V_1| - 1$ for vertices in bipartition class V_1. Then there is a labeling l_0 with the same α-deficit as l that assigns the same labels to the bipartition classes and $l_0^{-1}(0) < l_0^{-1}(|V_1| - 1)$.*

Proof: Assume that l does not have this property and that bipartition class V_1 is labeled $0, \ldots, |V_1| - 1$ and bipartition class V_2 is labeled $|V_1|, \ldots, |V| - 1$. By defining $l_0(v) = |V_1| - 1 - l(v)$ if $v \in V_1$ and $l_0(v) = |V_1| + |V| - 1 - l(v)$ otherwise, for an edge $\{v, w\}$ with $v \in V_1$ the induced label $l(e) = l(w) - l(v)$ becomes $l_0(e) = |V_1| + |V| - 1 - l(w) - (|V_1| - 1 - l(v)) = |V| - (l(w) - l(v)) = |V| - l(e)$. This defines a bijective mapping between the image sets of the two labelings proving that both labelings have the same deficit. $\square$

This result is used by backtracking immediately as soon as the labels 0 and $|V| - 1$ are assigned and the labeling does not have the property in this remark. As we will see, these labels are assigned very early, so the search space is reduced by a factor of 2 without much overhead.

Our algorithm does not try to assign vertex labels in every possible way, but the basic recursion is over the edge labels to assign. For every edge label all combinations of vertex labels are tried that induce this label and for each combination of vertex labels, each (still possible) edge is tried. If no labeling with α-deficit 0 is found, also the possibility is tried that this edge label is not induced. Assume for the following that the tree tested is not a star. For stars deficit 0 is returned immediately.

For efficient branch and bound algorithms it is important to restrict the branching especially in the beginning when hardly any bounding criteria are applicable. To this end we order the edge labels so that the number of corresponding vertex label pairs is decreasing. So the list starts with edge labels 1 and $|V|-1$ which correspond to unique vertex labels. Then labels 2 and $|V|-2$ follow, etc. Label 1 can only be obtained by assigning the vertex labels $|V_1|-1$ and $|V_1|$ and label $|V|-1$ can only be obtained by vertex labels $|V|-1$ and 0. So after these two steps in the case of looking for α-deficit 0 (where these edge labels must be present) Remark B.2 can already be applied.

So when testing for α-deficit 0 we have $|V|-1$ choices in the first step and $|V|-2-i$ for the second with i the number of edges adjacent with the first chosen edge. After these two steps already 4 vertices are labeled giving rise to a lot of restrictions for the following recursion steps.

Another optimisation is based on the symmetry group of the tree:

Assume that a partially labeled tree T is given and that γ is the automorphism group of T fixing already labeled vertices. If edge label l is to be assigned to an edge, it is obvious that in each orbit of the group on the edges of the tree only one edge e has to be chosen because the other edges only lead to labelings with the same deficit as the one obtained by labeling e. We used *nauty* (McKay (1981)) to determine the automorphism group. Even though nauty is very efficient, it was of course necessary to reduce the number of calls to nauty as much as possible. So we stopped calling nauty as soon as the only nontrivial automorphisms only permuted leaves neighbouring the same inner node (this can be easily detected) and also didn't call nauty if the newly assigned vertex labels were assigned to vertices that formed a trivial vertex orbit already under the old group. In this case we could reuse the old group.

Nevertheless for maximum degree 3 trees with deficit 0 the method without using symmetries was faster because obviously α-labelings were found very fast. For maximum degree 3 trees with deficit 1 the method was so much faster that, for example, for 23 vertices it is 2 times faster to use symmetries for all trees (because of 2 trees with deficit) while for 24 vertices (there are no maximum degree 3 trees with 24 vertices and nonzero α-deficit) it is two times slower to use symmetries. We will only give running times for the algorithm exploiting symmetries.

The order in which the edges are chosen is also of importance, but while it turned out to be a general principle to better start with edges at vertices of small degree, the best order partially also depends on the numbering of the input trees. Note that these are often not random and reflect some structure exploited by the generation algorithms. We tested B.D. McKay's program *geng* (McKay (1998)) and F. Ruskey's program *freetree* (Li and Ruskey (1999)) to generate the input trees for this program and inside the groups of vertices with the same degree different orders turned out to strongly effect the performance.

The ideas just sketched form the basis of the algorithm. Of course an efficient implementation (in C) and efficient data structures are also essential, but these details can best be seen in the source code (which can be obtained from the authors). The time necessary to check a tree depends heavily on whether it has a non zero α-deficit or not: testing for example all trees with maximum degree 3 on 32 vertices (no trees with deficit) was 1.6 times faster than testing those on 31 vertices (trees with deficit exist) – in spite of the fact that the trees are larger and that there are more than twice as many. While testing all 392.658.842 trees with maximum degree 3 on 31 vertices took 406 hours (so 0.0037 seconds per tree on average), testing for example the 4th tree depicted in Figure 3 alone took 89 hours.

For trees without a bound on the vertex degree, the time needed per tree increases fast: on a 2.4 GHz Intel Xeon processor on average 15.000 trees with 15 vertices (and without degree restrictions) were tested per second. For 25 vertices the rate decreased to only 18.5 per second.

In order to test our program as well as possible we implemented a second approach using a branch and bound method assigning vertex labels directly. We used the program *freetree* to generate trees for the algorithm described and *geng* for the second program in order to have complete independence of the approaches. We compared the results for all trees with up to 19 vertices and all trees with maximum degree 3 and up to 26 vertices. We had complete agreement of the results in all these cases.