Some non-existence results on Leech trees^{*}

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This paper is dedicated to the memory of Dominique de Caen, who introduced his friend, LAS, to Leech trees.

Abstract

More than 25 years ago John Leech [2] posed the following beautiful problem: find, whenever possible, trees on n vertices with positive weights on the edges, such that the $\binom{n}{2}$ weighted distances among the n vertices are exactly the numbers $1, 2, 3, ..., \binom{n}{2}$. This paper makes a modest progress on this problem.

1 Examples for Leech trees

A tree is called Leech tree if one can assign positive edge weights to its edges, such that the $\binom{n}{2}$ path weights, i.e. the sums of weights along the $\binom{n}{2}$ distinct paths connecting the pairs of the *n* vertices of the tree, yield exactly the numbers $1, 2, 3, ..., \binom{n}{2}$. Since edges of the tree are also paths, the edge weights have to be positive integers as well. John Leech introduced these trees in [2]. Believe it or not, he was motivated by a problem of electrical engineering, where edge weights represented electrical resistances. He gave a list of small Leech trees (see Fig. 1) and posed the problem of their existence in general. The difficulty of the existence problem lies in the unusual way of mixing additive number theory with combinatorics, in particular in the exponential growth of the number of candidates for Leech

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trees. Leech wrote "I expect the resolution of this question to be very difficult".

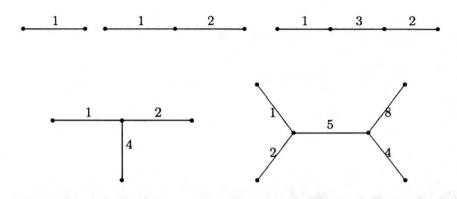


Figure 1: The known Leech trees.

Note that there are similar problems around that are notoriously hard. The Graceful Tree Conjecture of Ringel [3] states that for every tree with n vertices, there is a bijection f between the vertex set and $\{1, 2, ..., n\}$ such that $\{|f(v) - f(u)| : uv \text{ edge}\} = \{1, 2, ..., n-1\}$. The seventeen years old Prime Labeling Conjecture of Entringer states that for every tree with n vertices, there is a bijection f between the vertex set and $\{1, 2, ..., n\}$ such that $\gcd(f(v), f(u)) = 1$ whenever uv is an edge [4].

2 Results for the shape of Leech trees

Herbert Taylor [7] gave a beautiful proof restricting the number of vertices on which Leech trees can exist. For completeness we also show his proof.

Theorem 1. (H. Taylor) If there is a Leech tree on n vertices, then $n = k^2$ or $n = k^2 + 2$.

Proof. Let d(x, y) denote the sum of weights on the path connecting vertices x and y. The crucial observation is the fact that for any 3 vertices x, y, z in a tree, one has

$$d(x,y) \equiv d(x,z) + d(y,z) \pmod{2}.$$
(1)

Fix a vertex v and let A denote the set of vertices lying at an even distance from v (v is included), and let B denote the set of vertices lying at an odd distance from v. Now we have |A| + |B| = n. According to (1), two vertices define an odd-length path if and only if one of them belongs to A, and the other to B. Therefore the number of paths with odd weight is $|A| \cdot |B|$. If $\binom{n}{2}$ is even, there must be exactly $\frac{1}{2}\binom{n}{2}$ paths with odd weights. Hence

$$(|A| - |B|)^2 = (|A| + |B|)^2 - 4|A| \cdot |B| = n^2 - 2\binom{n}{2} = n$$

If $\binom{n}{2}$ is odd, there must be exactly $\frac{1}{2}\left(\binom{n}{2}+1\right)$ paths with odd weights.

Hence
$$(|A| - |B|)^2 = (|A| + |B|)^2 - 4|A| \cdot |B| = n^2 - 2\binom{n}{2} + 1 = n - 2.$$

Note that the proof gave seemingly more than the theorem: If there is a Leech tree on n vertices, then $n = k^2$ if $\binom{n}{2}$ is even, and $n = k^2 + 2$ if $\binom{n}{2}$ is odd. In fact, this more precise statement gives no more restriction. We leave this as an exercise to the readers.

Since no examples of Leech trees for n > 6 are known, and in this paper we show further non-existence results, one may arrive to the conjecture that

Conjecture 1. There are only finitely many Leech trees.

We give further support to this conjecture in the next section, showing that there are no Leech trees on n = 9 and 11 vertices. In the rest of this section we prove this conjecture for *particular* tree shapes.

Leech noted (without proof) that a path can be a Leech tree only for $n \leq 4$. Indeed, since $\binom{n}{2}$ must be among the path weights, it has to be the weight of the full tree. All n-1 edges of the tree must have distinct positive integer weights, and the i^{th} smallest of them is at least *i*. Since $1+2+\ldots+(n-1)=\binom{n}{2}$, it follows that the n-1 edge weights must be the numbers $1, 2, \ldots, (n-1)$. Weight 1 must be adjacent to (n-1) and nothing else, otherwise weight 1 and the edge adjacent to it would yield a path of weight < n, which is already present as an edge. Since 1 and (n-1) already give a path of length n, 2 can be adjacent only to (n-1), otherwise a path with weight $\leq n$ would be found. Now we cannot put any weighted edge to the other side of 2.

We can generalize this observation by proving that Leech trees cannot have very long paths: **Theorem 2.** If there is a Leech tree on n vertices, then it contains no paths of length larger than $\frac{n}{\sqrt{2}}(1+o(1))$.

Proof. Assume that $a_1, a_2, ..., a_t$ are the weights along a path in a Leech tree on n vertices in this order. Observe the following inequalities:

$$\sum_{i=1}^{t} (a_i) \leq \binom{n}{2} \tag{2}$$

$$\sum_{i=1}^{t-1} (a_i + a_{i+1}) \leq 2\binom{n}{2} \tag{3}$$

$$\sum_{i=1}^{t-j} (a_i + a_{i+1}... + a_{i+j}) \leq (j+1) \binom{n}{2}.$$
 (4)

Summing up these inequalities for j = 0, 1, 2, ..., k-1, we obtain that some $t + (t-1) + ... + (t-k+1) = tk - \binom{k}{2}$ distinct integers sum up to at most $\binom{k+1}{2}\binom{n}{2}$. Since the i^{th} smallest among these distinct integers is, again, at least i, we obtain that

$$\frac{1}{2} \left[tk - \binom{k}{2} \right] \left[tk - \binom{k}{2} + 1 \right] \leq \binom{k+1}{2} \binom{n}{2}.$$
(5)

Setting $k = \lfloor \sqrt{n} \rfloor$ in (5), we obtain the theorem.

We prove that largest Leech star consists of edges with weights 1,2, and 4. Indeed, it is easy to see that any Leech star with at least 3 leaves must contain these edge weights. Assume that there is a fourth leaf. Its edge must have weight 7. However, the star with edge weights 1,2,4, and 7 is not a Leech star, since 10 does not occur as a distance. If a Leech star with at least 5 leaves has edge weights 1,2,4,7, and 10, then 11 is represented twice as a distance, a contradiction. The theorem below shows that Leech trees cannot even go close to the star shape.

Theorem 3. In a Leech tree on n vertices, the maximum degree is at most $(\frac{\sqrt{8}}{3} + o(1))n$.

Proof. Let us be given a Leech tree on n vertices, which has a vertex v of degree d. Let W denote the set of d distinct integers, which are the weights of edges adjacent to v. Let D denote the set of d neighbors of v,

and let N denote the set of $\binom{d}{2}$ distinct distances among pairs of vertices in D. We will consider the intervals $I_1 = \begin{bmatrix} 1, \frac{1}{3} \binom{n}{2} \end{bmatrix} I_2 = \begin{pmatrix} \frac{1}{3} \binom{n}{2}, \frac{1}{2} \binom{n}{2} \end{bmatrix}$, and $I_3 = \begin{bmatrix} \frac{2}{3} \binom{n}{2}, \binom{n}{2} \end{bmatrix}$. Let i_l denote $|W \cap I_l|$, for l = 1, 2, 3. Let Z denote the set of $\binom{n}{2} - \binom{d}{2}$ distances which do not have both endpoints in D. Let j_l denote $|Z \cap I_l|$, for l = 1, 2, 3. We have the following inequalities:

$$\binom{i_1}{2} + j_1 \geq \left\lfloor \frac{1}{3} \binom{n}{2} \right\rfloor,$$
 (6)

$$\binom{i_2}{2} + j_3 \geq \left\lfloor \frac{1}{3} \binom{n}{2} \right\rfloor,$$
 (7)

$$j_1 + j_2 + j_3 \leq \binom{n}{2} - \binom{d}{2}.$$
(8)

Formula (6) follows from the fact that the elements of I_1 are represented as distances. Formula (7) follows from the fact that the elements of I_3 are represented as distances. Formulae (6), (7), and (8) immediately imply that for l = 1, 2

$$\frac{i_l^2}{2} \ge \frac{d^2}{2} - \frac{n^2}{3} + O(n). \tag{9}$$

Taking the square root of (9) for l = 1, 2, and summing it up, one obtains

$$d \ge i_1 + i_2 \ge 2\sqrt{2}\sqrt{\frac{d^2}{2} - \frac{n^2}{3} + O(n)}.$$
(10)

Solving the inequality (10) for d, we obtain the required $d \leq (\frac{\sqrt{8}}{3} + o(1))n$.

3 Computational results

Note that the smallest orders of a tree, where Theorem 1 leaves open the existence of Leech trees, is n = 9 and 11 vertices.

Theorem 4. There are no Leech trees on n = 9 and 11 vertices.

We will give the outline of the algorithm that we use to check the existence of Leech tree on 9 vertices. (The one for 11 is similar.) A backtrack algorithm is used to find whether there exists a Leech tree of 9 nodes. The weighted tree of 9 nodes will be represented as a 9×9 adjacency matrix. There are eight edges for a weighted tree of 9 nodes, which can be labeled as edge 1 through edge 8 such that their weights are in increasing order. Obviously the weight of edge 1 has to be one. And we can fix the position of edge 1 to be the (1,2) entry of the matrix. The algorithm will do as follows:

Initial step:

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set matrix m_1 to be the adjancency matrix with edge 1 assigned Step i \ (2 \le i \le 8) (handle edge i):
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weight \leftarrow Find-Next-Weight(m);

for all possible positions do:

if (Check-Validity(position,m)==FALSE), try next position;

 $copy(m_i, m_{i-1})$; Assign-Value $(m_i, weight, position)$;

if $(\text{Is-Valid}(m_i) = = \text{FALSE})$, try next position;

Do step i + 1;

Find-Next-Weight: find out the weights of all the existing paths, then take the smallest weight from $\{1, 2, ..., 36\}$ that is not in there, this has to be the weight of the next edge.

Check-Validity: since we are looking for a tree, we do not want cycles, so check the current graph for all possible paths, the new edge can not be in a position to connect two end vertices of an existing path (which will result in a cycle).

Is-Valid: check if any two paths of the existing graph has the same weight. Note that at step 8 when all the eight edges are assigned, we just need to check if it represents a valid Leech tree.

To find out the weights of all paths, we need to calculate the distance matrix of the graph. This was done using the classical all-pair shortest path algorithm. If all 8 edges are assigned and the matrix is still valid, the program ends with a Leech tree found. The code can be downloaded from [6].

We note that Wayne Goddard has independently arrived to the same computational results.

4 Buneman's 4-point condition

Consider some n vertices of a tree with positive edge weights. Define the distance of two vertices by the weight of the path connecting the vertices. It is well-known and easy to verify that these distances define a metric space on the vertex set. This metric space has a peculiar property, the so-called Buneman's 4-point condition: for any 4 vertices x, y, u, v, two out of the following three distance sums

$$d(x, y) + d(u, v), \quad d(x, u) + d(y, v), \quad d(x, v) + d(u, y)$$

are equal, and the third is not greater than the other two. A glimpse on the figure below shows why this holds.

In Figure 2, $a, b, c, d, e \ge 0$ are the lengths of the corresponding paths, and we have

$$d(x,y)+d(u,v)=a+b+d+e\leq$$

 $\leq a + b + 2c + d + e = d(x, u) + d(y, v) = d(x, v) + d(y, u).$

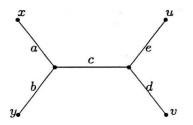


Figure 2: Buneman's 4-point condition.

Consider now the following problem: which finite metric spaces can be represented in the way described above? Buneman's theorem asserts that exactly those finite metric spaces have such a tree representation, for which Buneman's 4-point condition holds. It is worth noting that the triangle inequality of the metric space also follows from Buneman's 4-point condition, if it is extended to any four not necessarily distinct points. (Although Buneman's 4-point condition was actually discovered twice before Buneman did, see [5, 8], the result is still little known among those who do not work on phylogenetic tree reconstruction.)

One might pose the following conjecture, strengthening Conjecture 1:

Conjecture 2. For any finite metric space on $n > n_0$ vertices with distances $1, 2, 3, ..., \binom{n}{2}$, Buneman's 4-point condition fails.

This conjecture would say that $1, 2, 3, ..., \binom{n}{2}$ cannot be the distance set of *n* vertices in an edge-weighted tree that may have more than *n* vertices and not necessarily edge weighted with integers! Note, however, that Taylor's proof to Theorem 1 still works if we allow new vertices in the tree but require that all new vertices have integer distances to all old vertices.

We show an example that Conjecture 2 is false for any order. For any n, the following is an example of a tree T whose edge weights are half integers. There are n vertices in V(T) such that pairwise distance among these n vertices are $1, 2, 3, \ldots, \binom{n}{2}$.

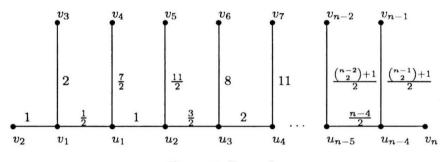


Figure 3: Example

In Figure 3, we assign half-integer weights to the edges as follows: $(v_1, v_2) = 1$, $(v_1, v_3) = 2$, $(v_1, u_1) = \frac{1}{2}$, $(u_{n-4}, v_n) = \binom{n}{2} - (u_{n-4}, v_{n-1})$; $(u_{i-1}, u_i) = \frac{i}{2}$ for $i = 2, 3, \ldots, n-4$; $(u_i, v_{i+3}) = \frac{\binom{i+3}{2}+1}{2}$ for $i = 1, 2, \ldots, n-4$. Then, if we consider the distance matrix for vertex $v_i, i = 1, 2, \ldots, n$, we have

	v_n	v_{n-1}	v_{n-2}		v_2	v_1
$v_n \\ v_{n-1}$	0	$\binom{n}{2}$	$\binom{n}{2} - 1$ $\binom{n-1}{2}$		$\binom{n-1}{2} + 2$ $\binom{n-2}{2} + 2$	$\binom{n-1}{2} + 1$ $\binom{n-2}{2} + 1$
v_{n-2}			·.	:	:	:
÷				0	3	2
v_2					0	1
v_1						0

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