Fully Leafed Tree-Like Polyominoes and Polycubes

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Abstract. We present and prove recursive formulas giving the maximal number of leaves in tree-like polyominoes and polycubes of size n. We call these objects *fully leafed tree-like polyforms*. The proof relies partly on a combinatorial algorithm that enumerates remarkable rooted and directed trees that we call abundant. We also show how to produce one family of fully leafed tree-like polyominoes and one family of fully leafed tree-like polycubes for each possible size, thus gaining insight on their geometric characteristics.

1 Introduction

Polyominoes and, to a lesser extent, polycubes have been the object of important investigations in the past 30 years either from a game theoretic or combinatorial point of view (see [11] and references therein). Recall that a polyomino is an edge-connected set of unit cells in the square lattice that is invariant under translation. The 3D equivalent of a polyomino is called a polycube, which is a face-connected set of unit cells in the cubic lattice, up to translation.

A central problem is the search for the number of polyminoes with n cells where n is called the size of the polyomino. This problem, still open, has been investigated from several points of view; asymptotic evaluation [14], computer generation and counting [13, 15, 16], random generation [12] and combinatorial description [2, 10]. Combinatorists have also concentrated their efforts in the description of various families of polyominoes and polycubes, such as convex polyominoes [4], parallelogram polyominoes [1, 8], tree-like polyominoes [9] and other families [5–7].

In this paper, we are interested in two related families: *tree-like polyominoes* and *tree-like polycubes* which are acyclic polyominoes in the graph theoretic sense. Our main results are recursive expressions giving the maximal number of leaves of tree-like polyominoes and polycubes of size n. A tree-like polyomino or polycube of size n is called *fully leafed* when it has the maximum possible number of leaves among all tree-like polyforms of size n. To our knowledge, these new classes of polyforms have not been considered yet. The number of leaves in a fully leafed tree-like polyomino and polycube with n cells are denoted respectively $L_2(n)$ and $L_3(n)$.

2 Preliminaries

Let $G = (V, E)$ be a simple graph, $u \in V$ and $U \subseteq V$. The set of neighbors of u in G is denoted $N_G(u)$, which is naturally extended to U by defining $N_G(U) = \{u' \in N_G(u) \mid u \in U\}$. For any subset of vertices $U \subseteq V$, the *subgraph induced by* U is the graph $G[U] = (U, E \cap \mathcal{P}_2(U))$, where $\mathcal{P}_2(U)$ is the set of 2-elements subsets of V. The *extension* of $G[U]$ is defined by $\mathrm{Ext}(G[U]) = G[U \cup N_G(U)]$ and the *interior* of $G[U]$ is defined by $\mathrm{Int}(G[U]) = G[\mathrm{Int}(U)]$, where $\mathrm{Int}(U) = \{u' \in U \mid N_G(u') \subseteq U\}$. Finally, the *hull* of $G[U]$ is defined by $\mathrm{Hull}(G[U]) = \mathrm{Int}(\mathrm{Ext}(G[U]))$.

The *square lattice* is the infinite simple graph $\mathcal{G}_2 = (\mathbb{Z}^2, A_4)$, where A_4 is the 4-*adjacency relation* defined by $A_4 = \{(p, p') \in \mathbb{Z}^2 \mid \mathrm{dist}(p, p') = 1\}$ where dist is the Euclidean distance of $\mathbb{R}^2$. For any $p \in \mathbb{Z}^2$, the set $c(p) = \{p' \in \mathbb{R}^2 \mid \mathrm{dist}_\infty(p, p') \leq 1/2\}$, where dist_∞ is the uniform distance of $\mathbb{R}^2$, is called the *square cell* centered in p. The function c is naturally extended to subsets of $\mathbb{Z}^2$ and subgraphs of $\mathcal{G}_2$.

For any finite subset $U \subseteq \mathbb{Z}^2$, we say that $\mathcal{G}_2[U]$ is a *grounded polyomino* if it is connected. The set of all grounded polyominoes is denoted by $\mathcal{GP}$. Given two grounded polyominoes $P = \mathcal{G}_2[U]$ and $P' = \mathcal{G}_2[U']$, we write $P \equiv_t P'$ (resp. $P \equiv_i P'$) if there exists a translation $T : \mathbb{Z}^2 \to \mathbb{Z}^2$ (resp. an isometry I on $\mathbb{Z}^2$) such that $U' = T(U)$ (resp. $U' = I(U)$. A *fixed polyomino* (resp. *free polyomino*) is then an element of $\mathcal{GP}/\equiv_t$ (resp. $\mathcal{GP}/\equiv_i$). Clearly, any connected induced subgraph of $\mathcal{G}_2$ corresponds to exactly one set of square cells via the function c. Consequently, from now on, polyominoes will be considered as simple graphs rather than sets of edge-connected square cells.

All definitions above can be naturally extended to the *cubic lattice* with the 6-*adjacency relation*. Thus, we define *cubic cell*, *grounded polycube*, *fixed polycube* and *free polycube* accordingly.

We take advantage of the fact that grounded polyominoes and polycubes are connected subgraphs of $\mathcal{G}_2$ and $\mathcal{G}_3$ so that the terminology of graph theory becomes available. A (grounded, fixed or free) *tree-like polyomino* is therefore a (grounded, fixed or free) polyomino whose associated graph is a tree. *Tree-like polycubes* are defined similarly.

Let $G = (V, E)$ be any finite simple graph. We say that $u \in V$ is a *leaf* of G when $\deg(u) = 1$. Otherwise u is called an *inner vertex* of G. For any $d \in \mathbb{N}$, the number of vertices of degree d is denoted by $n_d(G)$ and $n(G) = |V|$ is the number of vertices of G which is also called the *size* of G. Leaves are of particular interest when G is a tree. Let $T = (V, E)$ be any simple nonempty tree. The *depth* of $u \in V$ in T, denoted by $depth_T(u)$, is defined recursively by

$$depth_T(u) = \begin{cases} 0, & \text{if } \deg_T(u) \leq 1; \\ 1 + depth_{T'}(u), & \text{otherwise,} \end{cases}$$

where T' is the tree obtained from T by removing all its leaves (see Figure 1).

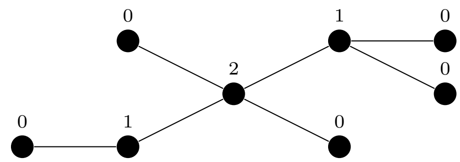


Fig. 1. The depth of the vertices in a tree.

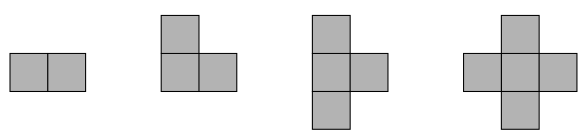
3 Fully Leafed Tree-Like Polyominoes

In this section, we describe the number of leaves of fully leafed tree-like polyominoes. For any integer $n \geq 2$, let the function $\ell_2(n)$ be defined as follows:

$$\ell_2(n) = \begin{cases} 2, & \text{if } n = 2; \\ n - 1, & \text{if } n = 3, 4, 5; \\ \ell_2(n-4) + 2, & \text{if } n \geq 6. \end{cases} \tag{1}$$

We claim that $\ell_2(n) = L_2(n)$. The first step is straightforward.

Lemma 1. *For all $n \geq 2$, $L_2(n) \geq \ell_2(n)$.*



(a) (b) (c) (d)

Fig. 2. Fully leafed tree-like polyominoes of size (a) 2, (b) 3, (c) 4 and (d) 5.

Proof. We build a family of tree-like polyominoes $\{T_n \mid n \geq 2\}$ whose number of leaves is given by (1). For $n = 2, 3, 4, 5$, the polyominoes T_n respectively in (a), (b), (c) and (d) of Figure 2 satisfy (1). For $n \geq 6$, let T_n be the polyomino obtained by appending the polyomino of Figure 2(c) to the right of T_{n-4}.

By induction on n, we have $n_1(T_n) = \ell_2(n)$ for all $n \geq 2$, since the fact that appending the T-shaped polyomino of Figure 2(c) adds 4 cells and 3 leaves, but removes 1 leaf. $\square$

In order to prove that the family $\{T_n \mid n \geq 2\}$ described in the proof of Lemma 1 is maximal, we need the following result characterizing particular subtrees that appear in possible counter-examples of minimum size.

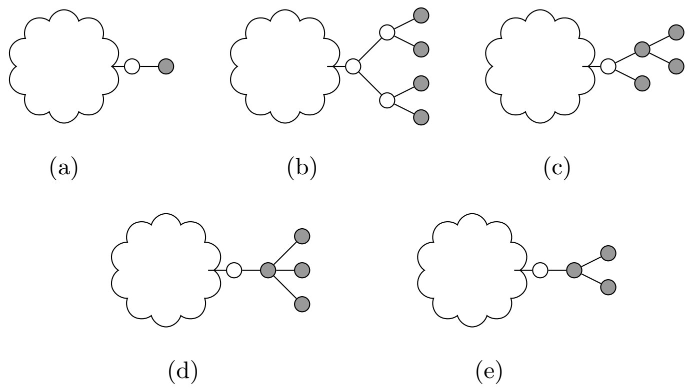


Fig. 3. The cases in the proof of Lemma 3.

Lemma 2. *Let T be a tree-like polyomino of minimum size such that $n_1(T) > \ell_2(n(T))$ and let T' be a tree-like polyomino such that $n(T') = n(T) - i$, for some $i \in \{1, 3, 4\}$. Also, let $\Delta\ell(1) = 0$, $\Delta\ell(3) = 1$ and $\Delta\ell(4) = 2$. Then*

$$n_1(T) > n_1(T') + \Delta\ell(i).$$

Proof. It is easy to prove by induction that for any $k \geq 2$, $\ell_2(k + i) \geq \ell_2(k) + \Delta\ell(i)$, where $i \in \{1, 3, 4\}$. Therefore,

$$\begin{aligned}
n_1(T) &> \ell_2(n(T)), && \text{by assumption,} \\
&= \ell_2(n(T') + i), && \text{by definition of } T', \\
&\geq \ell_2(n(T')) + \Delta\ell(i), && \text{by the observation above,} \\
&\geq L_2(n(T')) + \Delta\ell(i), && \text{by minimality of } n(T), \\
&\geq n_1(T') + \Delta\ell(i), && \text{by definition of } L_2,
\end{aligned}$$

concluding the proof. □

We are ready to prove that the family of tree-like polyominoes built in the proof of Lemma 1 is maximal.

Lemma 3. *For all $n \geq 2$, $L_2(n) \leq \ell_2(n)$.*

Proof. Suppose, by contradiction, that T is a tree-like polyomino of minimal size such that $n_1(T) > \ell_2(n(T))$.

We first show that all vertices of T of depth 1 have degree 3 or 4. Arguing by contradiction, assume that there exists a vertex u_1 of T such that $depth_T(u_1) = 1$ and $\deg_T(u_1) = 2$. Let T' be the tree-like polyomino obtained from T by removing the leaf adjacent to u_1 (see Figure 3(a)). Then $n(T') = n(T) - 1$ and $n_1(T') = n_1(T)$, contradicting Lemma 2.

Now, we show that T cannot have a vertex of depth 2. Again by contradiction, assume that such a vertex u_2 exists. Clearly, $\deg_T(u_2) \neq 4$, otherwise u_2 would have a neighbor of depth 1 and degree 2, which was just shown to be impossible. Also, if $\deg_T(u_2) = 3$, then we are either in case (b) or (c) of Figure 3. In each case, let T' be the tree-like polyomino obtained by removing the four gray cells. Then $n(T') = n(T) - 4$ and $n_1(T') = n_1(T) - 2$, contradicting Lemma 2. Finally, if $\deg_T(u_2) = 2$, then either (d) or (e) of Figure 3 holds, both leading to a contradiction with Lemma 2 when removing the gray cells.

Since every tree-like polyomino of size larger than 6 has at least one vertex of depth 2, the proof is completed by exhaustive inspection of all tree-like polyominoes of size at most 6.

Combining Lemmas 1 and 3, we have the following result.

Theorem 4. *For all integers $n \geq 2$, $L_2(n) = \ell_2(n)$ and the asymptotic growth of L_2 is given by $L_2(n) \sim \frac{1}{2}n$.* □

4 Fully Leafed Polycubes

The basic concepts introduced in Section 3 are now extended to tree-like polycubes with additional considerations that complexify the arguments.

Recall that for all integers $n \geq 2$,

$$L_3(n) = \max\{n_1(T) \mid T \text{ is a tree-like polycube of size } n\}$$

and define the function $\ell_3(n)$ as follows:

$$\ell_3(n) = \begin{cases} f_3(n) + 1, & \text{if } n = 6, 7, 13, 19, 25; \\ f_3(n), & \text{if } 2 \leq n \leq 40 \text{ and } n \neq 6, 7, 13, 19, 25; \\ f_3(n-41) + 28, & \text{if } 41 \leq n \leq 84; \\ \ell_3(n-41) + 28, & \text{if } n \geq 85. \end{cases} \tag{2}$$

where

$$f_3(n) = \begin{cases} \lfloor (2n+2)/3 \rfloor, & \text{if } 0 \leq n \leq 11; \\ \lfloor (2n+3)/3 \rfloor, & \text{if } 12 \leq n \leq 27; \\ \lfloor (2n+4)/3 \rfloor, & \text{if } 28 \leq n \leq 40. \end{cases} \tag{3}$$

The following key observations on ℓ_3 prove to be useful.

Proposition 5. *The function ℓ_3 satisfies the following properties:*

(i) *For all positive integers k, the sequence $((\ell_3(n+k) - \ell_3(n))_{n\geq 0}$ is bounded, so that the function $\Delta\ell_3 : \mathbb{N} \to \mathbb{N}$ defined by*

$$\Delta\ell_3(i) = \liminf_{n\to\infty}(\ell_3(n+i) - \ell_3(n))$$

is well-defined.

(ii) *For any positive integers n and k, if $\ell_3(n+k) - \ell_3(n) < \Delta\ell_3(k)$, then $n \in \{6, 7, 13, 19\}$.*

Proof. Omitted due to lack of space.

We now introduce rooted tree-like polycubes.

Definition 6. *A* rooted grounded tree-like polycube *is a triple* $R = (T, r, \overrightarrow{u})$ *such that*

(i) $T = (V, E)$ *is a grounded tree-like polycube of size at least* 2*;*
(ii) $r \in V$*, called the* root *of* R*, is a cell adjacent to at least one leaf of* T*;*
(iii) $\overrightarrow{u} \in \mathbb{Z}^3$*, called the* direction *of* R*, is a unit vector such that* $r + \overrightarrow{u}$ *is a leaf of* T*.*

The *height* of R is the maximun number of inner vertices that can be visited from the root r. *Rooted fixed tree-like polycubes* and *rooted free tree-like polycubes* are defined similarly. If R is a rooted, grounded or fixed, tree-like polycube, a unit vector $\overrightarrow{v} \in \mathbb{Z}^3$ is called a *free direction* of R whenever $r - \overrightarrow{v}$ is a leaf of T. A rooted grounded, fixed or free, tree-like polycube R is called *basic* if it has a single inner vertex. The 10 basic rooted free tree-like polycubes are illustrated in Figure 4.

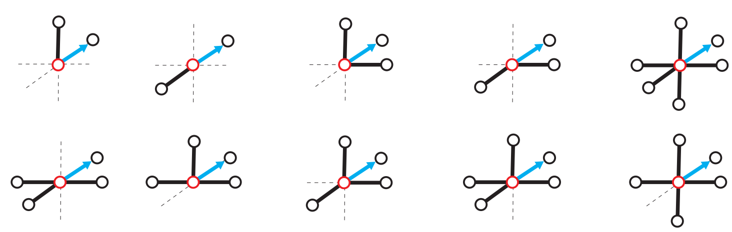


Fig. 4. Basic tree-like polycubes up to isometry

We now introduce a useful operation called the *graft union* of tree-like polycubes.

Definition 7 (Graft union). *Let* $R = (T, r, \overrightarrow{u})$ *and* $R' = (T', r', \overrightarrow{u'})$ *be two rooted grounded tree-like polycubes such that* $\overrightarrow{u'}$ *is a free direction of* R*. The* graft union *of* R *and* R'*, whenever it exists, is the rooted grounded tree-like polycube*

$$R \triangleleft R' = (\mathbb{Z}_3[V \cup \tau(V')], r, \overrightarrow{u}),$$

where V*,* V' *are the sets of vertices of* T*,* T' *respectively and* τ *is the translation with respect to the vector* $\overrightarrow{r'r} - \overrightarrow{u'}$*.*

The graft union is naturally extended to fixed and free tree-like polycubes. In the latter case however, $R \triangleleft R'$ is not a single rooted free tree-like polycube, but rather the set of all possible graft unions obtained from an isometry. Observe that graft union is a partial application on rooted grounded tree-like polycubes,

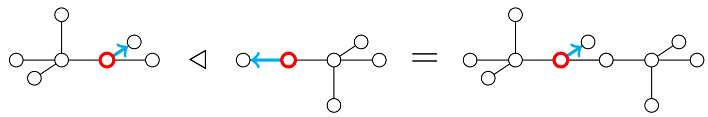


Fig. 5. A well-defined graft union of two rooted grounded tree-like polycubes

i.e. the triple $(\mathbb{Z}_3[V \cup \tau(V')], r, \vec{u})$ is not always a rooted tree-like polycube. More precisely, the induced subgraph $\mathbb{Z}_3[V \cup \tau(V')]$ is always connected, but not always acyclic. Also, $r + \vec{u}$ needs not be a leaf. Therefore, we say that a graft union $R \triangleleft R'$ is

(i) *non-final* if $R \triangleleft R'$ is a rooted grounded tree-like polycube;
(ii) *final* if the graph $G = \mathbb{Z}_3[V \cup \tau(V')]$ is a tree-like polycube, $\vec{u'} = -\vec{u}$ and $r + \vec{u}$ is not a leaf of G;
(iii) *well-defined* if it is either non-final or final;
(iv) *invalid* otherwise.

Figure 5 illusrates a well-defined graft union of two rooted tree-like polycubes. The graft union interacts well with the functions $n_i(T)$ giving the number of cells of degree i in T.

Lemma 8. *Let T_1, T_2 be rooted tree-like polycubes such that $T_1 \triangleleft T_2$ is well-defined. Then*

$$\begin{aligned} n_1(T_1 \triangleleft T_2) &= n_1(T_1) + n_1(T_2) - 2, \\ n_i(T_1 \triangleleft T_2) &= n_i(T_1) + n_i(T_2), \quad \textit{for } i \geq 2; \\ n(T_1 \triangleleft T_2) &= n(T_1) + n(T_2) - 2. \end{aligned}$$

Proof. This is an immediate consequence of Definition 7.

We are now ready to define a family of fully leafed tree-like polycubes.

Lemma 9. *For all $n \geq 2$, $L_3(n) \geq \ell_3(n)$.*

Proof. We exhibit a family of tree-like polycubes $\{U_n \mid n \geq 2\}$ realizing ℓ_3, i.e. such that $n_1(U_n) = \ell_3(n)$ for all $n \geq 2$. First, for $n = 6, 7, 13, 19, 25$, let U_n be the tree-like polycubes depicted in Figure 6(a), (b), (c), (d) and (e) respectively. It is easy to verify that $n_1(U_n) = \ell_3(n)$ in these cases.

Now, let $n \notin \{6, 7, 13, 19, 25\}$, let q and r be the quotient and remainder of the division of $n - 2$ by 41 and define the integers a, b, c, d, e as follow.

$$\begin{aligned} a &= \chi(r \geq 10) \\ b &= \chi(r \in \{1, 4, 7, 10, 11, 14, 17, 20, 23, 26, 27, 30, 33, 36, 39\}) \\ c &= \chi(r \in \{2, 5, 8, 12, 15, 18, 21, 24, 28, 31, 34, 37, 40\}) \\ d &= \lfloor (r - 10\,(\chi(r \geq 10) + \chi(r \geq 26)))\,/3 \rfloor \\ e &= \chi(r \geq 26), \end{aligned}$$

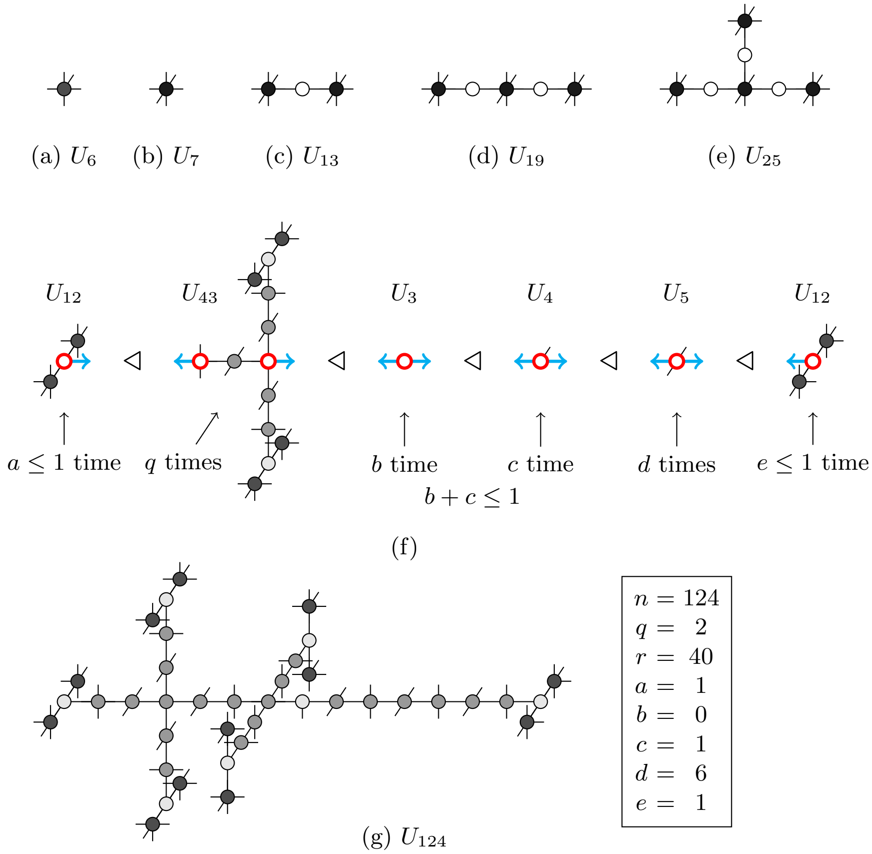


Fig. 6. Fully leafed tree-like polycubes

where χ is the usual characteristic function. Let U_n be a tree-like polycube obtained by the graft union

$$U_n = U_{12}^a \lhd U_{43}^q \lhd U_3^b \lhd U_4^c \lhd U_5^d \lhd U_{12}^e, \tag{4}$$

where the exponent notation of a tree-like polycube U_n is defined by

$$U_n^k = \begin{cases} U_2, & \text{if } k = 0; \\ R^{k-1}(U_n) \lhd U_n^{k-1}, & \text{if } k = 5, 43; \\ U_n \lhd U_n^{k-1}, & \text{otherwise.} \end{cases}$$

where $R^{k-1}(U_n)$ is the rotation of 90° of U_n about the "horizontal" axis in Figure 6 (f) and (g) applied $k-1$ times. In other words, when copies of U_5 and U_{43} are grafted to themselves, the new copy must be rotated by 90° before being grafted. We assume that the roots and directions used for the graft union are respectively as depicted in Figure 6 (f) by red dots and blue arrows. Note also that the two tree-like polycubes U_{12} at each end of Figure 6 (f) are shown in the proper position up to a rotation of 90°. Clearly, all graft unions in Equation (4) are well-defined. Therefore, for $2 \leq n \leq 85$ and $n \notin \{6, 7, 13, 19, 25\}$, it follows from Lemma 8 that

$$n(U_n) = 41q + 10(a+e) + b + 2c + 3d + 2 = n,$$
$$n_1(U_n) = 28q + 7(a+e) + c + 2d + 2 = \ell_3(n).$$

The recursive part in the definition of $\ell_3(n)$ is straightforward since q is arbitrarily large and $n_1(U_{43}) = 28$, concluding the proof. Figure 6 (g) shows the tree-like polycube obtained from Equation (4) when $n = 124$. □

In order to prove $L_3(n) \leq \ell_3(n)$ for all n, we introduce an appropriate notation for the operation dual to graft union which is the graft factorization of tree-like polycubes.

Definition 10 (Branch). *Let $T = (V, E)$ be a tree-like polycube and r, r' two adjacent vertices of T. Let V_r and $V_{r'}$ be the set of vertices of T defined by*

(i) $r \in V_r$, $r' \in V_{r'}$,
(ii) *the subgraphs of T induced by V_r and $V_{r'}$ are precisely the two connected components obtained from T by removing the edge $\{r, r'\}$.*

Then the rooted tree-like polycube $B = (T[V_r \cup \{r'\}], r, \overrightarrow{rr'})$ is called a branch *of T and the rooted tree-like polycube $B^c = (T[V_{r'} \cup \{r\}], r', \overrightarrow{r'r})$ is called the* co-branch *of B in T. When neither r nor r' are leaves of T, then we say that B is a* proper branch *of T.*

Proposition 11. *Let T be a tree-like polycube and B a proper branch of T. Then both $B \lhd B^c$ and $B^c \lhd B$ are well-defined and final, while their corresponding unrooted tree-like polycube is precisely T.*

Proof. This follows from Definitions 7 and 10.

We wish to identify branches that could appear in potential counter-examples. Intuitively, these branches would need to have many leaves with respect to their number of cells.

Definition 12. *Let R, R' be two rooted tree-like polycubes having the same direction. We say that R is* substitutable *by R' if, for any tree-like polycube T containing the branch R, $R^c \lhd R'$ is well-defined.*

Roughly speaking, Definition 12 means that R can always be replaced by R' without creating a cycle whenever it appears in some tree-like polycube T. A sufficient condition for finding substitutable rooteed tree-like polycubes is related to its *hull* (see Section 2).

Proposition 13. *Let R be a rooted tree-like polycube and R' a rooted subtree of* $\mathrm{Hull}(R)$ *having the same root as R. Then R is substitutable by R'.*

Algorithm 1 Generation of all abundant rooted tree-like polycubes.

```
function AbundantBranches(h : height) : pair of maps
    For i = 1, 2, ..., h, let A[i] ← ∅ and F[i] ← ∅
    A[1], F[1] ← {basic free tree-like polycubes of size 5 and 6}
    for i ← 1, 2, ..., h do
        for each basic rooted free tree-like polycube B do
            for each B′ ∈ B ◁ ∪_{j=0}^{i−1} A[j] of height i do
                if B′ is abundant then
                    if B′ is final then F[i] ← F[i] ∪ B′
                    else A[i] ← A[i] ∪ B′
                end if
            end for
        end for
    end for
    return (A, F)
end function
```

Proof. Omitted due to lack of space.

We are now ready to classify rooted tree-like polycubes.

Definition 14. *Let R be a rooted tree-like polycube. We say that R is* abundant *if one of the following two conditions is satisfied:*

(i) *R contains exactly two cells,*
(ii) *There does not exist another abundant rooted tree-like polycube R', such that R is substitutable by R', $n(R') < n(R)$ and*

$$n_1(R) - n_1(R') \leq \Delta\ell_3(n(R) - n(R')) \tag{5}$$

Otherwise, we say that R is sparse.

From Definition 14, one can enumerate all abundant rooted tree-like polycubes up to a given height, both final and nonfinal, using a brute-force approach as described by Algorithm 1. In the algorithm, for each height $i = 1, 2, \ldots, h$, where h is some positive integer, the abundant final and nonfinal rooted tree-like polycubes are stored respectively in the two lists $F[i]$ and $A[i]$.

Algorithm 1 was implemented in Python and run with increasing values of h [3]. It turned out that there exists no abundant rooted tree-like polycube for $h \geq 11$, i.e. there is a finite number of such objects. Due to a lack of space, we cannot exhibit all abundant rooted tree-like polycubes, but we can give some examples. For instance, in Figure 6, any rooted version of the trees U_6, U_7 and U_{12} is abundant, while U_3, U_4, U_5, U_{13}, U_{19},U_{25} and U_{43} are sparse.

The following facts are directly observed by computation.

Lemma 15. *Let $T = B \triangleleft B^c$ be a rooted tree-like polycube. If T is abundant, then its height is at most* 10 *and*

(i) *If T is final and both B and B^c are abundant, then $n_1(T) \leq \ell_3(n(T))$.*

(ii) *If* $n(T) \in \{6, 7, 13, 19\}$*, then either* B *or* B^c *is sparse.*

Proof. Let A and F be respectively the sets of abundant nonfinal and final rooted tree-like polycubes computed by Algorithm 1 with $h = 11$ [3]. Since $|F(11)| = 0$, the first observation is proved and exhaustive inspection of F implies (i).

For (ii), assume by contradiction that both B and B^c are abundant. By inspecting F, we must have $T \in F$, but F does not contain any final rooted tree-like polycube with 6, 7, 13 or 19 vertices. □

The nomenclature "sparse" and "abundant" is better understood with the following lemma, which asserts that a minimum counter-example may only contain abundant branches.

Lemma 16. *Assume that there exists a tree-like polycube* T *of minimum size such that* $n_1(T) > \ell_3(n(T))$*. Then every branch of* T *is abundant.*

Proof. Let B be any branch of T and C its co-branch so that $T = B \triangleleft C$. Assume that B is sparse, using the substitution by the abundant rooted tree-like polycube B' and let $T' = B' \triangleleft C$.

Suppose first that

$$\ell_3(n(B \triangleleft C)) - \ell_3(n(B' \triangleleft C)) \geq \Delta\ell_3(n(B) - n(B')) \geq n_1(B) - n_1(B'), \quad (6)$$

where the last inequality is deduced from Inequation (5). Then

$$\begin{aligned} \ell_3(n(T)) = \ell_3(n(B \triangleleft C)) &\geq n_1(B) - n_1(B') + \ell_3(n(B' \triangleleft C)) \\ &\geq n_1(B) - n_1(B') + n_1(B' \triangleleft C) \\ &= n_1(B \triangleleft C) = n_1(T), \end{aligned}$$

contradicting the hypothesis $n_1(T) > \ell_3(n(T))$.

Then it follows from the preceding paragraph that

$$\ell_3(n(B \triangleleft C)) - \ell_3(n(B' \triangleleft C)) < \Delta\ell_3(n(B) - n(B')). \quad (7)$$

By Proposition 5(ii), this implies that $n(B' \triangleleft C) \in \{6, 7, 13, 19\}$. Since B' is abundant, Lemma 15(ii) implies that C is sparse. Therefore, using the same reasoning as above, either we have Inequations (6) by swapping B and C, leading to a contradiction, or C can be substituted by some abundant branch C' such that $n(B \triangleleft C') \in \{6, 7, 13, 19\}$, so that $n(B \triangleleft C) \leq 19$. Therefore, $n(T) \leq 19$, but exhaustive inspection shows that there is no such counter-example. □

Hence, we have the following fact.

Lemma 17. *For all* $n \geq 2$, $L_3(n) \leq \ell_3(n)$.

Proof. By contradiction, assume that there exists a tree-like polycube T of minimum size such that $n_1(T) > \ell_3(n(T))$. By Lemma 16, every branch of T is abundant, so that there must exist two abundant branches B and B' such that $T = B \triangleleft B'$. The result follows from Lemma 15(i).

Combining Lemmas 9 and 17, we have proved our main result.

Theorem 18. *For all* $n \geq 2$, $L_3(n) = \ell_3(n)$ *and the asymptotic growth of* L_3 *is given by* $L_3(n) \sim \frac{28}{41}n$.

5 Concluding Remarks

Theorems 4 and 18 describe the maximal number of leaves that can be realized by tree-like polominoes and polycubes respectively. The next step would be to extend the results not only to other regular lattices, such as the hexagonal and the triangular lattice, but also to nonperiodic lattices.

References

1. J.-C. Aval, M. D'Adderio, M. Dukes, A. Hicks, and Y. Le Borgne. Statistics on parallelogram polyominoes and a q,t-analogue of the narayana numbers. *J. Comb. Th., Series A*, 123(1):271–286, 2014.
2. E. Barcucci, A. Frosini, and S. Rinaldi. On directed-convex polyominoes in a rectangle. *Discrete Mathematics*, 298(1-3):62–78, 2005.
3. A. Blondin Massé. A sagemath program to compute fully leafed tree-like polycubes, 2016. https://bitbucket.org/ablondin/fully-leafed-tree-polycubes.
4. M. Bousquet-Mélou and A. J. Guttmann. Enumeration of three dimensional convex polygons. *Annals of Combinatorics*, 1(1):27–53, 1997.
5. M. Bousquet-Mélou and A. Rechnitzer. The site-perimeter of bargraphs. *Adv. in Appl. Math.*, 31(1):86–112, 1997.
6. G. Castiglione, A. Frosini, E. Munarini, A. Restivo, and S. Rinaldi. Combinatorial aspects of l-convex polyominoes. *Europ. J. of Combinatorics*, 28(6):1724–1741, 2007.
7. J.-M. Champarnaud, J.-P. Dubernard, Q. Cohen-Solal, and H. Jeanne. Enumeration of specific classes of polycubes. *Electr. J. Comb.*, 20(4), 2013.
8. M.-P. Delest and G. Viennot. Algebraic languages and polyominoes enumeration. *Theoret. Comput. Sci.*, 34:169–206, 1984.
9. A. Goupil, H. Cloutier, and F. Nouboud. Enumeration of polyominoes inscribed in a rectangle. *Disc. Appl. Math.*, 158(18):2014–2023, 2010.
10. A. Goupil, M. E. Pellerin, and J. de Wouters d'Oplinter. Partially directed snake polyominos. *ArXiv:1307.8432v2*, 2014.
11. A. J. Guttmann. *Polygons, Polyominoes and Polycubes*. Springer, 2009.
12. W. Hochstättler, M. Loebl, and C. Moll. Generating convex polyominoes at random. *Discrete Mathematics*, 153(1-3):165–176, 1996.
13. I Jensen. Enumerations of lattice animals and trees. *J. Stat. Mechanics*, 102(18):865–881, 2001.
14. D.A. Klarner and R.L. Rivest. A procedure for improving the upper bound for the number of n-ominoes. *Canadian Journal of mathematics*, 25:585–602, 1973.
15. D.E. Knuth. Polynum, program available from knuth's home-page at http://sunburn.stanford.edu/knuth/programs.html#polyominoes, 1981.
16. D.H. Redelmeyer. Counting polyominoes: Yet another attack. *Discrete Mathematics*, 36(3):191–203, 1981.