AN IMPROVED UPPER BOUND ON THE GROWTH CONSTANT OF POLYIAMONDS

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Abstract. A polyiamond is an edge-connected set of cells on the triangular lattice. Let $T(n)$ denote the number of distinct (up to translation) polyiamonds made of n cells. It is known that the sequence $T(n)$ has an asymptotic growth constant, i.e., the limit $\lambda_T := \lim_{n\to\infty} T(n+1)/T(n)$ exists, but the exact value of λ_T is still unknown. In this paper, we improve considerably the best known upper bound on λ_T from 4 to 3.6108.

1. Introduction

An **animal** on a two-dimensional lattice is a connected set of cells on the lattice, where connectivity is by edges. Examples are polyominoes on the square lattice and polyiamonds on the triangular lattice. Two **fixed** lattice animals are regarded as equal if they are translates of each other, while rotations are not considered. The study of lattice animals began in parallel more than half a century ago in statistical physics [**13**] and in mathematics [**5**]. In this paper, we consider fixed animals on the triangular lattice in the plane (where all cells are equilateral triangles), and refer to them in the sequel simply as "polyiamonds."

Let $T(n)$ denote the number of polyiamonds of size n. Figure 1 shows polyiamonds of size up to 5. Early counts of polyiamonds were given by Lunnon [**9**] up to size 16, by Sykes and Glen [**12**] up to size 22, and by Aleksandrowicz and Barequet [**2**] up to size 31. The values $T(n)$ (sequence A001420 in the On-Line Encyclopedia of Integer Sequences [**1**]) have been computed up to $n = 75$ [**6**, p. 479], using a version of Jensen's subgraph-counting algorithm [**7**]. The largest known value is $T(75) = 15{,}936{,}363{,}137{,}225{,}733{,}301{,}433{,}441{,}827{,}683{,}823 \approx 1.6 \times 10^{34}$.

Due to results of Klarner [**8**] and Madras [**10**], we know that the limits $\lambda_T := \lim_{n\to\infty} \sqrt[n]{T(n)} = \lim_{n\to\infty} T(n+1)/T(n)$ exist and are equal. This number, λ_T, is called the **growth constant** of polyiamonds. Based on existing data, it is estimated [**12**] that $\lambda_T = 3.04 \pm 0.02$. Klarner [**8**, p. 857] showed that $\lambda_T \geq 2.13$, see also Lunnon [**9**, p. 98]. Rands and Welsh [**11**] improved the lower bound to 2.3011. However, as was already pointed out [**4**], they could easily have shown that $\lambda_T \geq 2.3500$, using the data available at the time. Moreover, using the

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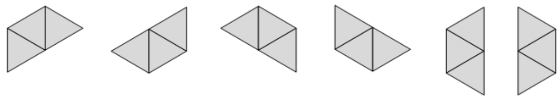
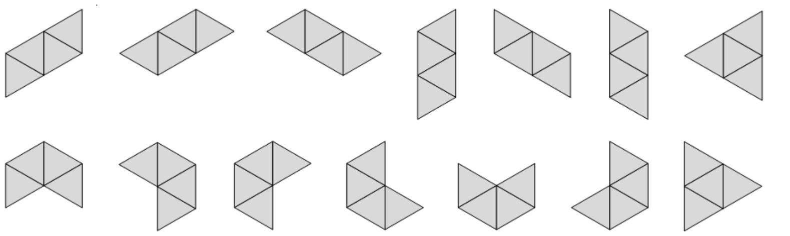
$n = 1$: Two moniamonds $n = 2$: Three diamonds



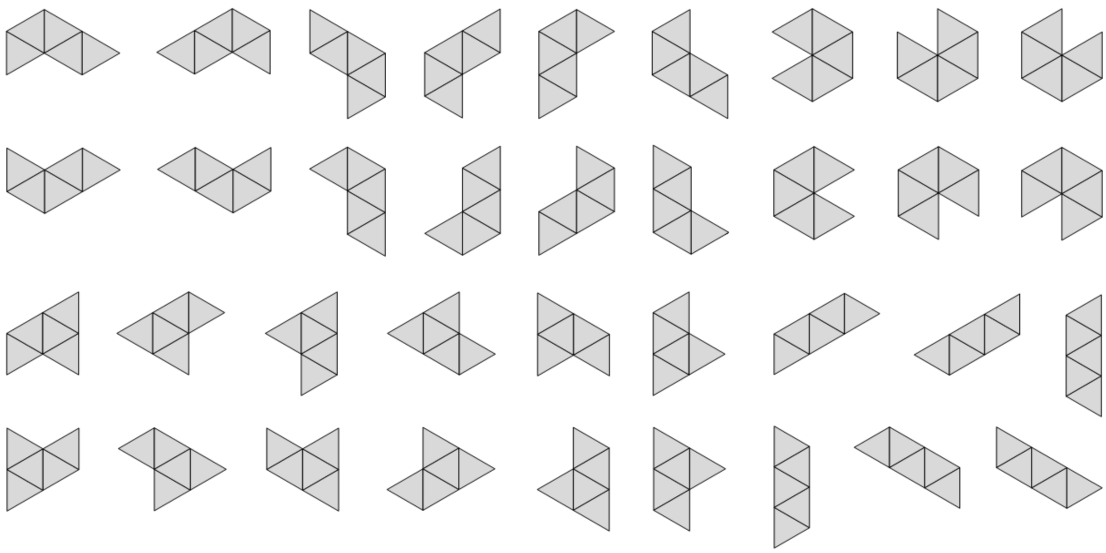
$n = 3$: Six triamonds



$n = 4$: 14 tetriamonds

n	$T(n)$
1	2
2	3
3	6
4	14
5	36
6	94
7	250
8	675
9	1 838
10	5 053
11	14 016
12	39 169
13	110 194
14	311 751
15	886 160
16	2 529 260

values of $T(n)$



$n = 5$: 36 pentiamonds

Figure 1. Polyiamonds of sizes $1 \le n \le 5$, and the first few values of $T(n)$.

same method but with more values $T(n)$ known today, one obtains the lower bound 2.7714. At any rate, the current best lower bound, $\lambda_T \ge 2.8424$, was obtained with a different method [**4**].

To the best of our knowledge, there is only a single work [**9**, p. 98] that proves an upper bound. It shows the rather easy bound $\lambda_T \le 4$. In this paper, we use a novel method in order to improve significantly the upper bound, showing that $\lambda_T \le 3.6108$. The new bound is obtained by investigating the growth constant of a sequence that bounds the number of polyiamonds from above.

2. The Method

We follow the method used recently [**3**] for polyominoes (animals on the **square** lattice). In fact, there is an error in this article, which invalidates the claimed improved upper bound on the growth constant of polyominoes. Theorem 2.5 therein claimed a **linear** upper bound on the number of **compositions** (see Section 3 below) of two polyominoes. However, G. Rote found a counterexample consisting of two polyominoes, each of size n, having $\Theta(n^{3/2})$ compositions. In a follow-up joint work with A. Asinowski, still unpublished, this counterexample was refined to construct, for any $\varepsilon > 0$, a pair of polyominoes, each of size n, having $\Omega(n^{2-\varepsilon})$ compositions. In the current work, we take a different approach for proving Theorem 2 below, proving a quadratic upper bound on the number of compositions.

Another difference between the current work and the original one [**3**] lies in the last step of the proof (Section 5 of the current paper). In both papers, the upper bound on the growth constant of the respective type of animals is computed by estimating the growth constant of a sequence which bounds from above the number of animals. While for the erroneous bound on the growth constant of polyominoes, the growth constant of the dominating sequence was computed using a nonrigorous numerical method, in this work we apply for the same purpose a rigorous and quite delicate mathematical induction.

3. Number of Compositions

Definition 1. *A polyiamond P can be **decomposed** into two polyiamonds P_1 and P_2 if the cell set of P can be split into two disjoint non-empty subsets, such that each subset comprises a valid (connected) polyiamond. We also say that the polyiamonds P_1, P_2 can be **composed**, with the appropriate relative translation, so as to yield the polyiamond P.*

A **composition** of two polyiamonds is a generalization of the widely-used notion of the **concatenation** of polyiamonds. Given a total order of the cells of a lattice, concatenation of two animals is simply a composition (possibly in more than one way) so that the lexicographically-largest cell of one animal is attached to the lexicographically-smallest cell of the other animal.

Theorem 2. (*Composition*) *Let P_1, P_2 be two polyiamonds of sizes n_1 and n_2, respectively. Then, at most $(n_1+2)(n_2+2)/2$ different polyiamonds can be obtained by composing P_1 and P_2.*

Proof. Every boundary edge of a polyiamond is either vertical, ascending, or descending. The inside of the polyiamond can be either to the left or to the right of the edge. Accordingly, we classify the boundary edges into six categories $v, a, d, \bar{v}, \bar{a}, \bar{d}$, see Figure 2 for an example. By counting the edges in each category, we get a 6-tuple of numbers, $(v, a, d, \bar{v}, \bar{a}, \bar{d})$, the **boundary signature** of the polyiamond, whose sum $v + a + d + \bar{v} + \bar{a} + \bar{d}$ equals the perimeter of the polyiamond.

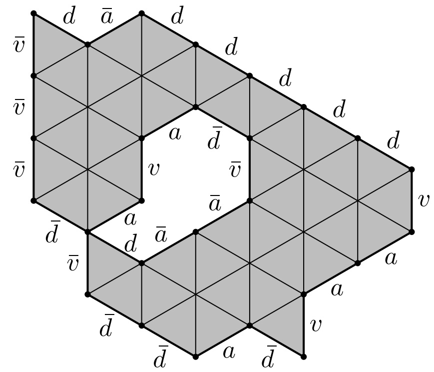


Figure 2. A polyiamond with boundary signature $(v, a, d, \bar{v}, \bar{a}, \bar{d}) = (3, 5, 7, 5, 3, 5)$.

Suppose that we are given two polyiamonds P_1, P_2 with respective perimeters p_1, p_2 and associated boundary signatures $(v_i, a_i, d_i, \bar{v}_i, \bar{a}_i, \bar{d}_i)$, for $i = 1, 2$. Then, a trivial upper bound on the number of compositions of P_1 and P_2 is $\sum_{t \in \{v,a,d,\bar{v},\bar{a},\bar{d}\}} (t_1 \cdot \bar{t}_2)$, using the convention $\bar{\bar{t}}_i = t_i$. The number of boundary edges of any type in a polyiamond of perimeter p cannot exceed $p/2$, otherwise there are not enough remaining edges to turn the boundary into one or more closed loops. The maximum of a bilinear function under linear inequality constraints on each operand is attained at an extreme point of the feasible region. Therefore, the maximum value of the upper bound under these constraints is attained, for example, by setting $(v_1, a_1, d_1, \bar{v}_1, \bar{a}_1, \bar{d}_1) = (\frac{p_1}{2}, 0, 0, \frac{p_1}{2}, 0, 0)$ and $(v_2, a_2, d_2, \bar{v}_2, \bar{a}_2, \bar{d}_2) = (\frac{p_2}{2}, 0, 0, \frac{p_2}{2}, 0, 0)$, leading to an upper bound of $2(p_1/2 \cdot p_2/2) = p_1 p_2/2$ on the number of compositions of P_1 and P_2. The perimeter of a polyiamond of size n is maximized when the cell-adjacency graph of the polyiamond is a tree, in which case the perimeter is $n+2$. (Indeed, the perimeter of a single triangle is 3, and each of the additional $n-1$ triangles adds at most 1 to the perimeter.) The claim follows. ☐

4. Balanced Decompositions

Definition 3. *A decomposition of a polyiamond of size n into two polyiamonds P_1, P_2 is **k-balanced** if $k \leq |P_1| \leq n - k$ (and hence $k \leq |P_2| \leq n - k$).*

Lemma 4. *Every polyiamond of size n has at least one $\lceil (n-1)/3 \rceil$-balanced decomposition.*

Proof. Let us rephrase the claim in graph terminology. In fact, we prove a more general claim which states that every connected graph G, with $|G| = n$ vertices and maximum degree $\Delta(G) \leq 3$, can be partitioned into two vertex-disjoint subgraphs A, B, such that A, B are connected and $\lceil (n-1)/3 \rceil \leq |A|, |B| \leq \lfloor (2n+1)/3 \rfloor$. Applying this claim to the cell-adjacency graph of the polyiamond gives the lemma.

We consider an arbitrary spanning tree T of G. Then, each edge of T induces a split of T, and hence of G, into two connected parts. Let e be the edge that gives the most balanced split of G into two parts A, B, and let s be the size of the smaller part (A). In addition, let x be the endpoint of e in B. The removal of x from B splits B into two parts B_1, B_2 (the smaller of which may be empty). Obviously, $|B_1| \leq s$ and $|B_2| \leq s$, otherwise the edge from x to the bigger of the two parts would then give a split of G which is more balanced than the split (A, B). Consequently, $n = |A| + |B_1| + |B_2| + 1 \leq 3s + 1$. Hence, $s \geq (n-1)/3$, and the claim follows from the fact that s must be integral. □

Remark. The bound $\lceil (n-1)/3 \rceil$ in the lemma is tight, as can be seen by a Y-shaped graph with three paths of length approximately $n/3$ ending in a common central vertex of degree 3, or in other words, a subdivision of the star graph $K_{1,3}$. This graph can arise as the cell-adjacency graph of a polyiamond.

5. A Dominating Sequence

We can now prove our main result.

Theorem 5. $\lambda_T \leq 3.6108$.

Proof. First, we show that the combination of Theorem 2 and Lemma 4 implies the following bound:

$$T(n) \leq \sum_{k=\lceil \frac{n-1}{3} \rceil}^{\lfloor \frac{2n+1}{3} \rfloor} \frac{(k+2)(n-k+2)}{4} T(k)T(n-k) + \frac{(n/2+2)^2}{4} T(\tfrac{n}{2}) \tag{1}$$

Indeed, every polyiamond P of size n can be decomposed in at least one $\lceil (n-1)/3 \rceil$-balanced way into a pair of polyiamonds P_1, P_2 of sizes $n_1 = k$ and $n_2 = n - k$, respectively. There are at most $(n_1+2)(n_2+2)/2$ possibilities to compose P_1, P_2 in order to reconstruct P. The extra factor $1/2$ is introduced to compensate for double counting. The term $T(k)T(n-k)$ counts the **ordered pairs** (P_1, P_2) of polyiamonds of appropriate sizes. Clearly, the opposite pair (P_2, P_1) generates the same composite polyiamonds. Every unordered pair $\{P_1, P_2\}$ occurs twice, except when $P_1 = P_2$. These exceptional pairs of equal elements exist only for $k = n-k = \frac{n}{2}$, and their number is $T(\frac{n}{2})$. The last term makes the necessary adjustment to ensure that these pairs are fully counted. In order to avoid clumsy case distinctions, we define $T(x) = 0$ if x is not an integer.

The following sequence, $U(n)$, is therefore an upper bound on $T(n)$: It starts with the known values of $T(n)$ for $n \leq 75$, and extends them by the relation (1).

$$U(n) = \begin{cases} 0 & \text{for } n \notin \mathbb{N} \\ T(n) & \text{for } n \leq 75 \\ \left\lfloor \displaystyle\sum_{k=\lceil \frac{n-1}{3} \rceil}^{\lfloor \frac{2n+1}{3} \rfloor} \frac{(k+2)(n-k+2)}{4} U(k)U(n-k) + \frac{(n/2+2)^2}{4} U(\tfrac{n}{2}) \right\rfloor & \text{for } n > 75 \end{cases} \tag{2}$$

We are done if we can show the following bound:

$$U(n) \leq \frac{C\mu^n}{(n+2)^3}, \text{ for } n \geq 1000, \tag{3}$$

with $\mu = 3.6108$ and $C = 1/1.46 \approx 0.685$. We prove this by induction on n. The induction basis covers the range $n = 1000, \ldots, 3000$, and can be checked by computing $U(n)$ according to the recursion (2) for $n \le 3000$, using a computer. For this purpose, we wrote a straightforward program[1] in the SAGE system,[2] which supports integer arithmetic with unbounded precision.

For $n > 3000$, we use again the recursion for the inductive step, and n is big enough so that the induction hypothesis can be applied on the right-hand side:

$$U(n) = \left\lfloor \sum_{k=\lceil \frac{n-1}{3} \rceil}^{\lfloor \frac{2n+1}{3} \rfloor} \frac{(k+2)(n-k+2)}{4} U(k)U(n-k) + \frac{(\frac{n}{2}+2)^2}{4} U(\tfrac{n}{2}) \right\rfloor$$

$$\le \sum_{k=\lceil \frac{n-1}{3} \rceil}^{\lfloor \frac{2n+1}{3} \rfloor} \frac{(k+2)(n-k+2)}{4} \frac{C\mu^k}{(k+2)^3} \frac{C\mu^{n-k}}{(n-k+2)^3} + \frac{(\frac{n}{2}+2)^2}{4} \frac{C\mu^{n/2}}{(\frac{n}{2}+2)^3}$$

$$= C^2\mu^n \sum_{k=\lceil \frac{n-1}{3} \rceil}^{\lfloor \frac{2n+1}{3} \rfloor} \frac{1}{4(k+2)^2(n-k+2)^2} + \frac{C\mu^{n/2}}{2n+8}$$

$$= C^2\mu^n \Big(S + \frac{1}{C\mu^{n/2}(2n+8)} \Big) = C^2\mu^n(S + S_0),$$

where S denotes the sum in the penultimate line, and S_0 is the second term in the parentheses in the last line. We will show that

$$S + S_0 \le \frac{1.46}{(n+4)^3} = \frac{1}{C(n+4)^3} < \frac{1}{C(n+2)^3}, \tag{4}$$

from which (3) follows. We estimate S by converting the sum to an integral. The summand, $f(k) = 1/[4(k+2)^2(n-k+2)^2]$, considered as a function of k, is first decreasing to a minimum at $k = n/2$, and then increasing. For such a function, the sum can be bounded from above by an integral as follows.

Lemma 6.

$$\sum_{k=a}^{b} f(k) \le \int_{k=a-1}^{b+1} f(k)\, dk.$$

Proof. Each summand $f(t)$ is bounded from above by $\int_{t-1}^{t} f(k)\, dk$ if t is on the decreasing branch, or by $\int_{t}^{t+1} f(k)\, dk$ if t is on the increasing branch. These integration intervals are disjoint, and they all lie inside the interval $[a-1, b+1]$. □

(The easy estimate $\sum_{k=a}^{b} f(k) \le (b-a+1)\max(f(a), f(b))$ would lead to a slightly weaker upper bound on λ_T.)

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[1] See `http://page.mi.fu-berlin.de/rote/Papers/abstract/An+improved+upper+bound+on+the+growth+constant+of+polyiamonds.html`

[2] `www.sagemath.org`

We can, therefore, bound the sum S from above as follows.

$$S \le \int_{k=(n-4)/3}^{(2n+4)/3} \frac{dk}{4(k+2)^2(n-k+2)^2} = \frac{1}{(n+4)^3} \int_{y=1/3-\alpha}^{2/3+\alpha} \frac{dy}{4y^2(1-y)^2}$$

with $\alpha = \frac{2}{3(n+4)}$, using the substitution $y = \frac{k+2}{n+4}$. Since $n > 3000$, α can be bounded by $\alpha_0 = 1/4500$, and the last integral is bounded from above by

$$(5) \qquad \int_{y=1/3-\alpha_0}^{2/3+\alpha_0} \frac{dy}{4y^2(1-y)^2} = \left[\frac{2y-1}{4y(1-y)} + \frac{1}{2}\ln\frac{y}{1-y}\right]_{y=1/3-\alpha_0}^{2/3+\alpha_0} \le 1.45.$$

We still have to deal with the term S_0. It is tiny, and we can afford a generous bound. Since $\mu = 3.6108$ and $n > 3000$, the bound

$$S_0 = \frac{1}{C\mu^{n/2}(2n+8)} \le \frac{0.01}{(n+4)^3}$$

is a gross overestimate. Putting everything together, we get

$$S + S_0 \le \frac{1.45}{(n+4)^3} + \frac{0.01}{(n+4)^3} = \frac{1.46}{(n+4)^3},$$

establishing (4) and, thus, concluding the inductive step. □

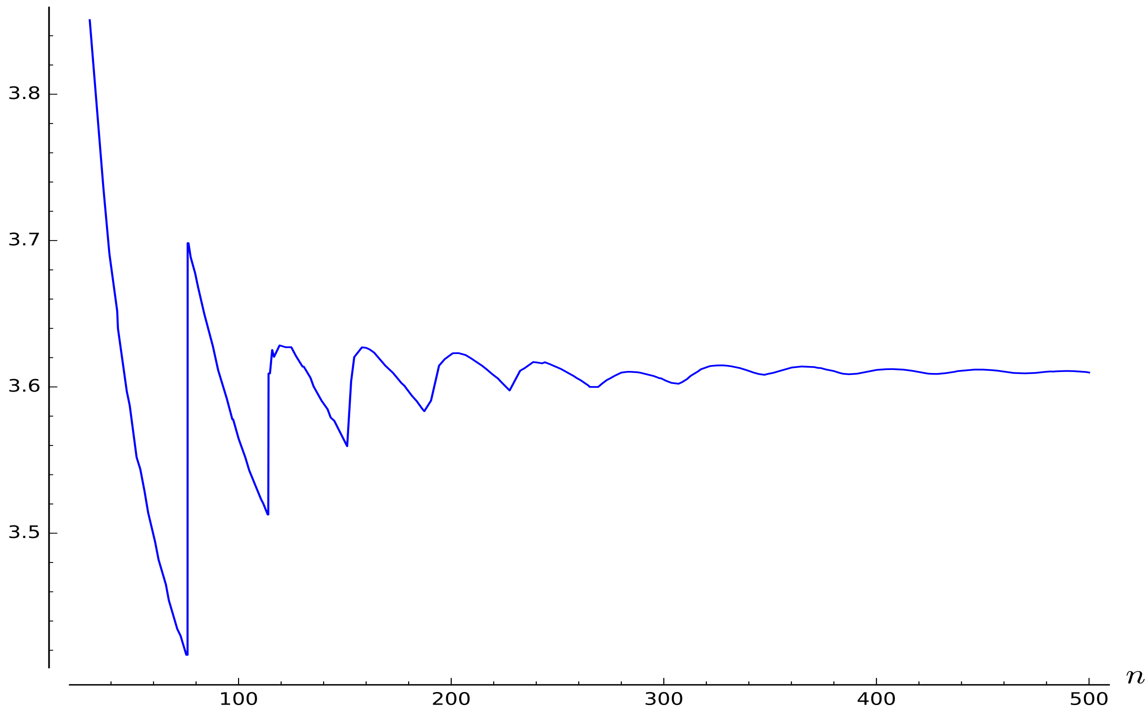

Figure 3. $\sqrt[n]{U(n)(n+2)^3/C}$ as a function of n.

Note that the validity of the inductive step does not depend on the value of μ, except for the term S_0, which is negligible. In fact, when setting up the proof, we first had to determine C from the integral (5) to make the induction work, and then we fixed μ so as to satisfy the hypothesis (3) for $1000 \le n \le 3000$, which we could accomplish by choosing $\mu \geq \max\{\sqrt[n]{U(n)(n+2)^3/C} \mid 1000 \leq n \leq 3000\}$. Figure 3 shows a plot of an initial segment of these values. They decrease for the range where the true values $T(n)$ are used ($n \leq 75$). There is a jump when the recursion sets in. The recursion reproduces the jump as soon as the large values start to be used on the right-hand side of (2). The jumps get damped into smaller and smaller waves as n increases. It pays off to let the induction start at $n = 3000$ instead of, say, $n = 300$, but the possible improvement for even higher values of n is marginal. Experimentally, the limit growth constant of $U(n)$ is approximately 3.6050. The true value of λ_T should, of course, be much smaller: It lies at the limit of the leftmost descending branch of the plot in Figure 3, if that branch were continued.

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