Applications of Concatenation Arguments to Polyominoes and Polycubes*

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Abstract

We present several concatenation arguments for polyominoes and polycubes, and show their applications to setting lower and upper bounds on the growth constants of some of their families, whose enumerating sequences are pseudo sub- or super-multiplicative. *Inter alia*, we provide bounds on the growth constants of general and tree polyominoes, and general polycubes.

1 Introduction

A *polycube* of size n is a connected set of n cells on $\mathbb{Z}^d$, where connectivity is through $(d-1)$-dimensional facets. Two-dimensional polycubes are also called *polyominoes*. Two *fixed* polycubes are *equivalent* if one can be translated into the other. We consider only fixed polycubes, hence we simply call them "polycubes." The study of polycubes began in statistical physics [4, 14], where they are called *lattice animals*. Counting polyominoes and polycubes is a long-standing problem. Let $A_d(n)$ denote the number of d-dimensional polycubes of size (area) n. Values of $A_2(n)$ are currently known up to $n = 56$ [8]. The growth constant of polyominoes also attracted much attention. Klarner [9] showed that $\lambda_d := \lim_{n\to\infty} \sqrt[n]{A_d(n)}$ exists. The convergence of $\frac{A_d(n+1)}{A_d(n)}$ to λ_d $(n\to\infty)$ was proven much later [11]. The best known lower [1] and upper [10] bounds on λ_2 are 4.0025 and 4.6496, respectively.

In this paper, we develop methods for deriving bounds on the growth constants of families of polyominoes and polycubes, for which the enumerating sequences are pseudo sub- or super-multiplicative. Such a property can be derived from a generalized polyomino-concatenation argument, as we show below. We demonstrate various applications of this method to general polyominoes and polycubes, as well as to specific families, such as tree polycubes.

2 Preliminaries

2.1 Concatenation and Sub-/Super-multiplicative Sequences

A sequence $(Z(n))$ is *super-multiplicative* (resp., *sub-multiplicative*) if $Z(m)Z(n) \le Z(m+n)$ (resp., $Z(m)Z(n) \ge Z(m+n)$) $\forall m,n \in \mathbb{N}$. It is known [13, p. 171] that a super-multiplicative (resp., sub-multiplicative) sequence $Z(n)$, with the property that $Z'(n) = \sqrt[n]{Z(n)}$ is bounded from above (resp., below), has a *growth constant*. That is, the quantity $\lim_{n\to\infty} Z'(n)$ exists.

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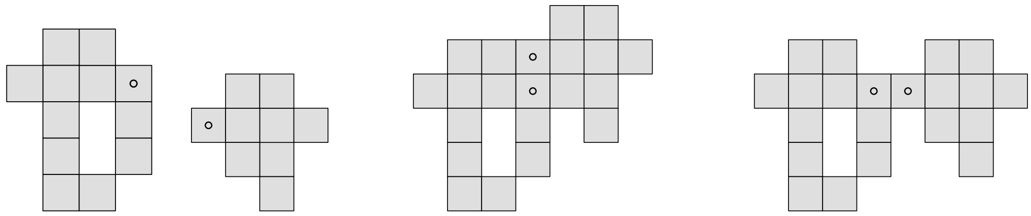


(a) Two polyominoes (b) Vertical concatenation (c) Horizontal concatenation

Figure 1 Concatenations of two polyominoes.

Let us define a total order on cells of the cubical lattice: First by x_1 (x in two dimensions), then by x_2 (y in two dimensions), and so on. Thus, in two dimensions, the *smallest* (resp., *largest*) square of a polyomino P is the lowest (resp., highest) cell in the leftmost (resp., rightmost) column of P. The vertical (resp., horizontal) *concatenation* of two polyominoes P_1, P_2 is the positioning of P_2 such that its smallest cell lies immediately *above* (resp., *to the right of*) the largest cell of P_1 (see Figure 1).

Similarly, two d-dimensional polycubes can be concatenated in d ways. Concatenating two polycubes always yields a valid polycube (connected and with no overlapping cells), and two different pairs of polycubes of sizes m, n always yield by concatenation two different polycubes of size $m+n$. Many polycubes, however, can be represented as the concatenations of several pairs of polycubes, whereas others cannot be represented at all as concatenations of smaller polycubes.

The following is a folklore concatenation argument for polyominoes, setting a rather weak lower bound on their growth constant. A direct consequence of the discussion above is that $A_2^2(n) < A_2(2n)$. That is, $\sqrt[n]{A_2(n)} < \sqrt[2n]{A_2(2n)}$. Hence, a sequence of the form $A^* = \left(\sqrt[n_0 2^i]{A_2(n_0 2^i)}\right)_{i=0}^{\infty}$ is monotone increasing for any natural number n_0. Since the entire sequence $A = (A_2(n))$ is super-multiplicative, and the sequence $A' = \left(\sqrt[n]{A_2(n)}\right)$ is bounded from above [6], the sequence A has a growth constant λ_2. Obviously, every subsequence of A' also converges to λ_2. In addition, since any such subsequence A^* is monotone increasing, any element of it, $\sqrt[n_0]{A_2(n_0)}$, is a lower bound on λ_2. Empirically, the best (largest) lower bound is obtained this way by setting $n_0 = 56$ (the largest value of n for which $A_2(n)$ is known), yielding the bound $\lambda_2 > 3.7031$.

Remarks. 1. Although A^* is a subsequence of A', the upward monotonicity of the former does *not* imply the monotonicity of the latter. Nevertheless, the known values of $A_d(n)$ (in all dimensions) *suggest* that A' be also monotone increasing. We later refer to this as "the unproven monotonicity of the root sequence" ("$\sqrt{\ }$UM," in short).
2. A stronger observed phenomenon is the upward monotonicity of the *ratio* sequence, *i.e.*, $A_d(n)/A_d(n-1) < A_d(n+1)/A_d(n)$ (for $n \geq 2$). Equivalently, $A_d^2(n) < A_d(n+1)A_d(n-1)$, and in a more general form, $A_d^2(n) < A_d(n+k)A_d(n-k)$ (for $n > k \geq 1$).
3. Yet another observation is that $\sqrt[n]{A_d(n)} < \frac{A_d(n)}{A_d(n-1)}$ for all $n > 1$, and in a more general form (using the convention $A(0) = 1$), $\sqrt[n]{A_d(k)A_d(n-k)} < \frac{A_d(n-k)}{A_d(n-1-k)}$ (for $n > k \geq 0$).
4. Property (2) implies Properties (1) and (3). If all are true, then the ratio sequence $(\sqrt[n]{A_d(n)})$ converges to λ_d faster than the root sequence $(\frac{A_d(n+1)}{A_d(n)})$, as is widely believed to be case.

Similarly, for any sub-multiplicative sequence $(B(n))$, for which $B'(n) = \sqrt[n]{B(n)}$ is bounded from below, and for which we can show that $B'(n) \geq B'(2n)$ for any $n \in \mathbb{N}$, any known value $B(n_0)$ sets the upper bound $B'(n_0)$ on the growth constant of $(B(n))$.

2.2 Pseudo Super- and Sub-Multiplicativity

A sequence $(Z(n))$ is *pseudo super-multiplicative* (resp., *pseudo sub-multiplicative*) if $P(m+n)Z(m)Z(n) \le Z(m+n)$ (resp., $Z(m)Z(n) \ge P(m+n)Z(m+n)$), for all $m,n \in \mathbb{N}$ and for a positive subexponential function $P(\cdot)$. (Hereafter, we will consider cases in which this function is polynomial.) In such cases, we use the fact that $\lim_{n\to\infty} \sqrt[n]{P(n)} = 1$ and obtain bounds on the growth constant of $Z(n)$ from known values of $Z(n)$.

▶ **Theorem 2.1.** *Assume that for a sequence $(Z(n))$, the limit $\mu := \lim_{n\to\infty} \sqrt[n]{Z(n)}$ exists. Let c_i ($c_1 \ne 0$) be some constants, and $\diamond \in \{`\le', `\ge'\}$. Then:*

(a) (multiplicative polynomial) If $c_1 n^{c_2} Z^2(n) \diamond Z(2n)$ $\forall n \in \mathbb{N}$, then $\sqrt[n]{c_1(2n)^{c_2} Z(n)} \diamond \mu$ $\forall n \in \mathbb{N}$.

(b) (index shift) If $c_1 Z^2(n+c_3) \diamond Z(2n)$ $\forall n \in \mathbb{N}$, then $\sqrt[n]{c_1 Z(n+2c_3)} \diamond \mu$ $\forall n \in \mathbb{N}$. Equivalently, if $c_1 Z^2(n) \diamond Z(2n+c_3)$ $\forall n \in \mathbb{N}$, then $\sqrt[n]{c_1 Z(n-c_3)} \diamond \mu$ $\forall n > c_3$.

Proof. In both cases, we manipulate the given relation and reach a relation of the form $\zeta(n) \diamond \zeta(2n)$. Then, we follow closely the logic of the basic argument given in the introduction.

(a) Simple manipulations of the given relation show that $\sqrt[n]{c_1(2n)^{c_2} Z(n)} \diamond \sqrt[2n]{c_1(4n)^{c_2} Z(2n)}$. Then, by setting $\zeta(n) = \sqrt[n]{c_1(2n)^{c_2} Z(n)}$, we see that $\zeta(n) \diamond \zeta(2n)$. It follows that the subsequence $(\zeta(2^{i+1} n_0))_{i=0}^{\infty}$ is monotone increasing (if $\diamond = `\le'$) or monotone decreasing (if $\diamond = `\ge'$), and converging to μ, for any natural number n_0. The claim follows.

(b) In this case, we substitute $n := m+c_3$ in the given relation and manipulate as above, obtaining that $c_1^2 Z^2(m+2c_3) \diamond c_1 Z(2m+2c_3)$. Hence, $\sqrt[m]{c_1 Z(m+2c_3)} \diamond \sqrt[2m]{c_1 Z(2m+2c_3)}$. Elementary calculus shows that the limits of the sequences $\left(\sqrt[m]{c_1 Z(m)}\right)$ and $\left(\sqrt[m]{c_1 Z(m+2c_3)}\right)$, as $m \to \infty$, are equal. Finally, we fix $\zeta(m) = \sqrt[m]{c_1 Z(m+2c_3)}$ and continue as above. The equivalent case, where the shift is in the right side of the relation, is treated similarly. ◀

3 Methods of Concatenation

We now list a few concatenation methods. For ease of exposition, we use relations that yield lower bounds on the growth constants. The sequence and its growth constant are denoted by $Z(n)$ and λ_Z, respectively. Polycubes P_1, P_2 are to be concatenated, and the largest (resp., smallest) cell of P_1 (P_2) is a_1 (a_2). Consistently with $\sqrt{}$UM, we observed that the best (largest) lower bounds on λ_d were obtained by using the largest known $A_d(n)$.

[E] The most elementary method of concatenation attaches cell a_1 to cell a_2 in a *single* way. This leads to the relation $Z^2(n) \le Z(2n)$, which implies that $\lambda_Z \ge \sqrt[n]{Z(n)}$ for all $n \in \mathbb{N}$.

[C] A simple improvement on Method [E] is achieved by considering all possible (lattice dependent) c ways of attaching a_1 to a_2, s.t. a_1 is smaller than a_2. This leads to the relation $cZ^2(n) \le Z(2n)$, which, by Theorem 2.1(a), implies that $\lambda_Z \ge \sqrt[n]{cZ(n)}$ $\forall n \in \mathbb{N}$.

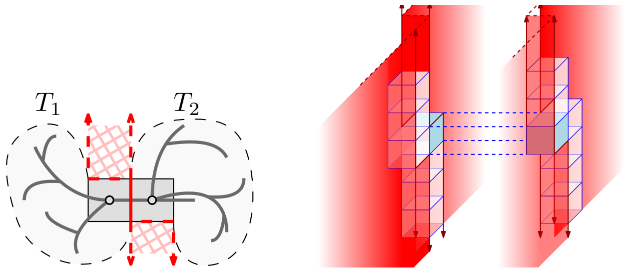
[M] A possible improvement on Method [C] can be obtained by considering all possible polycubes of size k concatenated in between P_1 and P_2. As in Method [C], there are c ways of attachments. This leads to the relation $c^2 Z(k) Z^2(n) \le Z(2n+k)$, which, by Theorem 2.1(b), implies that $\lambda_Z \ge \sqrt[n]{c^2 Z(k) Z(n-k)}$ for all $k,n \in \mathbb{N}$, such that $n > k$.

[O1] One can also *overlap* cells a_1 and a_2. This always yields a valid polycube, and different pairs of polycubes generate by this method different polycubes. This leads to $Z^2(n) \le Z(2n-1)$, which, by Theorem 2.1(b), implies that $\lambda_Z \ge \sqrt[n]{Z(n+1)}$ for all $n \in \mathbb{N}$.

[MO] One can also concatenate P_1 and P_2 through all possible polycubes of size k, using 1-cell overlaps in the middle concatenations. This leads to $Z(k) Z^2(n) \le Z(2n+k-2)$, which, by Thm. 2.1(b), implies that $\lambda_Z \ge \sqrt[n]{Z(k) Z(n-k+2)}$ for all $k,n \in \mathbb{N}$, s.t. $n > k-2$.

	Known	OEIS	Concatenation Methods			Other
Dimensions	Values	Sequence	[E]	[C]	[O1]	Methods
2	56	A001168	3.703120	3.749241	3.792324	**4.00253** [1]
3	19	A001931	**6.021134**	6.379548	6.652636	—
4	16	A151830	**8.462728**	9.228670	9.757631	—
5	15	A151831	**10.909365**	12.144998	12.939813	—
6	15	A151832	**13.523756**	15.239618	16.288833	—
7	14	A151833	**15.598535**	17.924538	19.269014	—
8	12	A151834	**16.647767**	19.797643	21.497519	—
9	12	A151835	**18.841772**	22.627780	24.606050	—

Table 1 Lower bounds on the growth constants of polycubes, obtained by different methods. (Best previously-published lower bounds appear in boldface.)



(a) Two dimensions (b) Three dimensions

Figure 2 Concatenating trees.

4 Simple Applications

4.1 General

We applied methods [E], [C], and [O1] to polyominoes and polycubes, and found lower bounds on λ_d (for $2 \le d \le 9$). Table 1 summarizes our findings. (In two dimensions, the bounds are inferior to the bound 4.00253 obtained by the much stronger *twisted cylinders* method [1], which, unfortunately, cannot be generalized efficiently to higher dimensions because it becomes computationally intractable.) We show in Section 5 how to improve all known bounds in $d \ge 3$ dimensions.

4.2 Trees

A polycube is a *tree* if its cell-adjacency graph is acyclic. Tree polycubes and their respective growth constants also attracted interest in the literature (see, *e.g.*, [5]). In order to preserve the tree property, special restrictions must be enforced while concatenating them. Figures 2(a,b) show two tree polycubes T_1, T_2, having cells c_1, c_2 as their largest and smallest cells, resp., concatenated by Method [E]. To remain a tree, the only valid concatenation is the one in which c_1 and c_2 are aligned with the most dominant axis of the lexicographic order. This leaves a $(d-1)$-dimensional buffer that prevents cycles in the concatenation of T_1 and T_2.

Let $A_{d;T}(n)$ and $\lambda_{d;T}$ denote the number of n-cell tree polycubes in d dimensions, and their growth constant, respectively. As in similar examples, we obtain the relation $A^2_{d;T}(n) \le A_{d;T}(2n)$, which, by Theorem 2.1(b), implies that $\lambda_{d;T} \ge \sqrt[n]{A_{d;T}(n)}$ for all $n \in \mathbb{N}$. Table 2 shows the best lower bounds obtained this way in dimensions 2–8, in all cases using the largest known values of the respective sequences.

Dimensions	Known Values	OEIS Sequence	Method [E]
2	44	A066158	3.4045
3	17	A118356	5.5592
4	10	A191094	6.7698
5	10	A191095	8.8035
6	8	A191096	9.4576
7	7	A191097	10.0909
8	7	A191098	11.4891

Table 2 Lower bounds on the growth constants of tree polycubes of various dimensions.

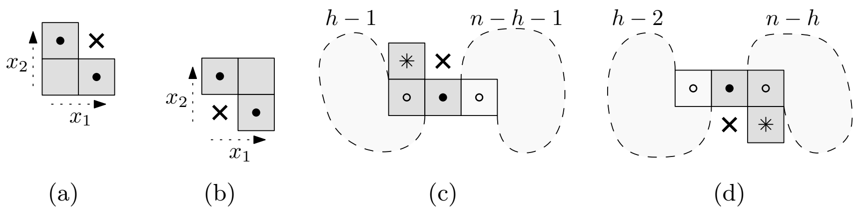


Figure 3 Constructions for the proof of Theorem 5.1.

5 Recursive Bounding

We now present a recursive scheme for improving bounds obtained by all methods described above. Let us demonstrate the scheme by a concrete example of setting lower bounds on the growth constants of polycubes. As observed earlier, the sequence enumerating d-dimensional polycubes is super-multiplicative and it has a growth constant, hence, by concatenation Method [O1], any term of the form $\sqrt[n-1]{A_d(n)}$ is a lower bound on λ_d. In practice, we can prove relations which are tighter than the super-multiplicativity condition, for example:

▶ **Theorem 5.1.** *Let $h = \lfloor (n+1)/2 \rfloor$. Then, for every $n \geq 4$, we have that*

$$A_d(n) \geq A_d(h)A_d(n-h+1) + \frac{d(d-1)^2}{2}(A_d(h-1)A_d(n-h-1) + A_d(h-2)A_d(n-h)). \quad (1)$$

Proof. The term on the left side of Relation 1 is the number of all d-dimensional polycubes of size n, whereas the terms on the right count a subset of these polycubes.

We distinguish between three types of polycubes by the connectedness of their cells.

The first term, $A_d(h)A_d(n-h+1)$, counts d-dimensional polycubes obtained by concatenating two polycubes of sizes h and $n-h+1$ with a 1-cell overlap. In these combinations, the lower h cells, as well the upper $n-h+1$ cells, form valid polycubes which share the hth cell.

The second factor of the second term, $A_d(h-1)A_d(n-h-1) + A_d(h-2)A_d(n-h)$, counts two types of constructions. In both types, we place 3-cell L-shapes (Figures 3(a,b)) in the middle in order to force the hth cell to be disconnected from either the upper $n-h$ cells or the lower $h-1$ cells (Figures 3(c,d)). The largest (smallest) cell of the lower (upper) polycube is marked by an empty circle, and the hth cell of the resulting polycube is marked by an asterisk. The trick is to mix between no-overlap and 1-overlap on the two sides of the L. To this aim, the L-shape in Figure 3(a) is overlapped with the lower polycube of size $h-1$, and concatenated to the upper polycube of size $n-h-1$ (Figure 3(c)). Similarly, the L-shape in Figure 3(b) is concatenated to the lower polycube of size $h-2$ and overlapped with the upper polycube of size $n-h$ (Figure 3(d)).

d	Bound
2	3.7944
3	**6.6621**
4	**9.7714**
5	**12.9569**
6	**16.3087**
7	**19.2927**
8	**21.5298**
9	**24.6416**

Table 3 Improved lower bounds on λ_d for $3 \le d \le 9$.

Let us finally explain the first factor of the second term. First, there are $\binom{d}{2}$ options for choosing the orientation of L. (Directions are denoted by x_1 and x_2, where x_1 has precedence over x_2 in the lexicographic order.) Second, the no-overlap concatenation (on one of the sides) can be done in $d-1$ ways: All directions are valid *except* direction x_2, the direction which would cover the forbidden cell (marked with an "$\times$" in Figures 3(a,b)). This constraint avoids multiple counting; otherwise, we would have in the middle a 2×2 square which can be created in more than one way. Overall, we have a factor of $\binom{d}{2}(d-1) = d(d-1)^2/2$.

It is easy to see that all resulting polycubes are different by construction. ◀

Unfortunately, we cannot derive from Relation (1) "chains" of lower bounds. However, we can apply a recursive procedure for bounding from below any value of $A_d(n)$. Since we know values of $A_d(n)$ up to some $n = n_0$, we can construct a sequence $B(n)$, such that $B(n) \le A_d(n)$ for every n: For $1 \le n \le n_0$, let $B(n) = A_d(n)$; and for $n > n_0$, set $B(n)$ recursively to the value calculated from the right side of Relation 1.

One can apply this method for large values of n *ad infinitum*, or, more practically, until the available computing resources are exhausted, and choose the best value encountered. We ran this procedure up to $n \approx$ 12,000,000 for $2 \le d \le 9$. This improved the lower bounds on λ_d in *all* of $3 \le d \le 9$ dimensions. Table 3 summarizes the obtained bounds.

6 Conclusion

We explore concatenation arguments and their applications to setting lower bounds on the growth constants of polycubes and tree polycubes. In the full version of the paper, we also provide a much more complex application of the method to setting an upper bound on the growth constant of *convex* polyominoes.

A possible direction for future work is analyzing the quality of our lower bounds. It was conjectured [2] that λ_d behaves asymptotically like $(2d-3)e + O(1/d)$ (as $d \to \infty$); see the blue line in the graph shown in Figure 4. Bounds obtained by the recursive-bounding method also exhibit a linear dependence on d, surprisingly similar to $3.13d{-}2.63$ (obtained with Rvalue=0.9998, using Python's linear least-squares regression tool `scipy.stats.linregress`); see the orange line in the same figure. Are the approximate slope π and intercept $-e$ a coincidence, or are they inherently related to the concatenation method?

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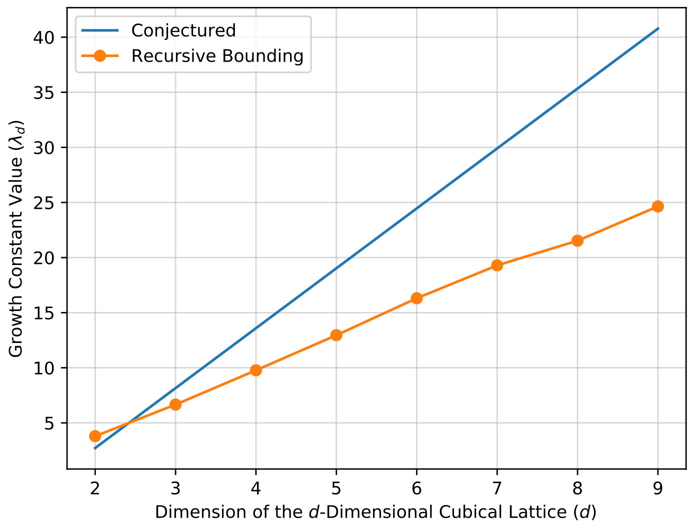

Figure 4 Conjectured growth constants (blue), and lower bounds we obtained (orange).

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