

# Improved Upper Bounds on the Growth Constants of Polyominoes and Polycubes\*

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## Abstract

A  $d$ -dimensional polycube is a facet-connected set of cells (cubes) on the  $d$ -dimensional cubical lattice  $\mathbb{Z}^d$ . Let  $A_d(n)$  denote the number of  $d$ -dimensional polycubes (distinct up to translations) with  $n$  cubes, and  $\lambda_d$  denote the limit of the ratio  $A_d(n+1)/A_d(n)$  as  $n \rightarrow \infty$ . The exact value of  $\lambda_d$  is still unknown rigorously for any dimension  $d \geq 2$ ; the asymptotics of  $\lambda_d$ , as  $d \rightarrow \infty$ , also remained elusive as of today. In this paper, we revisit and extend the approach presented by Klarner and Rivest in 1973 to bound  $A_2(n)$  from above. Our contributions are:

- Using available computing power, we prove that  $\lambda_2 \leq 4.5252$ . This is the first improvement of the upper bound on  $\lambda_2$  in almost half a century;
- We prove that  $\lambda_d \leq (2d - 2)e + o(1)$  for any value of  $d \geq 2$ , using a novel construction of a rational generating function which dominates that of the sequence  $(A_d(n))$ ;
- For  $d = 3$ , this provides a substantial improvement of the upper bound on  $\lambda_3$  from 12.2071 to 9.8073;
- However, we implement an iterative process in three dimensions, which improves further the upper bound on  $\lambda_3$  to 9.3835;

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# 1 Introduction

*Polyominoes* are edge-connected sets of squares on the square lattice. The size of a polyomino is the number of squares it contains. All polyominoes of size up to 4 are shown in Figure 1. Likewise, *polycubes* are facet-connected sets of  $d$ -dimensional unit cubes, where connectivity is through  $(d-1)$ -dimensional faces. Two *fixed* polycubes are considered identical if one can be obtained by a translation of the other. In this paper, we consider only fixed polycubes. Polyominoes and polycubes are specific types of *lattice animals*, the term used in the statistical physics literature to refer to connected sets of cells on *any* lattice.

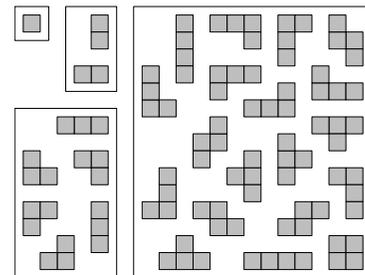


Figure 1: Polyominoes of sizes  $1 \leq n \leq 4$

The fundamental combinatorial problem concerning polycubes is “How many polycubes with  $n$  cubes are there?” This problem originated in parallel in the theory of *percolation* [14, 29], in the analysis of chemical graphs [10, 12, 20, 23], and in the graph-theoretic treatment of cell-growth problems [18] more than half a century ago. However, despite much research in those areas, most of what is known relies primarily on heuristics and empirical studies, and very little is known rigorously, even for the low-dimensional lattices in  $2 \leq d \leq 4$  dimensions. The simplest instance of counting polyominoes is considered one of the fundamental open problems in combinatorial geometry [2].

Let  $A_d(n)$  (sequence A001168 in the On-line Encyclopedia of Integer Sequences [1]) denote the number of polycubes of size  $n$ . Since no analytic formula for  $A_d(n)$  is known for any dimension  $d > 1$ , many researchers have focused on efficient algorithms for *counting* polycubes by size, primarily the square lattice. These methods are based on either explicitly enumerating all polycubes (e.g., by an efficient back-tracking algorithm [25, 28]), or on implicit enumeration (e.g., by a transfer-matrix algorithm [9, 16]). The sequence  $A_2(n)$  has been determined so far up to  $n = 56$  [16]. Enumerating polycubes in higher dimensions is an even more elusive problem. Most notably, Aleksandrowicz and Barequet [3, 4] extended polycube counting by efficiently generalizing Redelmeier’s algorithm [28] to higher dimensions. The statistical-physics literature provides extensive enumeration data of polycubes [14, 24, 23, 13], the most comprehensive being by Luther and Mertens [21], in particular, listing  $A_3(n)$  up to  $n=19$ .

One key fact that holds in all dimensions was discovered in 1967 by Klarner [18], showing that the limit  $\lambda_2 := \lim_{n \rightarrow \infty} \sqrt[n]{A_2(n)}$  exists. This is a straightforward consequence of the fact that the sequence  $(\log A_2(n))$  is super-additive, i.e.,  $A_2(n)A_2(m) \leq A_2(n+m)$ . Since then,  $\lambda_2$  has been called “Klarner’s constant.” Only in 1999, Madras [22] proved the existence of the asymptotic growth rate, namely,  $\lim_{n \rightarrow \infty} A_2(n+1)/A_2(n)$ , which clearly equals  $\lambda_2$ . Klarner’s and Madras’s results hold, in fact, in any dimension.

A great deal of attention has been given to estimating the values of  $\lambda_d$ , especially for  $d=2,3$ . Their exact values are not known and have remained elusive for many years. Based on interpolation methods, applied to the known values of the sequences  $(A_2(n))$  and  $(A_3(n))$ , it is estimated (without a rigorous proof), that  $\lambda_2 \approx 4.06$  [16] and  $\lambda_3 \approx 8.34$  [15]. There have been several attempts to bound  $\lambda_2$  from below, with significant progress over the years [6, 7, 11, 17, 18, 26, 27], but almost nothing is known for higher dimensions. For  $d = 2$ , it has been proven that  $\lambda_2 \geq 4.0025$  [7]. For  $d > 2$ , the only known way to set a lower bound on  $\lambda_d$  is by using the fact [18] that  $\lambda_d = \lim_{n \rightarrow \infty} \sqrt[n]{A_d(n)} = \sup_{n \geq 1} \sqrt[n]{dA_d(n)}$ . In particular, for  $d=3$ , the value  $A_3(19)=651,459,315,795,897$  yields the lower bound  $\lambda_3 \geq \sqrt[19]{3A_3(19)} \approx 6.3795$ , which is quite far from the best estimate of  $\lambda_3$  mentioned above.

On the other hand, only one procedure (Eden [11]) is known for bounding  $\lambda_d$  from above.<sup>1</sup> This

<sup>1</sup>Another method for bounding  $\lambda_2$  from above was presented elsewhere [5], but G. Rote (personal communication) discovered

procedure (explained in detail in the next section) shows that  $\lambda_2 \leq 6.7500$ ,  $\lambda_3 \leq 12.2071$  and that  $\lambda_d \leq (2d - 1)e$ . It was shown in [8] that  $\lambda_d \sim 2ed - o(d)$  as  $d$  tends to infinity, and conjectured (based on an unproven assumption) that  $\lambda_d$  is asymptotically equal to  $(2d-3)e+O(1/d)$ .

As we detail in the next section, Klarner and Rivest [19] enhanced Eden’s method by using a more sophisticated system of “twigs,” proving that  $\lambda_2 \leq 4.6496$ . In this paper, we extend this enhancement to higher dimensions, and show that it results in the two-variable rational generating function

$$g^{(d)}(x, y) = \sum_{n,m=0}^{\infty} l_d(n, m)x^n y^m = \sum_{n=0}^{\infty} xy^n \left( (1+x)^{2(d-1)} + x^2 \right)^n = \frac{x}{1-y\left((1+x)^{2(d-1)} + x^2\right)},$$

whose diagonal function  $\sum_{n=0}^{\infty} l_d(n, n)x^n y^n$  generates a sequence which dominates the sequence  $(A_d(n))$ . Using elementary calculus, Klarner and Rivest [19] proved that for  $d = 2$ ,  $l_2(n, n) \leq 4.8285^n$ . Similarly, we prove that for  $d = 3$ , we have that  $l_3(n, n) \leq 9.8073^n$ , giving the first nontrivial upper bound on  $\lambda_3$ . Finally, we prove that  $\lambda_d \leq (2d-2)e + 1/(2d-2)$ , by proving that  $l_d(n, n) \leq ((2d-2)e + 1/(2d-2))^n$ . To the best of our knowledge, this is the first generalization of Klarner and Rivest’s method to higher dimensions, and the first algorithmic approach for improving the upper bound on  $\lambda_d$  for any value of  $d > 2$ . An important result of this enhancement for dimensions  $d \geq 3$  is an improved upper bound on the space complexity required to encode polycubes, namely, a polycube of size  $n$  can be encoded with  $O(2d-2)n$  bits.

Lastly, we revisit the computer-assisted approach that Klarner and Rivest [19] used to further improve the upper bound on  $\lambda_2$  to 4.6495. We are not aware of any published attempt to reproduce their result. With the computing resources currently available to us, we improve the upper bound on  $\lambda_2$  to 4.5252. We also extend the approach to  $d = 3$ , and prove that  $\lambda_3 \leq 9.3835$ .

## 2 Previous Works by Eden, and Klarner and Rivest

For two  $d$ -dimensional cubes with centers  $c_1 = (x_1, \dots, x_d)$  and  $c_2 = (y_1, \dots, y_d)$ , we say that  $c_1$  is *lexicographically smaller* than  $c_2$  if  $x_i < y_i$  for the first value of  $i$  where they differ. Let  $P$  be an  $n$ -cell polycube in  $d$  dimensions.  $P$  can be uniquely encoded with a binary string  $W_P$  of length  $(2d-1)n-1$  [8, 11], as follows. Let  $G$  be the cell-adjacency graph of  $P$ . (The vertices of  $G$  are the centers of the cubes in  $P$ , and two vertices are connected by an edge if their corresponding cubes are adjacent.) Perform a breadth-first search on  $G$ , starting at cell 1 (the lexicographically smallest cell of  $P$ ).

In the course of this procedure, every cell  $c \in P$  is reached through an incoming edge  $e$  since  $P$  is connected. (An imaginary edge incoming into cell 1 is fixed so as to supposedly originate from a cell that cannot belong to  $P$ .) Clearly, the cell  $c$  is connected by edges of  $G$  to at most  $2d-1$  additional neighboring cells. The procedure now traverses all these outgoing edges according to a fixed order determined by their orientations relative to  $e$ . (For example, for polyominoes, the outgoing edges are traversed according to their clockwise order relative to  $e$ .) Then, if such an edge leads to a cell of  $P$  which has not been labeled yet, this cell is assigned the next unused number, and we update  $W_P := W_P \cdot 1$ , where “ $\cdot$ ” is the concatenation operator. Otherwise, if the cell does not belong to  $P$ , or it is already assigned a number, we set  $W_P := W_P \cdot 0$ . Since each cell can be assigned a number only once, this procedure maps polycubes in a one-to-one manner into

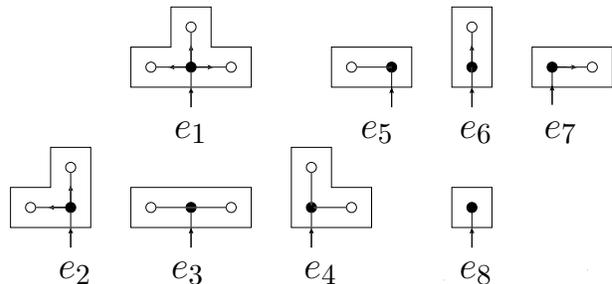


Figure 2: Eden’s set of twigs [19, Figure 3]

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an error in the computations thereof. Fixing this error raised the obtained upper bound above the known bound [19].

binary sequences with  $n-1$  ones and  $(2d-2)n$  zeros. Hence, using Stirling's formula,

$$A_d(n) \leq \binom{(2d-1)(n-1)}{n-1} \leq \left( \frac{(2d-1)^{2d-1}}{(2d-2)^{2d-2}} \right)^n. \quad (1)$$

For polyominoes, this procedure is equivalent to assigning an element of  $\mathbf{E} = \{e_1, \dots, e_8\}$  (Figure 2) to each square of  $P$  (in the same order).

In three dimensions, one obtains that  $\lambda_3 \leq 5^5/4^4 \leq 12.2071$ . In general, since  $\frac{(2d-1)^{2d-1}}{(2d-2)^{2d-2}} = (2d-1) \left(1 + \frac{1}{2d-2}\right)^{2d-2} < (2d-1)e$ , it follows that  $\lambda_d \leq (2d-1)e$ . (In fact, a more thorough analysis of the last relation shows that  $\lambda_d \leq (2d-1.5)e$ .) (The latter value is also known as the ‘‘Bethe approximation’’ of  $\lambda_d$ ; see Gaunt et al. [14, p. 1904, Eq. 3.9], and Gaunt and Peard [?, p. 7523, Eq. 4.9].)

Now refer to Figure 3. Around any square  $u$  on the square lattice, there are eight L-shaped 4-sets of squares, called the ‘‘L-contexts’’ of  $u$  [19]. Let us use the term *status* of a cell to refer to whether or not the cell belongs to a given polyomino. In their beautiful paper [19], Klarner and Rivest designed a set of *twigs*  $\mathbf{L}$  (see Figure 4), which is more compact than  $\mathbf{E}$ . They showed that similarly to  $e_1, \dots, e_8$ ,  $L_1, \dots, L_5$  can serve as building blocks for polyominoes: Every  $n$ -cell polyomino  $P$  corresponds to a unique  $n$ -term sequence of elements of  $\mathbf{L}$ , however, not every such sequence represents a polyomino, immediately implying that  $\lambda_2 < |\mathbf{L}| = 5$ , which is already a substantial improvement over 6.75.

The key idea behind the design of  $\mathbf{L}$  is that one can perform a breadth-first search on the cell-adjacency graph of a polyomino, such that at each step, each cell can be assigned one of the eight L-contexts shown in Figure 3, such that the statuses of *all* cells in this L-context are already encoded. Therefore, while  $\mathbf{E}$  encodes all  $2^3 = 8$  possible status configurations of *three* neighbors at every step of the traversal,  $\mathbf{L}$  encodes the statuses of just *two* neighbors at each step. The sequence  $\mathbf{L}_p$ , encoding a polyomino  $P$ , can be constructed algorithmically as follows. Assume, w.l.o.g., that in the lexicographic order defined over the cells of  $P$ , the cells are ordered first according to their  $y$ -coordinate, and secondly according to their  $x$ -coordinate. Maintain a queue (initially empty) of *white* (or *open*) cells. White cells are cells that have not yet been visited by the algorithm. Start from the lexicographically-smallest cell of  $P$ , and put it in the queue. The L-context of this cell is the one shown in Figure 3(a), since, by definition, the cells in this L-context of the cell do not belong to  $P$ . The addition of twigs to the configuration  $T$  constructed so far proceeds as follows until the queue is empty. Let  $u$  be the oldest cell in the queue. Remove  $u$  from the queue. Let  $a, b$  denote the cells connected to  $u$  (as shown in Figure 3),  $c (\neq u)$  denote the cell connected to  $a, b$ , and  $\ell$  denote the last label assigned to a cell of  $P$  (initially  $\ell = 0$ ). Refer to Figure 4. The twig  $L$  assigned to  $u$  is  $L_1$  if  $a, b, c \notin P$ ;  $L_2$  if  $b, c \notin P$  and  $a \in P$ ;  $L_3$  if  $b \notin P$  and  $a, c \in P$ ;  $L_4$  if  $a \notin P$  and  $b \in P$ ; or  $L_5$  if  $a, b \in P$ . A new configuration  $T * L$  is then constructed as follows:

1. The root cell of  $L$  (shown in black in Figure 4) is placed over  $u$ , such that the orientation (L-context) of  $L$  and  $u$  coincide (this may require a reflection and/or rotation of  $L$ ).
2. The white cell, where  $L$  has been added, is turned black (*dead*).

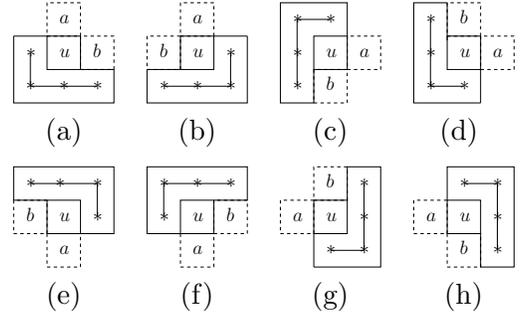


Figure 3: L-contexts of [19, Figure 6]

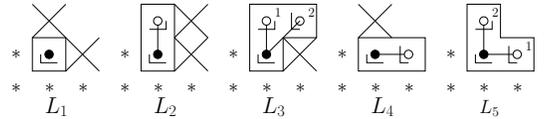


Figure 4: Twig set  $\mathbf{L}$  [19, Figure 7]

3. The cells of  $L$  marked with an  $\times$  (called *forbidden*) become forbidden in  $T$ , namely, they will never become cells of  $T$ .
4. The white cells of  $L$  are added (in their indicated order) to the queue. Note that each white cell has an assigned  $\mathbf{L}$ -context (indicated by the shape  $\mathbf{L}$ ), and that the statuses of all cells in this  $\mathbf{L}$ -context are known (and thus, already encoded).
5. The white cell(s) of  $L$  are assigned the label  $\ell+1$  (or  $\ell+1$  and  $\ell+2$ , in order).

Note that when  $a \in P$  and  $b \notin P$ , it is necessary to encode whether or not  $c$  is in  $P$  (twigs  $L_3$  and  $L_2$ , resp.), so that when  $a$  is inserted to the queue, the statuses of all cells in its indicated  $\mathbf{L}$ -context are encoded. Note also that the linear order of the white cells in  $L_3$  and  $L_5$  is necessary to ensure the uniqueness of the construction. For the second white cell in either  $L_3$  or  $L_5$ , the statuses of all cells in its indicated  $\mathbf{L}$ -context are known only after assigning a twig to the first open cell. An example of this process is shown in Fig. 5(b): Let  $u_i$  be the cell visited at step  $i$ , and  $a_i, b_i$  be the cells connected to  $u_i$  (Figure 3). The cell  $u_1$  is assigned the label 1 and the twig  $L_5$  since  $a_1, b_1 \in P$ . In order to assign a twig  $L_i \in \mathbf{L}$  to  $u_2$ ,  $L_i$  is rotated by  $90^\circ$  and reflected around the  $x$  axis. Note that a cell can be discovered and labeled only once. Therefore,  $u_5$  is assigned the twig  $L_1$  (not  $L_4$ ) since the cell on its right was already discovered at the fourth iteration and assigned the label 8.

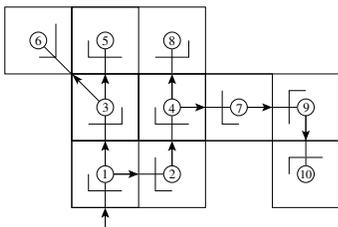


Figure 5: [19, Figure 8]

$L_P = (L_5, L_4, L_3, L_5, L_1, L_1, L_2, L_1, L_4, L_1)$ .

**Observation 2.1** *Two different polyominoes are encoded with different sequences of twigs.*

With this construction, Klarner and Rivest reduced the number of building blocks of polyominoes from 8 to 5. It is natural to ask if a more compact set of building blocks exists. We can now answer this question on the negative, since the existence of such set of size 4 would imply that  $\lambda_2 \leq 4$ , while we already know that  $\lambda_2 \geq 4.0025$  [7].

## 2.1 Mathematical Formulation

The upper bound  $\lambda_2 \leq 5$  can be improved by a more delicate analysis, which assigns different “weights” to different elements of  $\mathbf{L}$ , as follows. Each twig  $L \in \mathbf{L}$  is assigned a weight  $w(L) = x^a y^b$ , where  $a$  denotes the number of cells in  $L$  minus 1, and  $b$  denotes the number of black cells in  $L$ . (Thus,  $w(L_1) = y$ ,  $w(L_2) = xy$ ,  $w(L_3) = x^2 y$ ,  $w(L_4) = xy$ , and  $w(L_5) = x^2 y$ .) The *weight* of a sequence  $S = (\ell_1, \dots, \ell_k) \in \mathbf{L}^k$  is defined as  $W(S) = x \cdot w(\ell_1) \cdot \dots \cdot w(\ell_k)$ , and the weight of the empty sequence is defined to be  $x$ .

Let  $P$  be a polyomino of size  $n$ , and let  $L_P = \{\ell_1, \dots, \ell_n\} \in \mathbf{L}^n$  denote the sequence of twigs encoding  $P$ . For each  $\ell_i \in \mathbf{L}$ , we clearly have that  $w(\ell_i) = x^{a_i} y$ , such that  $a_i \in \{0, 1, 2\}$  equals the number of open cells in  $\ell_i$ . Thus,  $w(L_P) = x \cdot x^{\sum_{i=1}^n a_i} y^n$ . Moreover,  $\sum_{i=1}^n a_i = n-1$  because each cell of  $P$  (other than the smallest cell) becomes open only once, and is thus accounted for by some  $a_j$  in the sum. The smallest cell is accounted for by the term  $x$  in  $w(L_P)$ .

**Corollary 2.2**  $w(L_P) = x^n y^n$ .

Now, let  $\mathbf{L}^k$  denote the set of all sequences of  $k \geq 0$  elements of  $\mathbf{L}$ . The sum of weights of all finite sequences of elements of  $\mathbf{L}$  is

$$\sum_{k=0}^{\infty} \sum_{S \in \mathbf{L}^k} W(S) = \sum_{k=0}^{\infty} x \left( \sum_{\ell \in \mathbf{L}} w(\ell) \right)^k = x \left( 1 - \sum_{\ell \in \mathbf{L}} w(\ell) \right)^{-1}. \quad (2)$$

Clearly,  $\sum_{\ell \in \mathbf{L}} w(\ell) = y(2x^2 + 2x + 1)$ , thus, the generating function given by (2) is

$$\sum_{m,n=0}^{\infty} l(m,n)x^m y^n = \frac{x}{1 - y(2x^2 + 2x + 1)} = \sum_{n=0}^{\infty} xy^n (2x^2 + 2x + 1)^n, \quad (3)$$

where  $l(m,n)$  is the coefficient of the term  $x^m y^n$ .

By Observation 2.1 and Corollary 2.2, there is an injection of the set of polyominoes of size  $n$  into the set of finite sequences of elements of  $\mathbf{L}$  having weight  $x^n y^n$ . Thus, the coefficient  $l(n,n)$  of  $x^n y^n$  in Equation (3) is an upper bound on  $A_2(n)$ . In Section 3.3.1, we follow the proof of Klarner and Rivest [19] for showing that  $l(n,n) \leq 4.8285^n$ . In the next two sections, we extend the concept of “ $\mathbf{L}$ -context” to higher dimensions.

## 3 Higher Dimensions

### 3.1 Three Dimensions

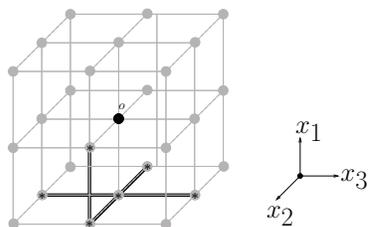


Figure 6: The  $+\mathbf{L}$  context (bold black lines) of a cell  $o$  on the 3D cubical lattice

We generalize the twigs idea to three dimensions as follows. Refer to Figure 6. Let  $o = (0, 0, 0)$  be the lexicographically-smallest cell of the polycube. Thus, by definition, all cubes that lie in the planes  $x_1 = -1$  and  $x_2 = 1$  do not belong to the polycube. We define the “ $+\mathbf{L}$ -context” of  $o$  (this name indicates a composition of a “Plus” and an “Ell”) to be the six cells around  $o$  shown in asterisks in Figure 6. Observe that the set of 2-dimensional twigs  $\mathbf{L}$  (Figure 4) captures all possible occupancy configurations of the neighbors of  $o$  that lie in the  $x_1 x_2$  plane. For the remaining neighbors of  $o$  (namely, cells  $(0, 0, -1)$  and  $(0, 0, 1)$ ), there are  $2^2 = 4$  possible encodings of whether or not they belong to the polycube. This yields the set  $\mathbf{L}^{(3)}$  of seventeen 3-dimensional twigs, shown in Figure 7. Similarly to two dimensions, the cells of a twig are either black or white, and the  $+\mathbf{L}$  context and linear order of the open cells is indicated. Similarly to  $L_1, \dots, L_5$  (in Figure 2), it is easy to check that  $T_1, \dots, T_{17}$  (in Figure 4) serve as complete building blocks for polycubes since they cover all possible situations (a formal proof is given in the next section). Every  $n$ -cell polycube  $P$  corresponds to a unique  $n$ -term sequence of elements of  $\mathbf{L}^{(3)}$ , and different polycubes are assigned different sequences. The sequence corresponding to a polycube can be constructed algorithmically by a breadth-first search as in two dimensions. Every twig is assigned a weight in the same manner, and we get that

$$\sum_{\ell \in \mathbf{L}^{(3)}} w(\ell) = y(1 + 4x + 7x^2 + 4x^3 + x^4) = y((x+1)^4 + x^2).$$

Thus, the generating function given by Eq. (2) is

$$\frac{x}{1 - y(1 + 4x + 7x^2 + 4x^3 + x^4)} = \sum_{n=0}^{\infty} xy^n (1 + 4x + 7x^2 + 4x^3 + x^4)^n. \quad (4)$$

See Section 3.3 for the full analysis of this generating function.

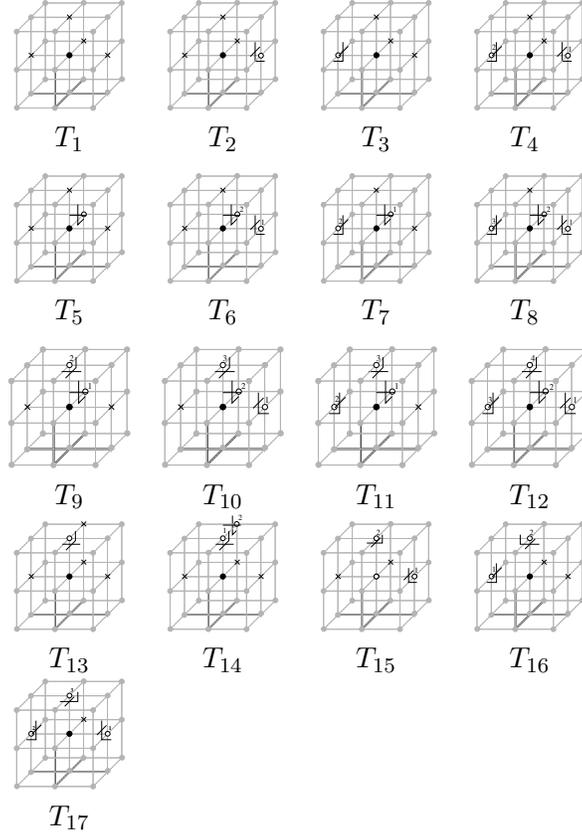


Figure 7: 3-dimensional twigs

### 3.2 $d > 3$

Our construction in three dimensions can be applied inductively for  $d > 3$ . The base of the induction is  $d=2$ , where we fix a square in the  $x_1x_2$  plane (as in Figure 6) together with its L-context. Going to  $d=3$ , the square gains two new neighbors in the third dimension  $x_3$ . In general, when we go from  $d-1$  to  $d$  dimensions, a cube gains two neighbors in the new dimension  $x_d$ . Let  $o = (0, 0, \dots, 0)$  be a  $d$ -dimensional cube ( $d > 2$ ). We define the  $+_d\mathbf{L}$ -context of  $o$  in a recursive way. The base of the definition is  $+_2\mathbf{L} := \mathbf{L}$  and  $+_3\mathbf{L} := +_3\mathbf{L}$ , and the recursion is  $+_d\mathbf{L} := +_{d-1}\mathbf{L} \cup \{c_1, c_2\}$ , where  $c_{1,2} = (-1, 0, \dots, 0, \pm 1)$ . The geometric interpretation of the  $+_d\mathbf{L}$ -context of  $o$  is an L-shape around  $o$  in the  $x_1x_2$  plane, which intersects  $d-2$  lines in the  $x_1 = -1$  plane at the point  $(-1, 0, \dots, 0)$ .

The set of twigs  $\mathbf{L}^{(d)}$  (where  $\mathbf{L}^{(2)} = \mathbf{L}$ ) is comprised of all  $2^{2d-2}$  occupancy options for the cells neighboring  $o$  (which are not in its  $+_d\mathbf{L}$ -context): In dimensions  $x_3, \dots, x_d$ , the construction simply covers all  $2^{2(d-2)}$  occupancy options for the two neighbors of  $o$ . In the  $x_1x_2$  plane, the occupancies of the neighbors of  $o$  are captured by  $\mathbf{L}$ , as in Fig. 4, and the only “problematic” case is when the cube  $(1, 0, \dots, 0)$  is white and all other neighbors of  $o$  are not (as is the case with the twigs  $L_2, L_3$  in Figure 4, and  $T_{13}, T_{14}$  in Figure 7). It is, thus, necessary to encode the status of the cell  $(1, -1, 0, \dots, 0)$ , since, by construction, it is contained in the  $+_d\mathbf{L}$  context of the cell  $(1, 0, \dots, 0)$ . This results in  $2^{2(d-2)} \cdot 2^2 + 1 = 2^{2(d-1)} + 1$  twigs, and compares favorably with the generalization of Eden’s construction, which contains about two times more ( $2^{2d-1}$ ) twigs.

In order to prove that our construction works better, all we need to show is that for any white cell  $u$  in every twig in  $\mathbf{L}^{(d)}$ , there is a set of  $4 + 2(d-2) = 2d$  cells around  $u$ , which can be completely ignored by the

construction when visiting  $u$ . Those cells can form its  $+_d\mathbf{L}$ -context. Note that except the second white cell in the problematic case mentioned above, all white cells are neighbors of  $o$ . In case a new neighbor of  $o$ , namely,  $(0, 0, \dots, 0, \pm 1)$ , is open, the  $\mathbf{L}$ -shape in its  $+_d\mathbf{L}$ -context is formed by  $c_1$  (or  $c_2$ ),  $(-1, 0, \dots, 0)$ ,  $o$ , and  $(1, 0, \dots, 0)$ ; the rest of the cells in its  $+_d\mathbf{L}$ -context are  $(0, \pm 1, 0, \dots, 0)$ ,  $\dots$ ,  $(0, \dots, 0, \pm 1, 0)$  (that is, all coordinates are 0, except one coordinate in the range  $2, \dots, (d-1)$ , which is  $\pm 1$ ). Note that the statuses of these cells are known by construction. For the other possible white neighbors  $n = (0, \dots, 0, \pm 1, 0, \dots, 0)$  of  $o$ ,  $+_d\mathbf{L} = +_{d-1}\mathbf{L} \cup (0, \dots, 0, \pm 1)$  since, by construction,  $o$  is where the ‘ $\mathbf{L}$ ’ and the ‘ $+$ ’ in the  $+_{d-1}\mathbf{L}$ -context of  $n$  intersect. Thus, the union  $+_{d-1}\mathbf{L} \cup (0, \dots, 0, \pm 1)$  forms its  $+_d\mathbf{L}$ -context; The statuses of the cells in its  $+_{d-1}\mathbf{L}$ -context and of  $(0, \dots, 0, \pm 1)$  are known by induction and construction, respectively. Finally, we need to address the second white cell  $p = (1, -1, 0, \dots, 0)$  in the problematic twig mentioned above. This cell will *always* be visited after the first open cell  $q = (0, 1, 0, \dots, 0)$  of the twig is visited and assigned a twig. Once  $q$  is assigned a twig, the statuses of all its neighbors will be encoded. Then, it is easy to check that the cells  $(1, 0, \dots, 0)$ ,  $o$ ,  $(0, 1, 0, \dots, 0)$ , and  $(0, 2, 0, \dots, 0)$  form the  $\mathbf{L}$ -shape in the neighborhood of  $p$ , and together with the remaining  $2(d-1)$  neighbors of  $q$ , they form the  $+_d\mathbf{L}$ -context of  $p$ . The statuses of these cells are already encoded by construction.

Finally, we need to compute the weight function  $W^{(d)}(x, y) = \sum_{t \in \mathbf{L}^{(d)}} w(t)$ . Since  $o$  has  $2(d-1)$  neighbors that are not in its  $+_d\mathbf{L}$ -context, there are  $\binom{2(d-1)}{i}$  twigs in  $\mathbf{L}^{(d)}$  with exactly  $i$  white cells and one black cell ( $o$ ), and the weight of each such twig is  $x^i y$ . Recall the problematic case mentioned above, which results in an additional twig with three cells—1 black and 2 white—whose weight is therefore  $x^2 y$ . Hence,

$$W^{(d)}(x, y) = \sum_{t \in \mathbf{L}^{(d)}} w(t) = \sum_{i=0}^{2(d-1)} \left[ \binom{2(d-1)}{i} x^i y \right] + x^2 y = y((x+1)^{2(d-1)} + x^2).$$

Substituting  $W^{(d)}(x, y)$  in the generating function from Equation (2), we obtain

$$g^{(d)}(x, y) = l_d(n, m) x^m y^n = \sum_{n=0}^{\infty} x y^n \left( (1+x)^{2(d-1)} + x^2 \right)^n = \frac{x}{1 - y \left( (1+x)^{2(d-1)} + x^2 \right)},$$

Similarly to polyominoes, polycubes of size  $n$  are mapped uniquely to sequences of elements of  $\mathbf{L}^{(d)}$  having weight  $x^n y^n$ .

### 3.3 Analysis of the Generating Functions

It can be easily observed that  $l_d(n, n)$ , the coefficient of  $x^n y^n$  in  $g^{(d)}(x, y)$ , is the coefficient of  $x^{n-1}$  in  $\left( (1+x)^{2(d-1)} + x^2 \right)^n$ . We now show how to compute  $l_d(n, n)$ . Let  $h^{(d)}(x) = \left( (1+x)^{2(d-1)} + x^2 \right)^n$ . We start with the simple cases of  $d = 2, 3$ , and then generalize the calculation to any value of  $d$ .

#### 3.3.1 $d = 2$

In two dimensions,  $h^{(2)}(x) = \left( (1+x)^2 + x^2 \right)^n = (1 + 2x + 2x^2)^n$ . By the Multinomial Theorem, we have that

$$(1 + 2x + 2x^2)^n = \sum_{i_1, i_2} \left[ \binom{n}{n - i_1 - i_2, i_1, i_2} (2x)^{i_1} (2x^2)^{i_2} \right].$$

Since we want to compute the coefficient of  $x^{n-1}$ , we require that  $i_1+2i_2 = n-1$ , i.e.,  $i_1 = n-2i_2-1$ . Thus,

$$\begin{aligned} l_2(n, n) &= \sum_{i_2} \left[ \binom{n}{i_2+1, n-2i_2-1, i_2} 2^{n-i_2-1} \right] = \frac{2^n}{2} \sum_{i_2} \left[ \binom{n}{i_2+1, n-2i_2-1, i_2} \left(\frac{1}{2}\right)^{i_2} \right] = \\ &= \frac{2^n}{\sqrt{2}} \sum_{i_2} \left[ \binom{n}{i_2+1, n-2i_2-1, i_2} \left(\frac{1}{\sqrt{2}}\right)^{i_2} \left(\frac{1}{\sqrt{2}}\right)^{i_2+1} \right] <_* \frac{2^n}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} + 1\right)^n = \frac{(2(\sqrt{2}+1))^n}{\sqrt{2}}. \end{aligned}$$

(The relation “ $<_*$ ” is because the summation in its left-hand side contains only a subset of the terms whose sum is equal to the exponential term on the right-hand side.) Hence,  $\lambda_2 \leq 2(\sqrt{2}+1) \approx 4.82843$ .

### 3.3.2 $d = 3$

**Theorem 3.1**  $\lambda_3 \leq 9.8073$ .

*Proof:* We repeat the calculation in the same manner as above.

$$\begin{aligned} h^{(3)}(x) &= ((1+x)^4 + x^2)^n = (1+4x+7x^2+4x^3+x^4)^n = \\ &= \sum_{i_1, i_2, i_3, i_4} \left[ \binom{n}{(n-\sum_{j=1}^4 i_j), i_1, i_2, i_3, i_4} 4^{i_1} 7^{i_2} 4^{i_3} x^{i_1+2i_2+3i_3+4i_4} \right]. \end{aligned}$$

Similarly to the 2-dimensional case, we require that  $i_1+2i_2+3i_3+4i_4 = n-1$ , that is,  $i_1 = n-1-2i_2-3i_3-4i_4$ . Substituting  $i_1$  in the right-hand side of the equality above, we obtain

$$l_3(n, n) = \sum \left[ \binom{n}{i_2+2i_3+3i_4+1, n-1-2i_2-3i_3-4i_4, i_2, i_3, i_4} 4^{n-1-2i_2-3i_3-4i_4} 7^{i_2} 4^{i_3} \right].$$

Therefore, by the Multinomial Theorem, we have that

$$\begin{aligned} l_3(n, n) &= \frac{4^n}{4} \sum_{i_2, i_3, i_4} \left[ \binom{n}{i_2+2i_3+3i_4+1, n-1-2i_2-3i_3-4i_4, i_2, i_3, i_4} \left(\frac{7}{4^2}\right)^{i_2} \left(\frac{4}{4^3}\right)^{i_3} \left(\frac{1}{4^4}\right)^{i_4} \right] < \\ &= \frac{4^n}{4} \left(\frac{7}{4^2} + \frac{1}{4^2} + \frac{1}{4^4} + 1 + 1\right)^n = \frac{1}{4} \left(\frac{641}{64}\right)^n. \end{aligned}$$

Thus,  $\lambda_3 \leq \frac{641}{64} \approx 10.016$ , already improving significantly on the known upper bound of  $\lambda_3 \leq 12.2071$  (see Section 2). However, we can do better than that. Let  $b > 0$  be some constant, whose value will be specified later, and rewrite the multinomial expression above as

$$l_3(n, n) = \frac{4^n}{4} \sum_{i_2, i_3, i_4} \left[ \binom{n}{i_2+2i_3+3i_4+1, n-1-2i_2-3i_3-4i_4, i_2, i_3, i_4} \underbrace{\left(\frac{7}{(b\frac{4}{b})^2}\right)^{i_2} \left(\frac{4}{(b\frac{4}{b})^3}\right)^{i_3} \left(\frac{1}{(b\frac{4}{b})^4}\right)^{i_4}}_{c(b)} \right],$$

and rearrange the three terms in  $c(b)$  as follows.

$$\begin{aligned}
c(b) &= \left(\frac{1}{b^2}\right)^{i_2} \left(\frac{7}{\left(\frac{4}{b}\right)^2}\right)^{i_2} \left(\frac{1}{b^3}\right)^{i_3} \left(\frac{4}{\left(\frac{4}{b}\right)^3}\right)^{i_3} \left(\frac{1}{b^4}\right)^{i_4} \left(\frac{1}{\left(\frac{4}{b}\right)^4}\right)^{i_4} = \\
&= \left(\frac{1}{b}\right)^{i_2} \left(\frac{1}{b}\right)^{i_2} \left(\frac{7}{\left(\frac{4}{b}\right)^2}\right)^{i_2} \left(\frac{1}{b^2}\right)^{i_3} \left(\frac{1}{b}\right)^{i_3} \left(\frac{4}{\left(\frac{4}{b}\right)^3}\right)^{i_3} \left(\frac{1}{b^3}\right)^{i_4} \left(\frac{1}{b}\right)^{i_4} \left(\frac{1}{\left(\frac{4}{b}\right)^4}\right)^{i_4} = \\
&= \left(\frac{1}{b}\right)^{i_2} \left(\frac{7}{\frac{16}{b}}\right)^{i_2} \left(\frac{1}{b}\right)^{2i_3} \left(\frac{4}{\frac{4^3}{b^2}}\right)^{i_3} \left(\frac{1}{b}\right)^{3i_4} \left(\frac{1}{\frac{4^4}{b^3}}\right)^{i_4} = \left(\frac{1}{b}\right)^{i_2+2i_3+3i_4} \left(\frac{7}{\frac{16}{b}}\right)^{i_2} \left(\frac{4}{\frac{4^3}{b^2}}\right)^{i_3} \left(\frac{1}{\frac{4^4}{b^3}}\right)^{i_4}.
\end{aligned}$$

Thus,

$$\begin{aligned}
l_3(n, n) &= \\
&= \frac{4^n}{4} \sum_{i_2, i_3, i_4} \left[ \binom{n}{i_2+2i_3+3i_4+1, n-1-2i_2-3i_3-4i_4, i_2, i_3, i_4} \left(\frac{1}{b}\right)^{i_2+2i_3+3i_4} \left(\frac{7}{\frac{16}{b}}\right)^{i_2} \left(\frac{4}{\frac{4^3}{b^2}}\right)^{i_3} \left(\frac{1}{\frac{4^4}{b^3}}\right)^{i_4} \right] \\
&< 4^n \left( \frac{1}{b} + 1 + \frac{7b}{16} + \frac{b^2}{4^2} + \frac{b^3}{4^4} \right)^n,
\end{aligned}$$

where the last relation is again due to the Multinomial Theorem and due to the partial summation.

The heart of our trick is that the partial summation allows us to choose the value of  $b$  that minimizes the sum of the chosen summands (by assigning appropriate weights to the five components). Define

$$f(b) = \frac{1}{b} + 1 + \frac{7b}{16} + \frac{b^2}{4^2} + \frac{b^3}{4^4}.$$

Our goal, then, is to choose  $b$  so as to minimize  $f(b)$ . Elementary calculus shows that  $f(b)$  assumes its minimum at  $b_0 = 1.274306378$  and that  $f(b_0) = 2.451823893$ . Recall that  $l_3(n, n) < 4^n f^n(b)$  for *any*  $b$ , in particular, for  $b = b_0$ . Hence, finally,

$$l_3(n, n) < 4^n \cdot 2.451823893^n = 9.807295572^n.$$

(Had we chosen  $b = 1$ , we would have obtained again the bound  $\lambda_3 \leq 10.016$ .) The claim follows.  $\square$

### 3.3.3 General value of $d$

**Theorem 3.2**  $\lambda_d \leq (2d - 2)e + 1/(2d - 2)$ .

*Proof:* The proof for a general value of  $d > 3$  is similar to that for  $d = 2, 3$ . For simplicity, let us fix  $a = 2(d - 1)$ . We have that

$$\begin{aligned}
h^{(d)}(x) &= ((1+x)^a + x^2)^n = \left( 1 + ax + \left( \binom{a}{2} + 1 \right) x^2 + \sum_{j=3}^a \binom{a}{j} x^j \right)^n = \\
&= \sum_{i_1, \dots, i_a} \left[ \binom{n}{n - \sum_{j=1}^a i_j, i_1, \dots, i_a} a^{i_1} \left( \binom{a}{2} + 1 \right)^{i_2} \left( \prod_{j=3}^a \binom{a}{j}^{i_j} \right) x^{i_1+2i_2+\dots+ai_a} \right].
\end{aligned}$$

Again, we require that  $i_1 + 2i_2 + \dots + ai_a = n - 1$ , that is,  $i_1 = n - 1 - \sum_{j=2}^a (j \cdot i_j)$ . Thus,

$$l_d(n, n) = \sum_{i_2, \dots, i_a} \left[ \binom{n}{(\sum_{j=2}^a (j-1)i_j + 1), (n-1 - \sum_{j=2}^a (j \cdot i_j)), i_2, \dots, i_a} a^{n-1 - \sum_{j=2}^a (j \cdot i_j)} \left( \binom{a}{2} + 1 \right)^{i_2} \left( \prod_{j=3}^a \binom{a}{j}^{i_j} \right) \right].$$

Therefore,

$$l_d(n, n) = \frac{a^n}{a} \sum_{i_2, \dots, i_a} \left[ \binom{n}{(\sum_{j=2}^a (j-1)i_j + 1), (n-1 - \sum_{j=2}^a (j \cdot i_j)), i_2, \dots, i_a} \frac{\left( \binom{a}{2} + 1 \right)^{i_2}}{a^{2i_2}} \prod_{j=3}^a \frac{\binom{a}{j}^{i_j}}{a^{ji_j}} \right] =$$

$$\frac{a^n}{a} \sum_{i_2, \dots, i_a} \left[ \binom{n}{(\sum_{j=2}^a (j-1)i_j + 1), (n-1 - \sum_{j=2}^a (j \cdot i_j)), i_2, \dots, i_a} \left( \frac{\binom{a}{2} + 1}{a^2} \right)^{i_2} \prod_{j=3}^a \left( \frac{\binom{a}{j}}{a^j} \right)^{i_j} \right].$$

It is well-known that for all values of  $m$  and  $k$ , such that  $1 \leq k \leq m$ , we have that  $\binom{m}{k} \leq \frac{m^k}{k!}$ . Hence, for  $j = 3, \dots, a$ , we have that  $\frac{\binom{a}{j}}{a^j} \leq \frac{1}{j!}$ . It is also known that  $e = \sum_{j=0}^{\infty} \frac{1}{j!}$ . Therefore,

$$l_d(n, n) \leq \frac{a^n}{a} \sum_{i_2, \dots, i_a} \left[ \binom{n}{(\sum_{j=2}^a (j-1)i_j + 1), (n-1 - \sum_{j=2}^a (j \cdot i_j)), i_2, \dots, i_a} \left( \frac{1}{2} + \frac{1}{a^2} \right)^{i_2} \prod_{j=3}^a \left( \frac{1}{j!} \right)^{i_j} \right]$$

$$< a^n \left( 1 + 1 + \left( \frac{1}{2} + \frac{1}{a^2} \right) + \sum_{j=3}^a \frac{1}{j!} \right)^n = a^n \left( \frac{1}{a^2} + \sum_{j=0}^a \frac{1}{j!} \right)^n < (ae + 1/a)^n$$

(The relation “ $<$ ” above is again because the summation in its left-hand side contains only a subset of the terms whose sum is equal to the exponential term on the right-hand side, and the factor  $1/a$  in its left-hand side.) Consequently,  $\lambda_d \leq (2d - 2)e + \frac{1}{2d-2}$ . □

This compares well with the conjecture that  $\lambda_d \sim (2d - 3)e$  [8], and improves upon Eden’s upper bound of  $(2d - 1)e$  (which can actually be shown to be  $(2d - 1.5)e$ ; see Section 2). For example, for  $d = 4$ , we obtain  $\lambda_4 \leq 15.1284$ , whereas the bound provided by the generalized Eden’s method is 17.6514.

## 4 Further Improvements of the Upper Bounds on $\lambda_2$ and $\lambda_3$

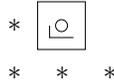


Figure 8: A twig with one open cell

Klarner and Rivest [19] developed their idea further, noting that it is possible to start with a configuration containing a single open cell (as shown in Figure 8), and keep adding twigs and updating the configuration, to construct from  $L$  increasingly larger sets  $C_1, C_2, C_3, \dots$ , where the set  $C_i$  contains all possible twigs with  $i$  black cells (and possibly some white cells) or less than  $i$  black cells (and no white cells). In particular,  $C_1 = L$ . The process for building all twigs with  $i$  black cells is as follows:

1. Set  $C_i := \emptyset$ ,  $B := \{\bar{s}\}$  (the twig shown in Figure 8, and  $W_i(x, y) := 0$ ;

2. If  $B = \emptyset$ , then output  $C_i$  and halt;
3. Remove some twig  $T$  from  $B$ ;
4. If  $T$  contains no open cells or exactly  $i$  dead cells, then add  $T$  to  $C_i$ , set  $W := W + w(T)$ , and goto Step 2;
5. For  $j = 1, \dots, 5$  do
  - Set  $T_j := T * L_j$ ;
  - If  $T_j$  meets condition (\*) below, then add  $T_j$  to  $B$ ;
 od
6. Goto Step 2.

**Condition (\*):** None of the cells of  $L_i$  (except of the black cell) overlap with any of the cells (black or white) of  $T$  nor with any of the cells of  $T$  marked with X.

Condition (\*) guarantees that adding a new twig to the configuration will not cause cells to overlap.

**Observation 4.1**  $A_2(i) \leq |C_i|$

Indeed, this relation is trivially justified by the facts that every polyomino of size  $i$  can be built with *some* sequence of  $i$  twigs, and the algorithm above constructs *all* valid sequences of  $i$  twigs.

The algorithm above can be viewed as a breadth-first-search traversal on an infinite tree (see Figure 9) rooted at the twig  $\bar{s}$  (Figure 8). All other vertices of the tree are twigs that can be “grown” from its root by repeatedly applying the operation ‘\*’ (defined in Section 2). The tree contains an edge directed from a twig  $T_1$  to another twig  $T_2$  if  $T_2 = T_1 * L_i$  (for some  $L_i \in \mathbb{L}$ ). Hence, each vertex of the tree has at most five outgoing edges, and its leaves are all twigs which have no open cells.

The key idea is that, given a polyomino  $P$ , it is possible to encode  $P$  with a sequence of elements of  $C_i$ , for any  $i \geq 1$ , and any such sequence can be converted into a sequence of elements of  $\mathbb{L}$ .

**Observation 4.2** *The set of converted sequences of elements of  $C_{i+1}$  is a proper subset of the set of converted sequences of elements of  $C_i$ , since the former contains less invalid sequences (those that do not represent polyominoes) than the latter.*

Similarly to  $\mathbb{L}$ , every twig  $T \in C_i$  is assigned a weight  $w(T) := x^a y^b$  (where  $a$  denotes the number of cells in  $T$  minus 1, and  $b$  denotes the number of black cells in  $T$ ), and, thus, it can be shown that every polyomino of size  $n$  gives rise to a unique sequence of elements of  $C_i$  of weight  $x^n y^n$ . Letting  $W_i(x, y) = \sum_{T \in C_i} w(T)$ , we can plug  $W_i(x, y)$  in the generating function in Equation (2) and obtain  $\sum_{m, n} c_i(m, n) x^m y^n = x / (1 - W_i(x, y))$ . Again, we are interested in the diagonal term  $c_i(n, n)$  of the series expansion  $\sum_{m, n} c_i(m, n) x^m y^n$ . Due to Observation 4.2, the sets  $C_1, C_2, \dots$  yield a sequence of improving (decreasing) upper bounds on  $\lambda_2$ . Thus, as  $i$  increases, the upper bound decreases. Therefore,

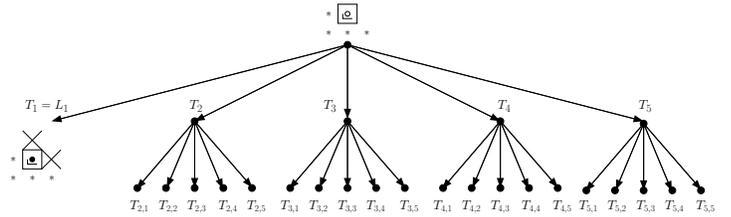


Figure 9: The tree modeling the algorithm that generates  $C_i$ . The root  $r$  is a twig with one open cell; its  $\mathbb{L}$ -context is shown in Fig. 3(a). For  $i, j = 1, \dots, 5$ , set  $T_i = L_i = r * L_i$ , and  $T_{i,j} = T_i * L_j$ . The twig  $T_1$  is a leaf because it has no open cells.

the goal is to compute an upper bound on  $c_i(n, n)$ . The main computational challenge in this approach is to construct algorithmically the sets  $C_i$  (in order to compute  $W_i(x, y)$ ), as  $|C_i|$  is increasing exponentially with  $i$ , like  $A_2(i)$  does. Klarner and Rivest carried their approach to the limit of the resources they had available at the time, and computed  $C_i$  up to  $i = 10$ . Their computations are summarized in Table 1.

## 4.1 Two Dimensions

**Theorem 4.3**  $\lambda_2 \leq 4.5252$ . ■

We implemented the algorithm described in the previous section for constructing the sets  $C_i$  in a parallel C++ program, using `Maple` (see Appendix D) to derive an upper bound on  $c_i(x, y)$ . Since the size of the set  $C_i$  is growing exponentially with  $i$ , we did not keep it in memory. Instead, we accumulated the weights of the twigs as in Step 4 in the algorithm. The “for loop” in Step 5 can be run in parallel since there are no dependencies between the twigs  $T_1, \dots, T_5$ , as illustrated in Figure 9. We used `OpenMP` and `OpenMPI` to run the program in parallel on a high-performance computer cluster at the Technion. We used 33 computing nodes, each having 12 cores, for a total of 396 cores. The time for computing  $C_{10}$  was negligible even without parallelizing the program. Results were systematically improved by increasing  $i$ , the number of dead cells of the twigs. However, as the size of  $C_i$  increases roughly by a factor of 4 as  $i$  is incremented by 1, constructing  $C_{i+1}$  requires more than four times the computing power needed to construct  $C_i$ . The improved upper bound  $\lambda_2 \leq 4.5252$  was obtained by using twigs with 21 dead cells. Computing  $C_{21}$  took roughly seven hours. Our results, alongside Klarner and Rivest’s results, are summarized in Table 1. The two sets of results differ for  $i = 6, \dots, 10$ . We address these differences in Section A. The weight functions  $W_1(x, y), \dots, W_{21}(x, y)$  are provided in Appendix B.

For  $i \geq 6$ , the number of twigs ( $|C_i|$ ) we found is slightly (but consistently) larger than the number reported by Klarner and Rivest [19] (see Table 1). As a result, the value of the upper bound we computed for  $C_{10}$  is slightly higher than the value they reported. Since they provided neither the computer program which generated the sets  $C_i$ , nor the functions  $W_6(x, y), \dots, W_{10}(x, y)$  which they obtained, we had no means for comparing our results to theirs.

## 4.2 Three Dimensions

We applied the process described in the previous section to construct sets  $C_1^3, C_2^3, \dots$  of larger 3-dimensional twigs. Again, we began with a single open cell on the cubical lattice, and constructed all twigs with  $i$  dead cells or fewer dead cells and no open cells. We were able to reach twigs with  $i = 9$  dead cells, obtaining a set of about  $17 \cdot 10^9$  twigs, by which we proved that  $\lambda_3 \leq 9.3835$ . Computing  $C_9^3$  took 3 hours on the same cluster mentioned in Section 4.1. Our results (reported in Table 2), and  $W_9(x, y) = \sum_{\ell \in C_9^3} w(\ell)$  are provided in Appendix C.

## 4.3 Code

Our code is available at [https://github.com/mshalah/polyominoes\\_polycubes\\_upperbounds](https://github.com/mshalah/polyominoes_polycubes_upperbounds).

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## A Comparison of Results

$i$	$ C_i $		$1/\sigma_i$		Time (Hours)
	Ref. [19]	Ours	Ref. [19]	Ours	Ours
1	5	5	4.828428	4.828427124	
2	21	21	4.828428	4.828427124	
3	93	93	4.828428	4.828427124	
4	409	409	4.796156	4.796155640	
5	1,803	1,803	4.765534	4.765532996	
6	7,929	<b>7,937</b>	4.738062	<b>4.738743624</b>	
7	34,928	<b>35,084</b>	4.714292	<b>4.716641912</b>	
8	151,897	<b>153,458</b>	4.690920	<b>4.695386599</b>	
9	656,363	<b>668,128</b>	4.669409	<b>4.676042980</b>	
10	2,821,227	<b>2,899,941</b>	4.649551	<b>4.658412767</b>	
11		<b>12,557,503</b>		<b>4.642235017</b>	
12		<b>54,137,703</b>		<b>4.627069746</b>	
13		<b>232,203,877</b>		<b>4.612780890</b>	
14		<b>991,607,177</b>		<b>4.599355259</b>	
15		<b>4,218,349,778</b>		<b>4.586741250</b>	
16		<b>17,881,987,659</b>		<b>4.574877902</b>	
17		<b>75,568,307,191</b>		<b>4.563716381</b>	
18		<b>318,489,941,731</b>		<b>4.553209881</b>	0:04
19		<b>1,339,093,701,964</b>		<b>4.543308340</b>	0:20
20		<b>5,617,897,764,831</b>		<b>4.533962650</b>	1:30
21		<b>23,521,568,438,976</b>		<b>4.525128839</b>	7:00

Table 1: Left: Results obtained by Klarner and Rivest [19, Table 1]; Right: Our results for  $d=2$ .

In fact, Klarner and Rivest claim to have used the following version of condition (\*):

### Condition (\*):

- None of the cells of  $L_i$  (except its root) overlap with any of the cells or forbidden cells of  $T$ ; and
- None of the forbidden cells of  $L_i$  overlap with any cells of  $T$ .

However, although they did not state the following explicitly, they probably did not use the second part of condition (\*) in their program. We motivate this claim by the two arguments provided below, emphasizing that indeed using the second part of this condition *as-is* is incorrect, as we explain in the second argument. Still, our results agree with those of Klarner and Rivest's only up to  $i = 5$ , and we were unable to trace further the causes for the differences for  $i \geq 6$ .

### Argument 1

Consider the set  $C_4$ , which contains all twigs that have exactly 4 black cells, or fewer black cells and no white cells. Let us enumerate the twigs that have one, two, or three black cells and no open cells. We can easily observe the following.

1. There is only *one* twig ( $L_1 \in \mathbf{L}$ , shown in Figure 4) with one dead cell and no open cells.

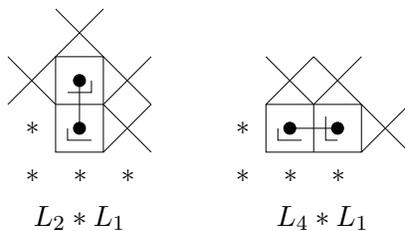


Figure 10: The only two twigs with two dead cells and no open cells

2. There are only *two* twigs (see Figure 10) with two dead cells and no open cells.
3. There are only *six* twigs with three dead cells and no open cells. The sequences corresponding to these six twigs are  $L_2 * L_2 * L_1$ ,  $L_2 * L_4 * L_1$ ,  $L_3 * L_1 * L_1$ ,  $L_4 * L_2 * L_1$ ,  $L_4 * L_4 * L_1$ , and  $L_5 * L_1 * L_1$ .

We now show that there are 400 twigs with 4 dead cells. Each such twig  $T$  corresponds to a sequence  $(\alpha, \beta, \gamma, \delta)$  of four elements of  $\mathbf{L}$  (Figure 4), such that  $T = \alpha * \beta * \gamma * \delta$ . Trivially, in total, there are  $|\mathbf{L}|^4 = 5^4 = 625$  sequences of four elements of  $\mathbf{L}$ . However, some of these sequences are invalid, namely, they do not represent valid twigs. For example, the only valid sequence that starts with  $L_1$  is of length 1 since  $L_1$  has no open cells. It is easy to verify that the following sequences are exactly those that are invalid since their prefixes correspond to configurations with less than four dead cells and no open cells:  $S_1 = (L_1, \beta, \gamma, \delta)$ ,  $S_2 = (L_2, L_1, \gamma, \delta)$ ,  $S_3 = (L_4, L_1, \gamma, \delta)$ ,  $S_4 = (L_2, L_4, L_1, \delta)$ ,  $S_5 = (L_4, L_2, L_1, \delta)$ ,  $S_6 = (L_2, L_2, L_1, \delta)$ ,  $S_7 = (L_4, L_4, L_1, \delta)$ ,  $S_8 = (L_3, L_1, L_1, \delta)$ , and  $S_9 = (L_5, L_1, L_1, \delta)$ .

Clearly, we have that  $|S_1| = 5^3 = 125$ ,  $|S_2| = |S_3| = 5^2 = 25$ , and  $|S_4| = |S_5| = |S_6| = |S_7| = |S_8| = |S_9| = 5$ . There remain exactly twenty invalid sequences. Refer to Figure 4. The twigs  $L_4$  and  $L_5$  cannot be concatenated to any of the configurations (a–j) (Figures 11 and 12) since this would violate the first part of condition (\*), that is, a cell of  $L_4$  or  $L_5$  would overlap with an occupied cell of the configuration or a cell marked as forbidden. This results in  $2 \cdot 10 = 20$  more invalid sequences. Thus, we obtain that the number of twigs with four dead cells is

$$|\mathbf{L}|^4 - \sum_{i=1}^9 |S_i| - 2 \cdot 10 = 625 - 125 - 2 \cdot 25 - 6 \cdot 5 - 20 = 400.$$

Hence, adding items (1–3) above, we obtain that  $|\mathbf{C}_4| = 400 + 1 + 2 + 6 = 409$ , which is the number provided for  $|\mathbf{C}_4|$  by Klarner and Rivest as well (see Table 1). On the other hand, restricting the construction of  $\mathbf{C}_4$  further with the second part of condition (\*) would imply that, for example, concatenating  $L_1$  to configuration (d) is invalid, which would decrease the size of  $\mathbf{C}_4$ . Therefore, we conclude that Klarner and Rivest most probably did not use the second part of condition (\*).

## Argument 2

Consider the pentomino  $P$  shown in Figure 13. The spanning tree of  $P$  corresponds to the sequence  $L_3 * L_2 * L_4 * L_1 * L_1$  (which is equivalent to concatenating  $L_1$  twice to configuration (d) in Figure 11). In terms of elements of  $\mathbf{C}_4$ , this is a sequence of length two: its first element  $T$  is the twig corresponding to adding  $L_1$  to configuration (d), and its second element is  $L_1$ . By definition, the two twigs  $T$  and  $L_1$  belong to  $\mathbf{C}_4$ . However, if we were to use the second part of condition (\*),  $T$  would be discarded as an element of  $\mathbf{C}_4$ . In such a situation,  $\mathbf{C}_4$  would not be a *complete* set of building blocks for polyominoes, and  $P$  would have no corresponding sequence of weight  $x^5 y^5$  of elements of  $\mathbf{C}_4$ . Therefore, the method would have failed to provide an upper bound on  $\lambda_2$  if the second part of condition (\*) had been used, as some polyominoes (such as  $P$ ) would be overlooked.

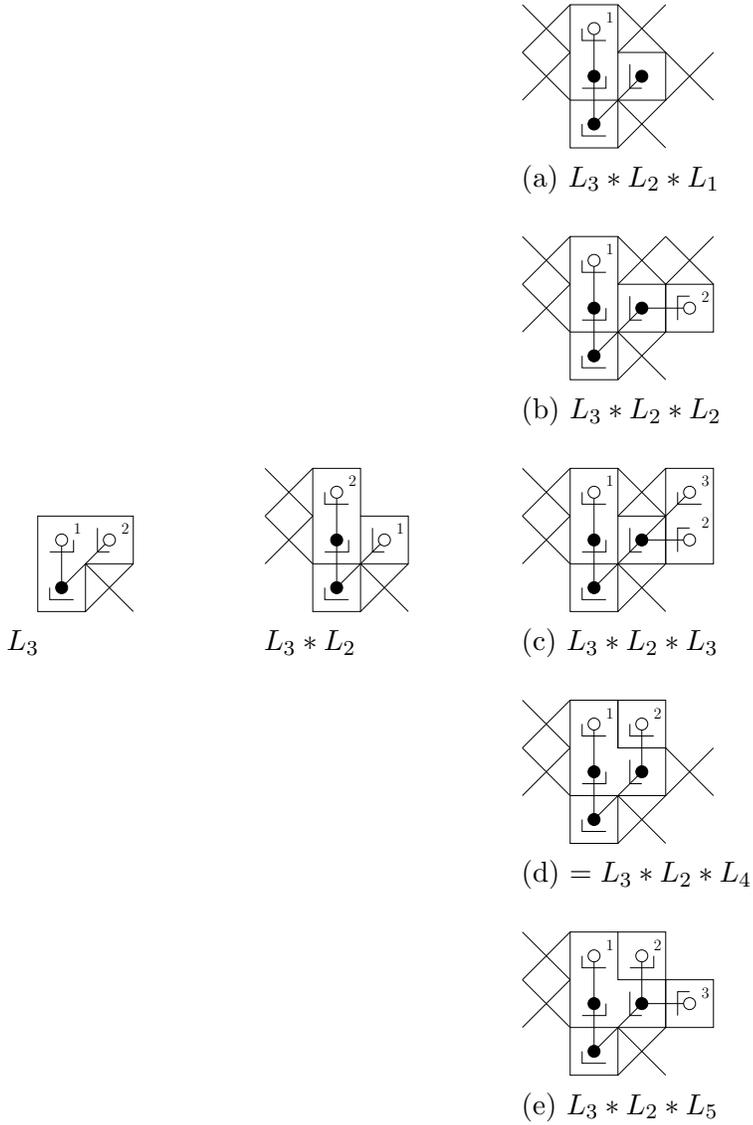


Figure 11: Concatenation of  $L_2$  and  $L_3$ .

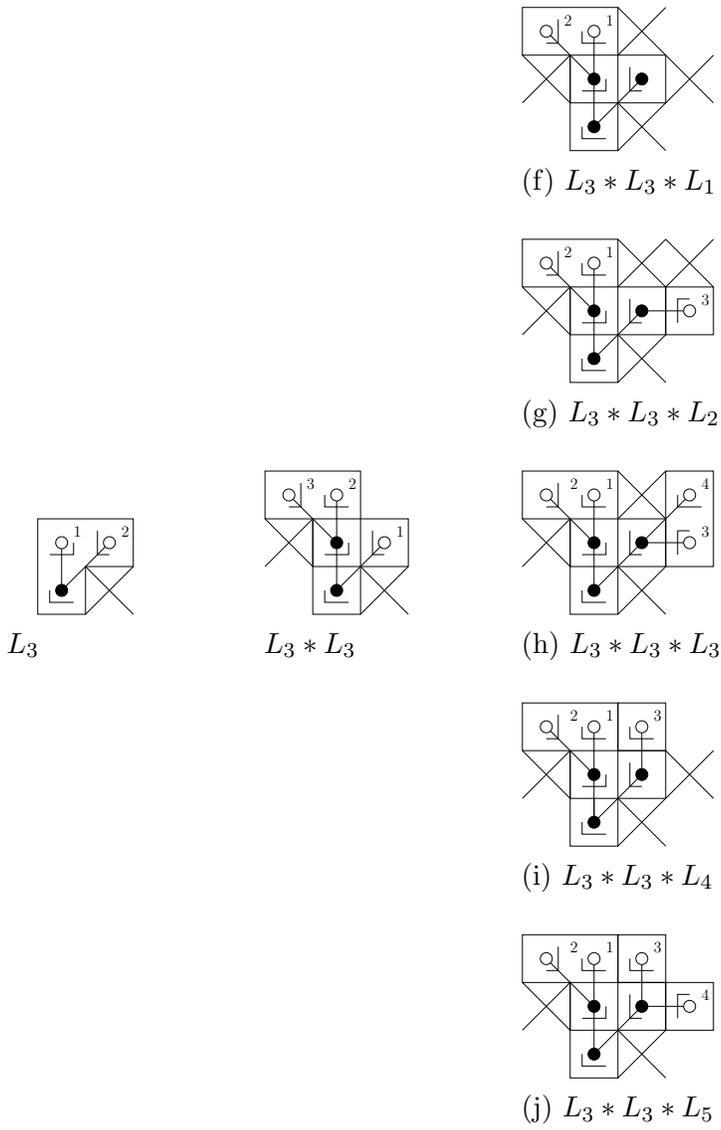


Figure 12: Concatenation of  $L_3$  and  $L_3$ .

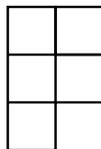


Figure 13: A pentomino

## B The Functions $W_i(x, y)$

Here are the weight functions  $W_1(x, y), \dots, W_{21}(x, y)$ :

$$W_1(x, y) = 2x^2y + 2xy + y$$

$$W_2(x, y) = 4x^4y^2 + 8x^3y^2 + 6x^2y^2 + 2xy^2 + y$$

$$W_3(x, y) = 8x^6y^3 + 24x^5y^3 + 32x^4y^3 + 20x^3y^3 + 6x^2y^3 + 2xy^2 + y$$

$$W_4(x, y) = 14x^8y^4 + 58x^7y^4 + 113x^6y^4 - 124x^5y^4 + 71x^4y^4 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y$$

$$W_5(x, y) = 24x^{10}y^5 + 124x^9y^5 + 317x^8y^5 + 494x^7y^5 + 483x^6y^5 + 261x^5y^5 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y$$

$$W_6(x, y) = 36x^{12}y^6 + 240x^{11}y^6 + 772x^{10}y^6 + 1550x^9y^6 + 2099x^8y^6 + 1895x^7y^6 + 984x^6y^6 + 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y$$

$$W_7(x, y) = 64x^{14}y^7 + 468x^{13}y^7 + 1750x^{12}y^7 + 4221x^{11}y^7 + 7177x^{10}y^7 + 8795x^9y^7 + 7489x^8y^7 + 3775x^7y^7 + 984x^6y^7 + 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y$$

$$W_8(x, y) = 88x^{16}y^8 + 780x^{15}y^8 + 3487x^{14}y^8 + 10135x^{13}y^8 + 20921x^{12}y^8 + 32015x^{11}y^8 + 36517x^{10}y^8 + 29738x^9y^8 + 14657x^8y^8 + 3775x^7y^8 + 984x^6y^7 + 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y$$

$$W_9(x, y) = 96x^{18}y^9 + 1092x^{17}y^9 + 6138x^{16}y^9 + 21679x^{15}y^9 + 53840x^{14}y^9 + 99208x^{13}y^9 + 139805x^{12}y^9 + 150644x^{11}y^9 + 118455x^{10}y^9 + 57394x^9y^9 + 14657x^8y^9 + 3775x^7y^8 + 984x^6y^7 + 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y$$

$$W_{10}(x, y) = 64x^{20}y^{10} + 1288x^{19}y^{10} + 9620x^{18}y^{10} + 41940x^{17}y^{10} + 124236x^{16}y^{10} + 271585x^{15}y^{10} + 455916x^{14}y^{10} + 600672x^{13}y^{10} + 618318x^{12}y^{10} + 472966x^{11}y^{10} + 226165x^{10}y^{10} + 57394x^9y^{10} + 14657x^8y^9 + 3775x^7y^8 + 984x^6y^7 + 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y$$

$$W_{11}(x, y) = 32x^{22}y^{11} + 1560x^{21}y^{11} + 15116x^{20}y^{11} + 77222x^{19}y^{11} + 265528x^{18}y^{11} + 671900x^{17}y^{11} + 1315757x^{16}y^{11} + 2043184x^{15}y^{11} + 2547938x^{14}y^{11} + 2528282x^{13}y^{11} + 1892135x^{12}y^{11} + 895513x^{11}y^{11} + 226165x^{10}y^{11} + 57394x^9y^{10} + 14657x^8y^9 + 3775x^7y^8 + 984x^6y^7 + 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y$$

$$W_{12}(x, y) = 32x^{24}y^{12} + 2448x^{23}y^{12} + 24984x^{22}y^{12} + 140612x^{21}y^{12} + 537148x^{20}y^{12} + 1535243x^{19}y^{12} + 3428784x^{18}y^{12} + 6148920x^{17}y^{12} + 8968766x^{16}y^{12} + 10700784x^{15}y^{12} + 10309921x^{14}y^{12} + 7582080x^{13}y^{12} + 3559132x^{12}y^{12} + 895513x^{11}y^{12} + 226165x^{10}y^{11} + 57394x^9y^{10} + 14657x^8y^9 + 3775x^7y^8 + 984x^6y^7 + 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y$$

$$W_{13}(x, y) = 64x^{26}y^{13} + 3376x^{25}y^{13} + 39052x^{24}y^{13} + 242230x^{23}y^{13} + 1029746x^{22}y^{13} + 3276965x^{21}y^{13} + 8225862x^{20}y^{13} + 16714930x^{19}y^{13} + 27959240x^{18}y^{13} + 38764654x^{17}y^{13} + 44612842x^{16}y^{13} + 41963681x^{15}y^{13} + 30425691x^{14}y^{13} + 14187563x^{13}y^{13} + 3559132x^{12}y^{13} + 895513x^{11}y^{12} + 226165x^{10}y^{11} + 57394x^9y^{10} + 14657x^8y^9 + 3775x^7y^8 + 984x^6y^7 + 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y$$

$$\begin{aligned}
W_{14}(x, y) = & 3872x^{27}y^{14} + 53860x^{26}y^{14} + 388828x^{25}y^{14} + 1856137x^{24}y^{14} + \\
& 6593524x^{23}y^{14} + 18410515x^{22}y^{14} + 41847658x^{21}y^{14} + 78846479x^{20}y^{14} + \\
& 124566489x^{19}y^{14} + 165600553x^{18}y^{14} + 184977014x^{17}y^{14} + 170581831x^{16}y^{14} + \\
& 122243680x^{15}y^{14} + 56691193x^{14}y^{14} + 14187563x^{13}y^{14} + 3559132x^{12}y^{13} + \\
& 895513x^{11}y^{12} + 226165x^{10}y^{11} + 57394x^9y^{10} + 14657x^8y^9 + 3775x^7y^8 + 984x^6y^7 + \\
& 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y
\end{aligned}$$

$$\begin{aligned}
W_{15}(x, y) = & 4400x^{29}y^{15} + 74688x^{28}y^{15} + 598128x^{27}y^{15} + 3182157x^{26}y^{15} + \\
& 12522050x^{25}y^{15} + 38772694x^{24}y^{15} + 97650143x^{23}y^{15} + 204840498x^{22}y^{15} + \\
& 362613604x^{21}y^{15} + 546205155x^{20}y^{15} + 701024617x^{19}y^{15} + 763765263x^{18}y^{15} + \\
& 692808602x^{17}y^{15} + 491675078x^{16}y^{15} + 226975964x^{15}y^{15} + 56691193x^{14}y^{15} + \\
& 14187563x^{13}y^{14} + 3559132x^{12}y^{13} + 895513x^{11}y^{12} + 226165x^{10}y^{11} + 57394x^9y^{10} + \\
& 14657x^8y^9 + 3775x^7y^8 + 984x^6y^7 + 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y
\end{aligned}$$

$$\begin{aligned}
W_{16}(x, y) = & 6912x^{31}y^{16} + 106640x^{30}y^{16} + 902716x^{29}y^{16} + 5194974x^{28}y^{16} + \\
& 22502316x^{27}y^{16} + 76836395x^{26}y^{16} + 213862804x^{25}y^{16} + 495599251x^{24}y^{16} + \\
& 972881530x^{23}y^{16} + 1634495588x^{22}y^{16} + 2365001740x^{21}y^{16} + 2946546711x^{20}y^{16} + \\
& 3143569000x^{19}y^{16} + 2812205702x^{18}y^{16} + 1979423214x^{17}y^{16} + 910239465x^{16}y^{16} + \\
& 226975964x^{15}y^{16} + 56691193x^{14}y^{15} + 14187563x^{13}y^{14} + 3559132x^{12}y^{13} + \\
& 895513x^{11}y^{12} + 226165x^{10}y^{11} + 57394x^9y^{10} + 14657x^8y^9 + 3775x^7y^8 + 984x^6y^7 + \\
& 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y
\end{aligned}$$

$$\begin{aligned}
W_{17}(x, y) = & 7488x^{33}y^{17} + 136064x^{32}y^{17} + 1260248x^{31}y^{17} + 8008422x^{30}y^{17} + \\
& 38155640x^{29}y^{17} + 143730425x^{28}y^{17} + 440598289x^{27}y^{17} + 1124991218x^{26}y^{17} + \\
& 2431711692x^{25}y^{17} + 4512423641x^{24}y^{17} + 7250819239x^{23}y^{17} + 10138105194x^{22}y^{17} + \\
& 12316094597x^{21}y^{17} + 12907416312x^{20}y^{17} + 11411126315x^{19}y^{17} + 7975518589x^{18}y^{17} + \\
& 3655351652x^{17}y^{17} + 910239465x^{16}y^{17} + 226975964x^{15}y^{16} + 56691193x^{14}y^{15} + \\
& 14187563x^{13}y^{14} + 3559132x^{12}y^{13} + 895513x^{11}y^{12} + 226165x^{10}y^{11} + 57394x^9y^{10} + \\
& 14657x^8y^9 + 3775x^7y^8 + 984x^6y^7 + 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y
\end{aligned}$$

$$\begin{aligned}
W_{18}(x, y) = & 6656x^{35}y^{18} + 144624x^{34}y^{18} + 1596016x^{33}y^{18} + 11499558x^{32}y^{18} + \\
& 61231243x^{31}y^{18} + 254612673x^{30}y^{18} + 859000063x^{29}y^{18} + 2406743605x^{28}y^{18} + \\
& 5707780042x^{27}y^{18} + 11616872329x^{26}y^{18} + 20533746813x^{25}y^{18} + 31753025591x^{24}y^{18} + \\
& 43111962291x^{23}y^{18} + 51254247441x^{22}y^{18} + 52900498537x^{21}y^{18} + 46293847405x^{20}y^{18} + \\
& 32158564611x^{19}y^{18} + 14696358415x^{18}y^{18} + 3655351652x^{17}y^{18} + 910239465x^{16}y^{17} + \\
& 226975964x^{15}y^{16} + 56691193x^{14}y^{15} + 14187563x^{13}y^{14} + 3559132x^{12}y^{13} + \\
& 895513x^{11}y^{12} + 226165x^{10}y^{11} + 57394x^9y^{10} + 14657x^8y^9 + 3775x^7y^8 + 984x^6y^7 + \\
& 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y
\end{aligned}$$

$$\begin{aligned}
W_{19}(x, y) = & 4160x^{37}y^{19} + 132864x^{36}y^{19} + 1806784x^{35}y^{19} + 15379120x^{34}y^{19} + \\
& 92764008x^{33}y^{19} + 429323463x^{32}y^{19} + 1592168897x^{31}y^{19} + 4883567215x^{30}y^{19} + \\
& 12646494275x^{29}y^{19} + 28110031644x^{28}y^{19} + 54277687090x^{27}y^{19} + 91972916089x^{26}y^{19} + \\
& 137593335616x^{25}y^{19} + 182153289931x^{24}y^{19} + 212563199986x^{23}y^{19} + \\
& 216507646418x^{22}y^{19} + 187791339852x^{21}y^{19} + 129752205674x^{20}y^{19} + \\
& 59145846645x^{19}y^{19} + 14696358415x^{18}y^{19} + 3655351652x^{17}y^{18} + 910239465x^{16}y^{17} + \\
& 226975964x^{15}y^{16} + 56691193x^{14}y^{15} + 14187563x^{13}y^{14} + 3559132x^{12}y^{13} + \\
& 895513x^{11}y^{12} + 226165x^{10}y^{11} + 57394x^9y^{10} + 14657x^8y^9 + 3775x^7y^8 + 984x^6y^7 + \\
& 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y
\end{aligned}$$

$i$	$ \mathbb{C}_i^3 $	$1/\sigma_i$
1	17	9.807295572
2	273	9.807295567
3	3,745	9.701430690
4	51113	9.631827042
5	693,725	9.573610717
6	9,047,959	9.517471577
7	114,736,608	9.467046484
8	1,428,690,351	9.422618063
9	17,538,443,750	9.383460515

Table 2: Our results in 3 dimensions

$$\begin{aligned}
W_{20}(x, y) = & 2176x^{39}y^{20} + 105984x^{38}y^{20} + 1912912x^{37}y^{20} + 19332440x^{36}y^{20} + \\
& 133729026x^{35}y^{20} + 690201840x^{34}y^{20} + 2818499583x^{33}y^{20} + 9436504653x^{32}y^{20} + \\
& 26597729598x^{31}y^{20} + 64253320144x^{30}y^{20} + 134933108961x^{29}y^{20} + \\
& 248868733815x^{28}y^{20} + 406568926658x^{27}y^{20} + 591104290770x^{26}y^{20} + \\
& 765646007641x^{25}y^{20} + 879150587033x^{24}y^{20} + 885155570880x^{23}y^{20} + \\
& 761751496919x^{22}y^{20} + 523818188901x^{21}y^{20} + 238239106019x^{20}y^{20} + \\
& 59145846645x^{19}y^{20} + 14696358415x^{18}y^{19} + 3655351652x^{17}y^{18} + 910239465x^{16}y^{17} + \\
& 226975964x^{15}y^{16} + 56691193x^{14}y^{15} + 14187563x^{13}y^{14} + 3559132x^{12}y^{13} + \\
& 895513x^{11}y^{12} + 226165x^{10}y^{11} + 57394x^9y^{10} + 14657x^8y^9 + 3775x^7y^8 + 984x^6y^7 + \\
& 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + 6x^2y^3 + 2xy^2 + y
\end{aligned}$$

$$\begin{aligned}
W_{21}(x, y) = & 1152x^{41}y^{21} + 96256x^{40}y^{21} + 2056288x^{39}y^{21} + 24172920x^{38}y^{21} + \\
& 187337816x^{37}y^{21} + 1070722580x^{36}y^{21} + 4785628001x^{35}y^{21} + 17443616434x^{34}y^{21} + \\
& 53301072439x^{33}y^{21} + 139441849789x^{32}y^{21} + 316994896043x^{31}y^{21} + \\
& 633630643451x^{30}y^{21} + 1123186767205x^{29}y^{21} + 1777867306642x^{28}y^{21} + \\
& 2521701005541x^{27}y^{21} + 3204911295924x^{26}y^{21} + 3628247213386x^{25}y^{21} + \\
& 3615763450791x^{24}y^{21} + 3089960078272x^{23}y^{21} + 2115755445262x^{22}y^{21} + \\
& 960344267887x^{21}y^{21} + 238239106019x^{20}y^{21} + 59145846645x^{19}y^{20} + \\
& 14696358415x^{18}y^{19} + 3655351652x^{17}y^{18} + 910239465x^{16}y^{17} + 226975964x^{15}y^{16} + \\
& 56691193x^{14}y^{15} + 14187563x^{13}y^{14} + 3559132x^{12}y^{13} + 895513x^{11}y^{12} + 226165x^{10}y^{11} + \\
& 57394x^9y^{10} + 14657x^8y^9 + 3775x^7y^8 + 984x^6y^7 + 261x^5y^6 + 71x^4y^5 + 20x^3y^4 + \\
& 6x^2y^3 + 2xy^2 + y
\end{aligned}$$

## C Three Dimensions

The following is the weight function for  $i = 8$ , from which we computed the upper bound  $\lambda_3 \leq 9.3835$ .

$$\begin{aligned}
W_8(x, y) = & y + 4xy^2 + 23x^2y^3 + 150x^3y^4 + 1051x^4y^5 + 7661x^5y^6 + 57337x^6y^7 + \\
& 437050x^7y^8 + 3376485x^8y^9 + 26352274x^9y^9 + 108757201x^{10}y^9 + 306714778x^{11}y^9 + \\
& 674917794x^{12}y^9 + 1222175063x^{13}y^9 + 1866911075x^{14}y^9 + 2434995919x^{15}y^9 + \\
& 2728046412x^{16}y^9 + 2631637304x^{17}y^9 + 2185885771x^{18}y^9 + 1560584567x^{19}y^9 + \\
& 954538066x^{20}y^9 + 497886496x^{21}y^9 + 220105634x^{22}y^9 + 81810253x^{23}y^9 + \\
& 25294655x^{24}y^9 + 6411687x^{25}y^9 + 1305352x^{26}y^9 + 207134x^{27}y^9 + 24462x^{28}y^9 + \\
& 1992x^{29}y^9 + 97x^{30}y^9 + 2x^{31}y^9);
\end{aligned}$$

## D Maple Code

Let  $f(x,y)$  be a rational two-variable generating function. Klarner and Rivest [19, §3] showed how to obtain the the radius of convergence of the diagonal of  $f(x,y)$ . This requires a change of variable in order to apply the residue theorem. The diagonal function  $f_D(z) = \sum_n l(n,n)z^n$  could then be written as a sum of residues. The following is our Maple implementation of this method.

```
g:=(x,y)->f(x,y)/x;
par := g(s,z/s);
d := denom(par);
with(Physics):
c := Coefficients(d,s,leading);
div := Coefficients(c,z,leading);
d := d / div;
dis := discrim(d,s);
sols := fsolve(dis=0,z);
maxroot := max(sols);
ub := evalf(1/maxroot);
```