

# On the Number of Compositions of Two Polycubes

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## Abstract

A composition of two polycubes is appending them to each other so that the union is a valid polycube. We provide almost tight (up to subpolynomial factors) bounds on the minimum and maximum possible numbers of compositions of two polycubes, either when each is of size  $n$ , or when their total size is  $N$ , in two and higher dimensions. We also provide an efficient algorithm for computing the number of compositions that two given polyominoes (or polycubes) have.

**Keywords and phrases** Polyominoes, polycubes.

**Digital Object Identifier** 10.57717/cgt.v3i1.41

**Related Version** A preliminary version of this paper appeared in Ref. [2].

**Funding** *Andrei Asinowski*: FWF Grant P28466

*Gill Barequet*: ISF Grant 575/15 and BSF Grant 2017684

**Acknowledgements** We thank the referees for their helpful remarks.

## 1 Introduction

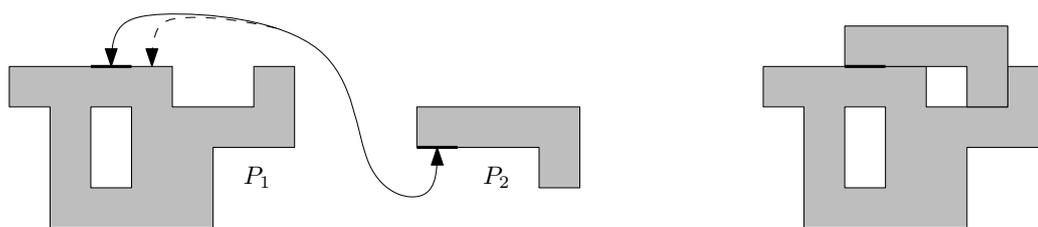
A  $d$ -dimensional *polycube* (*polyomino* if  $d = 2$ ) is a connected set of cells on the cubical lattice  $\mathbb{Z}^d$ , where the connectivity is through  $(d-1)$ -dimensional faces. Polycubes and other *lattice animals* (e.g., polyiamonds and polyhexes) play for more than half a century an important role in enumerative combinatorics [7] as well as in statistical physics [6].

The *size* (volume, or area in the plane) of a polycube is the number of  $d$ -dimensional cells it contains. The counts of  $n$ -cell polyominoes are currently known up to  $n = 70$  [4]. Counts of 3-dimensional polycubes are currently known up to size 22 (see sequence [A000162](#) in the On-line Encyclopedia of Integer Sequences [10]). Counts of higher-dimensional polycubes were published as well; see, e.g., Refs. [1, 9].

A *composition* of two  $d$ -dimensional polycubes is the placement of one of them relative to the other, such that they touch each other (sharing one or more  $(d-1)$ -dimensional faces) but do not overlap, so that the union of their cell sets is a valid (connected) polycube, see Figure 1 for an example in the plane. This definition generalizes for other lattice animals in a straightforward way. The number of compositions plays an important role in proving bounds on the growth constant of lattice animals. For example, it was used for obtaining an upper bound on the growth constant of polyiamonds (edge-connected sets of cells on the



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■ **Figure 1** Aligning the edges connected by the arrow-curve creates a composition of the two polyominoes  $P_1$  and  $P_2$ , as shown on the right. The alignment along the dotted curve does not create a valid composition because it would lead to an overlap between  $P_1$  and  $P_2$ .

■ **Table 1** The number of compositions of two polycubes of total size  $N$ .

Number of Compositions	Two Dimensions		$d \geq 3$ Dimensions	
	Lower Bound	Upper Bound	Lower Bound	Upper Bound
Minimum	$\Theta(N^{1/2})$		$2(N/2)^{1-1/d}$	$O(2^d d(N/2)^{1-1/d})$
Maximum	$N^2/2^{O(\log^{1/2} N)}$	$O(N^2)$	$\Theta(dN^2)$	

regular planar triangular lattice) [5].<sup>1</sup>

In this paper, we address the following.

Question 1: Given two polycubes **of total size  $N$** , how many different compositions do they have?

We can also ask a restricted version:

Question 2: Given two polycubes, **each of size  $n$** , how many different compositions do they have?

Notice that all the polycubes, as well as their compositions, are considered up to translations. That is, polycubes that can be obtained from each other by a parallel translation are considered as the same combinatorial object.

Since the situation in Question 2 is a special case of that in Question 1, some bounds for one of the questions carry over to the other question. Namely, any lower (resp., upper) bound on the minimum (resp., maximum) number of compositions in Question 1 also carries over to Question 2, and any upper (resp., lower) bound on the minimum (resp., maximum) number of compositions in Question 2 also carries over to Question 1. In fact, all our bounds apply to both versions of the question. In addition, any specific example provides both an upper bound on the minimum and a lower bound on the maximum of the respective number of compositions. To avoid confusion, we denote by  $N$  throughout the paper the total size of the two polycubes under discussion. We summarize our results in Table 1.

<sup>1</sup> A linear upper bound on the maximum possible number of compositions of polyominoes has been incorrectly claimed [3, Theorem 2.5], leading to an erroneous improvement of an upper bound on the growth constant of polyominoes [3, Theorem 2.6]. After finding a counterexample, we regarded it as a challenge how far away from the claimed linear upper bound we could push. An almost quadratic lower bound on the number of compositions is given below in Theorem 4, while a quadratic upper bound is trivial (Observation 3).

Interestingly, when it comes to finding the pair of polycubes, each of size  $n$ , with the largest number of compositions, there is a huge difference between two and higher dimensions: Obtaining the tight quadratic bound in higher dimensions is almost trivial, whereas the planar case requires considerable effort.

We also provide an efficient algorithm for computing the number of compositions of two given polyominoes (or polycubes) (Theorem 13 in Section 5).

## 2 Two dimensions

### 2.1 Minimum number of compositions

► **Theorem 1.** (i) Any two polyominoes of sizes  $n_1$  and  $n_2$  have  $\Omega((n_1 + n_2)^{1/2})$  compositions. (ii) For every two numbers  $n_1 \geq 1, n_2 \geq 1$ , there is a pair of polyominoes of sizes  $n_1$  and  $n_2$  with  $\Theta((n_1 + n_2)^{1/2})$  compositions.

**Proof.** Let  $N = n_1 + n_2$ , and consider a pair of polyominoes  $P_1, P_2$  of sizes  $n_1$  and  $n_2$ . Assume without loss of generality that  $n_1 \geq n_2$ , that is,  $n_1 \geq N/2$ . Assume, also without loss of generality, that the width ( $x$ -span) of  $P_1$  is greater than (or equal to) the height ( $y$ -span) of  $P_1$ . Hence, the width of  $P_1$  is at least  $n_1^{1/2}$ . Then,  $P_2$  may touch  $P_1$  from below or above in different ways at least twice this width: Simply put  $P_2$  below (or above)  $P_1$  so that the left column of  $P_2$  is aligned with the  $i$ th column of  $P_1$  (for  $1 \leq i \leq n_1^{1/2}$ ) and translate  $P_2$  upward (or downward) until it touches  $P_1$ . Hence, we have a least  $2n_1^{1/2} \geq (2N)^{1/2}$  compositions.

To see that this lower bound is tight, we take polyominoes that fit in a square with side lengths  $k_1 = \lceil n_1^{1/2} \rceil$  and  $k_2 = \lceil n_2^{1/2} \rceil$ . We form  $P_1$  and  $P_2$  by filling the respective squares row-wise until they have the desired size. Polyominoes  $P_1$  and  $P_2$  can be composed in at most  $4(k_1 + k_2 - 1) \leq 4(n_1^{1/2} + n_2^{1/2} + 1) \leq 4\sqrt{2}(n_1 + n_2)^{1/2} + 4 = 4\sqrt{2}N^{1/2} + 4$  ways. ◀

The following is a direct corollary of Theorem 1.

► **Corollary 2.** Any two polyominoes of total size  $N$  have  $\Omega(N^{1/2})$  compositions. This lower bound is attainable. ◀

### 2.2 Maximum number of compositions

In this section, we find bounds on the maximum number of compositions of two polyominoes of size  $n$ . First, we show a (quite trivial) upper bound of  $O(n^2)$ . Next, we show that it is “almost tight” by constructing an example that yields a lower bound of  $\Omega(n^{2-\varepsilon})$ , for any  $\varepsilon > 0$ .

#### 2.2.1 Upper bound

► **Observation 3.** Any two polyominoes of sizes  $n_1$  and  $n_2$  have  $O(n_1 n_2)$  compositions.

**Proof.** Let  $n_1, n_2$  denote the sizes of polyominoes  $P_1$  and  $P_2$ , respectively. Then, every cell of  $P_1$  can touch every cell of  $P_2$  in at most four ways, yielding  $4n_1 n_2$  as a trivial upper bound on the number of compositions. For  $N = n_1 + n_2$ , this directly gives the bound of  $O(N^2)$ . ◀

#### 2.2.2 Lower bound

It was claimed [3] that the number of compositions of two polyominoes of total size  $N$  is bounded from above by  $2N$ , which would be a substantial improvement of the bound  $O(N^2)$

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from Observation 3. Unfortunately, its proof contained an erroneous argument, and here we construct an example showing that in fact “almost”  $N^2$  compositions are possible.

► **Theorem 4.** *For every  $n \geq 1$ , there are two polyominoes, each of size at most  $n$ , that have at least*

$$\frac{n^2}{2^{8 \cdot \sqrt{\log_2 n}}} \tag{1}$$

*compositions.*

*Remarks.* From now on, “log” will always denote the binary logarithm. The denominator  $2^{8 \cdot \sqrt{\log n}}$  grows asymptotically more slowly than  $x^\varepsilon$  for any  $\varepsilon > 0$ . Hence, the maximum number of compositions is  $\Omega(n^{2-\varepsilon})$  for any  $\varepsilon > 0$ . On the other hand, if  $n \leq 2^{64}$ , then  $8 \geq \sqrt{\log n}$ , and the denominator of the bound (1) can be estimated as

$$2^{8 \cdot \sqrt{\log n}} \geq 2^{\sqrt{\log n} \cdot \sqrt{\log n}} = n.$$

Hence, the claimed bound (1) is not bigger than  $n$ , which is weaker (smaller) than the number  $4n$  of compositions of two  $1 \times n$  “sticks.” Thus, the bound in the general form (1) starts to beat the trivial bound only for *very large* values of  $n$ . The reason for this is that our analysis concentrates on getting bounds that are both *explicit* and *asymptotically strong*, at the expense of small  $n$ .

After we describe and analyze our construction, we discuss weaker bounds that can be derived from it and that exhibit superlinear growth already for moderate sizes.

**Proof.** We will recursively construct a series of polyominoes  $D_0, D_1, D_2, \dots$ , which we call *dense toothbrushes*, and a series of polyominoes  $S_0, S_1, S_2, \dots$ , which we call *sparse toothbrushes*; see Figure 2. We refer to  $D_k$  and  $S_k$  as *toothbrushes of order  $k$* . In addition to  $k$ , these polyominoes are also parameterized by a *degree parameter*,  $r \geq 2$ , that indicates how many copies of toothbrushes of order  $k-1$  are used to construct a toothbrush of order  $k$ . We use  $r = 3$  in Figure 2. The basic building elements of toothbrushes are *sticks*—rectangles of height 1 or width 1—with one extreme cell identified as *root* and another as *apex*, so that each stick is considered to be oriented from its root to its apex. Toothbrushes  $D_k$  and  $S_k$  consist of  $i$ -sticks—sticks at *levels*  $i = 0, 1, 2, \dots, k$ —where ( $< k$ )-sticks come recursively from toothbrushes of order  $< k$ , and they are attached to a “new”  $k$ -stick. The sticks cycle directions while opposing each other and have increasing lengths as shown in Table 2. (Level  $-1$  does not exist, but it is convenient to define  $\ell_{-1} = 1$ .)

The toothbrushes are constructed as follows. The 0-order toothbrushes  $D_0$  and  $S_0$  are simply 0-sticks, *i.e.*, horizontal  $1 \times 2$  dominoes, the root being the left cell for  $D_0$ , and the right cell for  $S_0$ . For  $k \geq 1$ , the toothbrush  $D_k$  (resp.,  $S_k$ ) consists of a *handle*—a  $k$ -stick of length  $\ell_k$ , oriented as specified in Table 2—to which  $r$  copies of  $D_{k-1}$  (resp., of  $S_{k-1}$ ) are attached, so that their roots coincide with the cells of the handle at distance  $\alpha \cdot o_k^D$  (resp.,  $\alpha \cdot o_k^S$ ),  $\alpha = 0, 1, \dots, r-1$  cells away of its apex. The factors  $o_k^D, o_k^S$  are listed in Table 2 as the *offsets* between successive copies of  $D_{k-1}$  (resp., of  $S_{k-1}$ ) along the handle of  $D_k$  (resp., of  $S_k$ ). *As an exception to this rule*, the smallest dense toothbrush  $D_1$  is constructed by attaching the copies of  $D_0$  at distances  $1, 3, 5, \dots, 2r-1$  from the apex, instead of the distances  $0, 2, 4, \dots, 2r-2$  that would conform to the general pattern.

Figure 2 illustrates the construction. Dense toothbrushes are green, and sparse toothbrushes red. For dense and sparse toothbrushes of order 0 and 1, the roots are marked by blue dots. Arrows indicate the positions where the toothbrushes are attached to the handle of the next order.

■ **Table 2** Orientations and sizes of  $i$ -sticks for the recursive construction; the offsets between successive copies of  $D_{i-1}$  or  $S_{i-1}$  along the  $i$ -sticks.

Level $i$	Orientation of $i$ -sticks		Stick length $\ell_i$	Offset $o_i^D$ in $D_i$	Offset $o_i^S$ in $S_i$
	in $D_i$	in $S_i$			
(-1)			1		
0	→	←	2		
1	↑	↓	$2r^2$	2	$2r$
2	←	→	$4r^2$	4	$4r$
3	↓	↑	$4r^4$	$4r^2$	$4r^3$
4	→	←	$8r^4$	$8r^2$	$8r^3$
5	↑	↓	$8r^6$	$8r^4$	$8r^5$
⋮	⋮	⋮	⋮	⋮	⋮
0 mod 4	→	←	$2^{(i+2)/2}r^i$	$2^{(i+2)/2}r^{i-2}$	$2^{(i+2)/2}r^{i-1}$
2 mod 4	←	→			
1 mod 4	↑	↓	$2^{(i+1)/2}r^{i+1}$	$2^{(i+1)/2}r^{i-1}$	$2^{(i+1)/2}r^i$
3 mod 4	↓	↑			

As a result of these rules, sub-brushes always fan off to the *right* of the handle when viewed from the root towards the apex. As  $k$  increases, the orientation of the brushes cycles counterclockwise in the order left-down-right-up.

Thus, the difference between dense and sparse toothbrushes is that the copies of  $(k - 1)$ -order toothbrushes are denser in  $D_k$  and sparser in  $S_k$ , and that  $D_0$  is oriented to the right and  $S_0$  to the left, and then similarly for higher levels: the sticks of the same level have opposite orientations in  $D_k$  and  $S_k$ .

For later reference, we record the relations between lengths and offsets from Table 2:

$$o_i^D = 2\ell_{i-2}, \quad o_i^S = r \cdot o_i^D, \quad \ell_i = r \cdot o_i^S = 2r^2\ell_{i-2}. \tag{2}$$

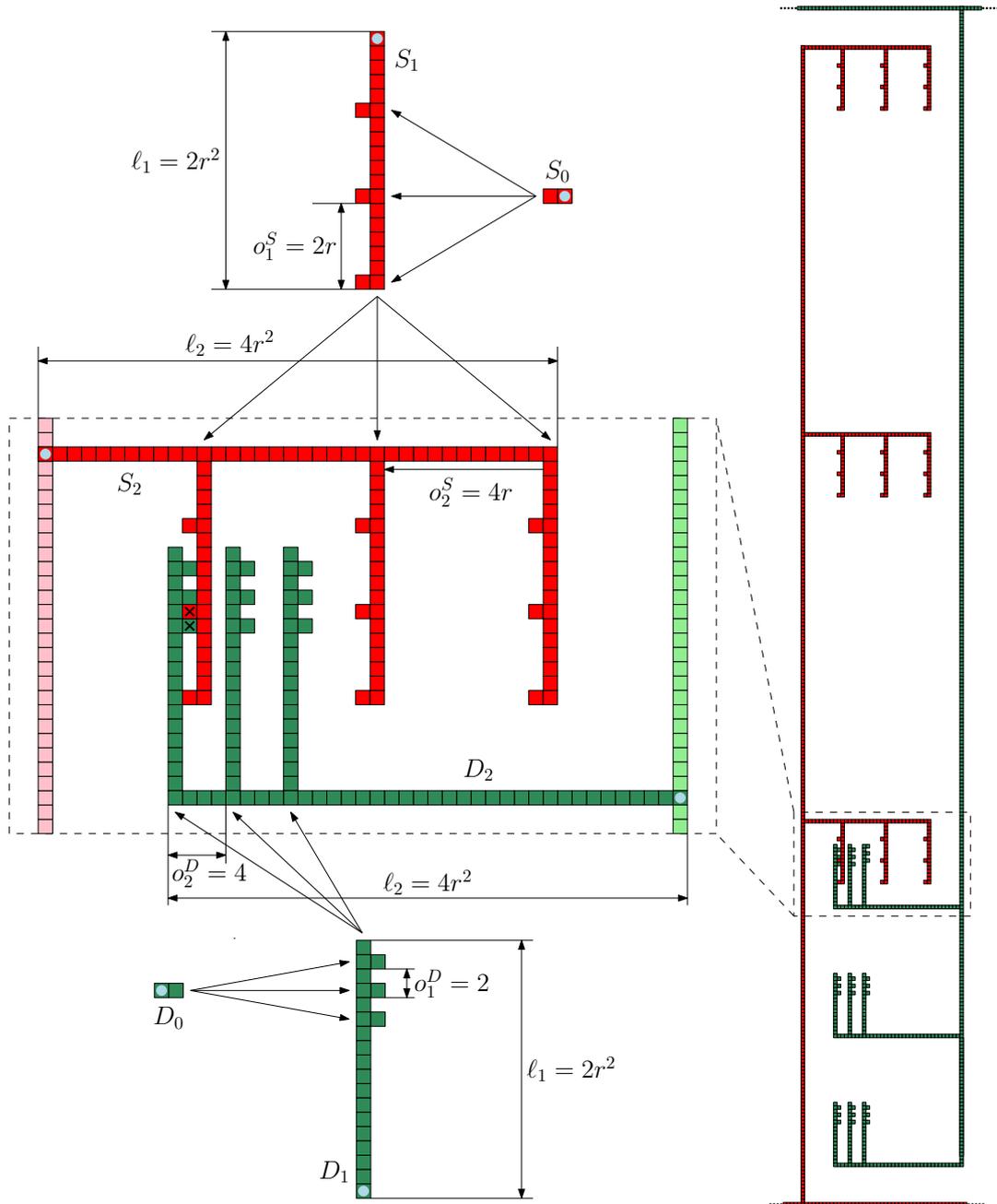
As a consequence, one can observe that when we increase the level  $i$  by two steps, all dimensions increase by a factor of  $2r^2$ .

The 0-sticks consist of two squares, but since one of these squares overlaps a vertical 1-stick, they appear as single-square protrusions, or *notches*. These notches will play a crucial role in counting the compositions. Each of the toothbrushes  $D_k$  and  $S_k$  has  $r^k$  notches. We represent each notch  $N$  of  $D_k$  by a sequence  $A = (\alpha_1, \alpha_2, \dots, \alpha_k)$ , where  $\alpha_i$  indicates that the copy of  $D_{i-1}$  that contains  $N$  is attached to the level- $i$  handle at distance  $\alpha_i o_i^D$  from its apex (or for  $i = 1$ , at distance  $1 + \alpha_1 o_1^D = 1 + 2\alpha_1$ ). The “digits”  $\alpha_i$  of this representation (for  $1 \leq i \leq k$ ) are in the range  $0 \leq \alpha_i \leq r - 1$ . We also use a similar encoding  $B = (\beta_1, \beta_2, \dots, \beta_k)$  for notches of  $S_k$ . In Figure 2, two notches are marked by crosses: the notch  $(2, 0, 2, \dots)$  of (green)  $D_k$  and the notch  $(1, 2, 2, \dots)$  of (red)  $S_k$ .

► **Lemma 5.** *The size of  $D_k$  and  $S_k$  is bounded from above by  $2^{(k+2)/2}r^{k+1}(1 + \frac{2}{r})$  for even  $k$ , and by  $2^{(k+3)/2}r^{k+1}(1 + \frac{1}{r})$  for odd  $k$ . A common upper bound for both cases is*

$$3(\sqrt{2} \cdot r)^{k+1}. \tag{3}$$

**Proof.** To get an upper bound, we simply add the sizes of all sticks, ignoring the overlaps. Let us begin with  $k$  being even. The handle of  $D_k$  or  $S_k$  is horizontal and has size  $2^{(k+2)/2}r^k$ .



■ **Figure 2** The construction for  $r = 3$ . The roots of  $D_0, S_0, D_1, S_1, D_2, S_2$  are marked with blue dots.

There are  $r$  copies of  $D_{k-1}$  or  $S_{k-1}$ , and their  $r$  vertical handles have total size  $r \times 2^{k/2} r^k$ . Together, the sticks at the top two levels have size

$$2^{k/2+1} r^k + 2^{k/2} r^{k+1} = 2^{k/2} r^{k+1} \left(1 + \frac{2}{r}\right). \quad (4)$$

When going down two levels, the stick length decreases by a factor of  $2r^2$ , but the number of sticks increases by a factor of  $r^2$ . Thus, the total size of the sticks decreases by a factor of 2. Counting separately the sticks at even and at odd levels, we therefore get an upper bound on the total size of all sticks if we multiply (4) by  $1 + \frac{1}{2} + \frac{1}{4} + \dots = 2$ . This proves the first statement.

For odd  $k$ , we obtain in a similar way

$$\left(2^{(k+1)/2} r^{k+1} + r \times 2^{(k+1)/2} r^{k-1}\right) \times \left(1 + \frac{1}{2} + \frac{1}{4} + \dots\right) = 2^{(k+3)/2} r^{k+1} \left(1 + \frac{1}{r}\right).$$

The factor 3 in (3) is large enough to cover the extra term  $\sqrt{2} \times \left(1 + \frac{2}{r}\right) \leq \sqrt{2} \times 2$  for the even case and  $2 \times \left(1 + \frac{1}{r}\right) \leq 2 \times \frac{3}{2}$  for the odd case.  $\blacktriangleleft$

► **Lemma 6.** *There are at least  $r^{2k}$  compositions of  $D_k$  and  $S_k$ .*

**Proof.** For each notch  $\mathbf{N}_D$  of  $D_k$  and for each notch  $\mathbf{N}_S$  of  $S_k$ , we can translate  $D_k$  and  $S_k$  so that the upper edge of  $\mathbf{N}_D$  coincides with the lower edge of  $\mathbf{N}_S$ . In the inset of Figure 2, the two involved notches are marked by crosses.

We claim that (1) Such  $r^{2k}$  compositions are distinct; and (2) Each of them is valid in the sense that  $D_k$  and  $S_k$  positioned in this way are disjoint. (We ignore many other compositions, but asymptotically, this gives the dominant term of the total number of compositions.)

(1) We first argue that all these compositions are distinct. Let  $\mathbf{N}_D$  be a notch of  $D_k$  represented by a sequence  $A = (\alpha_1, \alpha_2, \dots, \alpha_k)$ , as explained above. Let us position  $D_k$  so that the notch encoded by  $(0, 0, \dots, 0)$  has coordinates  $\binom{0}{0}$ . Then, the coordinates of the notch  $\mathbf{N}_D$  are

$$\begin{aligned} \binom{0}{0} + \alpha_1 \binom{0}{-o_1^D} + \alpha_2 \binom{o_2^D}{0} + \alpha_3 \binom{0}{o_3^D} + \alpha_4 \binom{-o_4^D}{0} + \dots = \\ \left( \begin{array}{c} 4 \cdot \alpha_2 - 8r^2 \cdot \alpha_4 + 16r^4 \cdot \alpha_6 - 32r^6 \cdot \alpha_8 + \dots \\ -2 \cdot \alpha_1 + 4r^2 \cdot \alpha_3 - 8r^4 \cdot \alpha_5 + 16r^6 \cdot \alpha_7 - \dots \end{array} \right). \end{aligned} \quad (5)$$

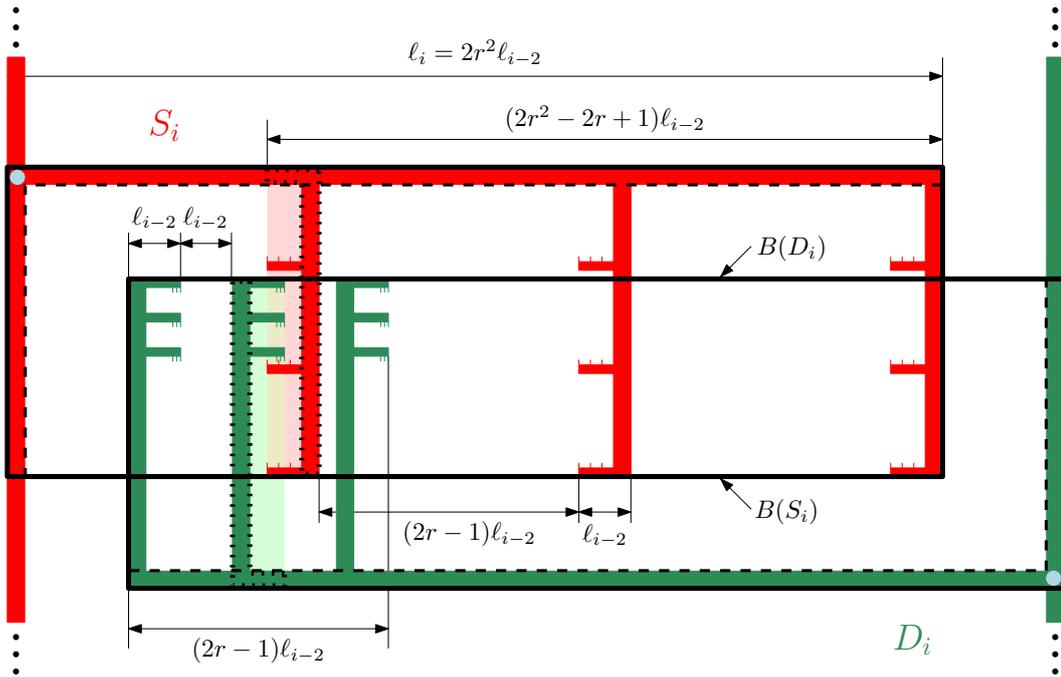
If we similarly encode the notch  $\mathbf{N}_S$  of  $S_k$  by  $B = (\beta_1, \beta_2, \dots, \beta_k)$  and position  $S_k$  so that the notch encoded by  $(0, 0, \dots, 0)$  has coordinates  $\binom{0}{0}$ , then the coordinates of the notch  $\mathbf{N}_S$  are

$$\begin{aligned} \binom{0}{0} + \beta_1 \binom{0}{o_1^S} + \beta_2 \binom{-o_2^S}{0} + \beta_3 \binom{0}{-o_3^S} + \beta_4 \binom{o_4^S}{0} + \dots = \\ \left( \begin{array}{c} -4r \cdot \beta_2 + 8r^3 \cdot \beta_4 - 16r^5 \cdot \beta_6 + 32r^7 \cdot \beta_8 - \dots \\ 2r \cdot \beta_1 - 4r^3 \cdot \beta_3 + 8r^5 \cdot \beta_5 - 16r^7 \cdot \beta_7 + \dots \end{array} \right). \end{aligned} \quad (6)$$

The translation of  $S_k$  that brings  $\mathbf{N}_S$  to the cell directly above  $\mathbf{N}_D$  is found by taking the difference between Equations (5) and (6), and adding  $\binom{0}{1}$ :

$$\left( \begin{array}{c} 4\alpha_2 + 4r\beta_2 - 8r^2\alpha_4 - 8r^3\beta_4 + \dots \\ 1 - 2\alpha_1 - 2r\beta_1 + 4r^2\alpha_3 + 4r^3\beta_3 - \dots \end{array} \right).$$

Since both the successive multipliers  $4, 4r, 8r^2, 8r^3, \dots$  for the  $x$ -coordinate and the successive multipliers  $2, 2r, 4r^2, 4r^3, \dots$  for the  $y$ -coordinate differ at least by a factor of  $r$ ,



■ **Figure 3** Schematic illustration of bounding boxes and rims for toothbrushes  $D_i$  and  $S_i$ .

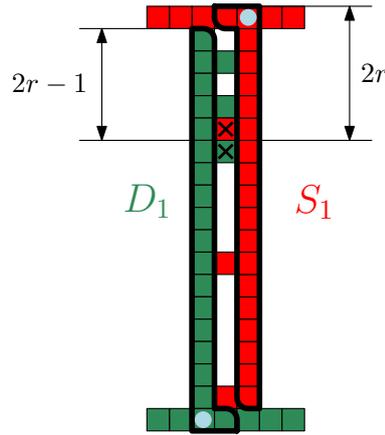
and the coefficients  $\alpha_i$  and  $\beta_i$  are between 0 and  $r-1$ , we conclude that distinct  $(2k)$ -tuples  $(\alpha_1, \alpha_2, \dots, \alpha_k, \beta_1, \beta_2, \dots, \beta_k)$  lead to distinct translations.

(2) It remains to prove that the  $r^{2k}$  compositions described above are valid. That is, to show that if we translate  $D_k$  and  $S_k$  so that some notch  $N_D$  of  $D_k$  is just below some notch  $N_S$  of  $S_k$ , then the union of  $D_k$  and  $S_k$  is disjoint. This will be accomplished by the following Claims 7 and 8.

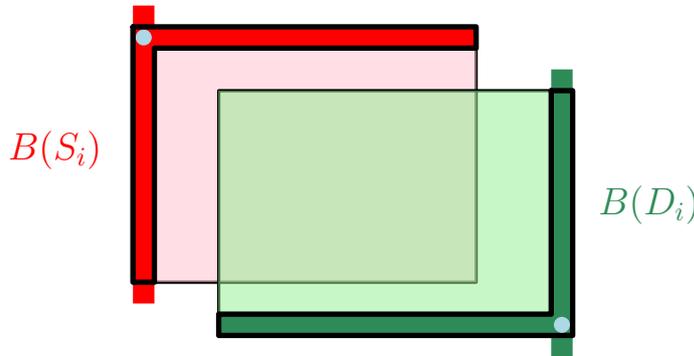
For each polyomino  $P$ , let its *bounding box*  $B(P)$  be the smallest (filled) grid rectangle that contains it. It is easy to see that the bounding boxes of  $D_i$  and of  $S_i$  have size  $\ell_i \times \ell_{i-1}$  or  $\ell_{i-1} \times \ell_i$  (using the convention  $\ell_{-1} = 1$ ). We define the *rim* of a toothbrush as the union of the sides—one horizontal and one vertical—of its bounding box that contain the root of its handle. In fact, one of the sides of the rim of an  $i$ -order toothbrush is its handle, and the other side is contained in the handle of the  $(i+1)$ -order toothbrush to which it belongs. In Figure 3, bounding boxes of two toothbrushes are shown by bold frames, and the bending point of the respective rims are marked by a blue dot. Bounding boxes of some toothbrushes of smaller order are shown by light green or pink background. Respective rims are shown by dashed lines. One should keep in mind that this figure is schematic and sticks of different levels are not to scale.

▷ **Claim 7.** Consider a composition of  $D_k$  and  $S_k$  as described above. Let  $1 \leq i \leq k$ , and suppose that the composition is established via the notches  $N_D$  of  $D_k$  and  $N_S$  of  $S_k$ .<sup>2</sup> Suppose further that  $N_D$  lies in some copy of  $D_i$  and the notch  $N_S$  lies in some copy of  $S_i$ . Then the bounding boxes  $B(D_i)$  and  $B(S_i)$  overlap, but neither bounding box overlaps the rim of the other toothbrush. (Refer to Figure 5 for a schematic depiction of the statement.)

<sup>2</sup> Recall that this means that  $N_D$  is just below  $N_S$ .



■ **Figure 4** Proof of Claim 7, case  $i = 1$ .



■ **Figure 5** Illustration of Claim 7: Bounding boxes overlap, but the rims never overlap. Since the situation is symmetric, it is sufficient to prove the claim for one of the rims.

**Proof.** We prove the claim by induction. For  $i = 1$ , it is easily checked by inspection; refer to Figure 4. The notches do not overlap since all the notches of  $D_1$  fit into gaps between notches in  $S_1$ . It remains to show that  $B(D_1)$  cannot reach the uppermost row of  $B(S_1)$ . Indeed, if  $N_D$  is the lowest notch of  $D_1$ , the vertical distance from its upper edge to the top of  $B(D_1)$  is  $r \cdot o_1^D - 1 = 2r - 1$ . If  $N_S$  is the highest notch of  $S_1$ , the vertical distance from its lower edge to the top of  $B(S_1)$  is  $o_1^S = 2r$ . Thus, if the upper edge of  $N_D$  coincides with the lower edge of  $N_S$ , the top of  $B(D_1)$  is still strictly below the top of  $B(S_1)$ .

Now let  $i \geq 2$ . Assume without loss of generality (and consistently with Figure 3) that the rim of  $D_i$  occupies the lower and the right side of  $B(D_i)$ , and the rim of  $S_i$  occupies the upper and the left side of  $B(S_i)$ , as shown by bold frames in Figure 3. Let  $D_{i-1}$  and  $S_{i-1}$  be specific copies of the lower-order toothbrushes that contain the notches  $N_D$  and  $N_S$ . Their bounding boxes are shown in the figure with a shaded background. Since  $B(D_{i-1})$  and  $B(S_{i-1})$  overlap by induction, we immediately get the overlap of  $B(D_i)$  and  $B(S_i)$ .

To prove that the rim of  $S_i$  does not overlap  $B(D_i)$ , we need to show that  $B(D_i)$  can reach neither the highest row nor the leftmost column of  $B(S_i)$ . The former claim is easy: If  $B(D_i)$  intersects the highest row of  $B(S_i)$ , then  $B(D_{i-1})$  intersects the rim of  $S_{i-1}$ , which contradicts the induction hypothesis.

To show that  $B(D_i)$  cannot reach the leftmost column of  $B(S_i)$ , we use the relations (2) in the calculation. The horizontal extension of each  $(i-1)$ -order sub-brush  $D_{i-1}$  or  $S_{i-1}$  is  $\ell_{i-2}$ .

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The  $(i-1)$ -order sub-brushes of  $D_i$  span in total a horizontal range of width  $(r-1)o_i^D + \ell_{i-2} = (2(r-1)+1)\ell_{i-2}$ , extending to the right from the left side of  $\mathbf{B}(D_i)$ . The  $(i-1)$ -order sub-brushes of  $S_i$  span in total a horizontal range of width  $(r-1)o_i^S + \ell_{i-2} = (2r(r-1)+1)\ell_{i-2}$ , extending to the left from the right side of  $\mathbf{B}(S_i)$ . The sum of these two distances is equal to  $\ell_i = 2r^2\ell_{i-2}$ , the horizontal extension of  $D_i$  and  $S_i$ . It follows that  $\mathbf{B}(D_i)$  cannot reach the leftmost column of  $\mathbf{B}(S_i)$  if the bounding boxes of some  $(i-1)$ -order sub-brushes overlap, which holds by induction for the specified copies of  $D_{i-1}$  and  $S_{i-1}$ . ◀

▷ **Claim 8.** Consider two (sub-)brushes  $D_i$  and  $S_i$  of order  $i \geq 2$ . If two of their sub-brushes  $D_{i-1}$  and  $S_{i-1}$  have overlapping bounding boxes, then no other pair of sub-toothbrushes  $D'_{i-1}$  and  $S'_{i-1}$  of order  $i-1$  can have overlapping bounding boxes.

**Proof.** We employ the same assumption as for the orientation of  $D_i$  and  $S_i$  as in the previous proof. The horizontal dimension of the bounding boxes of level  $i-1$  is then  $\ell_{i-2}$ . The offset between different copies of  $D_{i-1}$  is  $o_i^D = 2\ell_{i-2}$ , by (2). Hence, the distance between their bounding boxes is  $\ell_{i-2}$ , and, therefore, no toothbrush  $S_{i-1}$  can intersect with two different copies of  $D_{i-1}$ .

We also have to argue that no two copies of  $S_{i-1}$  can be intersected by some  $D_{i-1}$ . The offset between successive copies of  $S_{i-1}$  is  $o_i^S = 2r\ell_{i-2}$ , and, hence, the gap between their bounding boxes is  $(2r-1)\ell_{i-2}$ . On the other hand, all copies of  $D_{i-1}$  together fit in a box of horizontal extension  $(2r-1)\ell_{i-2}$ . Hence, no toothbrush  $D_{i-1}$  can intersect with two different copies of  $S_{i-1}$ . ◀

With Claims 7 and 8, we can now conclude that  $D_k$  and  $S_k$  are disjoint: It follows from Claim 7 that the handle of  $D_k$  is disjoint from  $S_k$  (even from its bounding box), and vice versa. All cells that are not in the handle are in the sub-brushes  $D_{k-1}$  and  $S_{k-1}$ . There is exactly one pair  $D_{k-1}, S_{k-1}$  that contains  $\mathbf{N}_D$  and  $\mathbf{N}_S$ , respectively, and by Claim 7, the respective bounding boxes overlap. By Claim 8, this means that all other pairs  $S'_{k-1}, L'_{k-1}$  are disjoint. It suffices, therefore, to prove the claim for sub-brushes  $D_{k-1}$  and  $S_{k-1}$  that contain  $\mathbf{N}_D$  and  $\mathbf{N}_S$ .

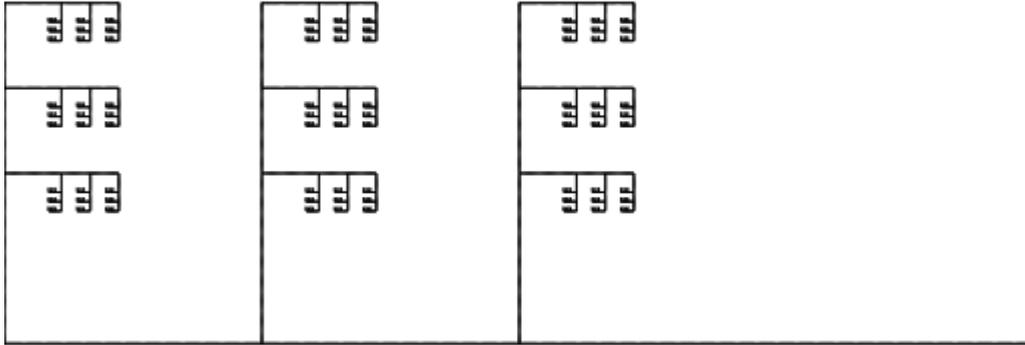
However, the proof above applies for sub-brushes of any order. In this way, we proceed by induction to toothbrushes of lower order until we reach the order-0 pair  $D_0, S_0$  containing the notches  $\mathbf{N}_D$  and  $\mathbf{N}_S$ , for which disjointness is obvious. This concludes the proof of Lemma 6. ◀

In order to finish the proof of Theorem 4, we apply the construction with the parameters  $k := \lfloor \sqrt{\log n} \rfloor - 1$  and  $r := 2^k$ . As discussed after the statement of the theorem, our claimed lower bound is implied by the trivial construction of two orthogonal sticks for  $n \leq 2^{64}$ . Thus, we may assume that  $n > 2^{64}$ . Hence,  $k \geq 7$  and  $r \geq 128$ .

We use Lemma 5 to show that the size of the polyominoes is at most  $n$ . The logarithm of the bound (3) is

$$\begin{aligned} \log((\sqrt{2} \cdot r)^{k+1} 3) &= \log((\sqrt{2} \cdot 2^k)^{k+1}) + \log 3 \\ &= (k + 1/2)(k + 1) + \log 3 \\ &\leq (\sqrt{\log n} - 1/2)\sqrt{\log n} + \log 3 \\ &= \log n - \sqrt{\log n}/2 + \log 3 \\ &\leq \log n, \end{aligned}$$

where the last relation holds for  $n \geq 1059$ .



■ **Figure 6** A rendering of a variation of our sparse toothbrush  $S_5$  as an L-system.

Now we apply Lemma 6 in order to estimate the number of compositions from below. Again, we compute the logarithm of the desired quantity:

$$\log(r^{2k}) = \log((2^k)^{2k}) = 2k^2 \geq 2(\sqrt{\log n} - 2)^2 = 2 \log n - 8\sqrt{\log n} + 8 \geq 2 \log n - 8\sqrt{\log n}.$$

From this, we directly get the bound (1). ◀

There are a few obvious local improvements of our construction. For example, the necessary spacing between the level-1 vertical sticks in  $D_2$  is only 3 instead of the 4 that we use. Removing all notches allows to reduce the spacing even further, without reducing the number of compositions that we count. Alternatively, we could replace the notches by sticks of length  $r$  and adjust all horizontal dimensions accordingly. This would increase the number of compositions by the factor  $r-1$ , while increasing the sizes only by a constant factor. By contrast, our proof strives to make the description of the construction as easy as possible and to keep simple expressions for the dimensions in terms of powers of 2 and  $r$ .

By choosing a small constant order  $k$ , we already obtain superlinear bounds from Lemmata 5 and 6. For example,  $k = 3$  leads to toothbrushes of size  $n = O(r^4)$  with at least  $r^6$  compositions, *i.e.*,  $\Omega(n^{3/2})$  compositions. Setting  $k = 4$  leads to toothbrushes of size  $n = O(r^5)$  with at least  $r^8$  compositions, *i.e.*,  $\Omega(n^{8/5})$  compositions, etc. For any fixed  $k$ , we get  $\Omega(n^{2-2/(k+1)})$  compositions.

**Remark:** As  $k \rightarrow \infty$ , the toothbrushes  $D_k$  and  $S_k$ , properly scaled and rotated, converge to tree-like structures whose substructures are “similar” to the whole structure: thus, it bears some similarity to fractals. The limits are different for  $D_k$  and  $S_k$ , and, in addition, we have to distinguish between even and odd values of  $k$ . When going down two orders, all lengths are uniformly scaled by  $1/(2r^2)$ , and, hence, we find self-similar substructures. However, since the number of substructures is only  $r^2$ , the total length is finite, and the fractal dimension is 1. Hence, we don’t have a fractal in the strict sense. We mention that our toothbrushes, like many fractals, can be modeled by L-systems,<sup>3</sup> for example, as follows:

```

Constants: X
Axiom:    --X
Rule1:    X=[-FFXFXFX]
Rule2:    F=FFF
    
```

<sup>3</sup> <https://en.wikipedia.org/wiki/L-system>

An L-system renderer (<http://www.kevs3d.co.uk/dev/lsystems/>) produces, using the specification above, the fractal shown in Figure 6. In this L-system, a string of symbols is converted to an image by interpreting the symbols as turtle graphics commands: The letter F makes a step forward, and the symbol ‘-’ makes a right turn by 90°. The symbol ‘[’ saves the current position and orientation on a stack, and ‘]’ returns to the previously saved state. The letter X is ignored for the drawing. In one iteration, all occurrences of X and F in the current string are simultaneously substituted according to the two rules. Figure 6 is produced from the starting string (axiom) “-X” after 6 iterations.

We note that the fractal dimension [11] is not the relevant parameter for our problem since it measures the length of a fractal curve (the boundary of the polyomino, in our setting) in terms of the diameter. However, for our application, we also want the *size* (the area enclosed by the boundary) to be small.

### 3 Higher dimensions

#### 3.1 Minimum number of compositions

##### 3.1.1 Lower bound

► **Theorem 9.** *Any two  $d$ -dimensional polycubes of total size  $N$  have at least  $2(N/2)^{1-1/d}$  compositions.*

**Proof.** The proof is similar to that of Theorem 1. Consider two polycubes  $P_1, P_2$  of total size  $N$ . Assume, without loss of generality, that  $P_1$  is the larger of the two polycubes, that is, the size ( $d$ -dimensional volume) of  $P_1$  is at least  $n=N/2$ . Let  $V_i$  (for  $1 \leq i \leq d$ ) be the  $(d-1)$ -dimensional volume of the projection of  $P_1$  orthogonal to the  $x_i$  axis. An isoperimetric-like inequality of Loomis and Whitney [8] ensures that  $\prod_{i=1}^d V_i \geq n^{d-1}$ . Let  $V_k \geq n^{1-1/d}$  be largest among the numbers  $V_1, \dots, V_d$ . Then, there are at least  $2V_k \geq 2n^{1-1/d}$  different ways for how  $P_2$  may touch  $P_1$ . Indeed, the polycube  $P_1$  has  $V_k$  “columns” in the  $x_k$  direction. Pick one specific such “column” of  $P_2$  and align it with each “column” of  $P_1$ , putting it either “below” or “above”  $P_1$  along direction  $x_k$ , and find the unique translation along  $x_k$  by which they touch for the first time while being translated one towards the other. ◀

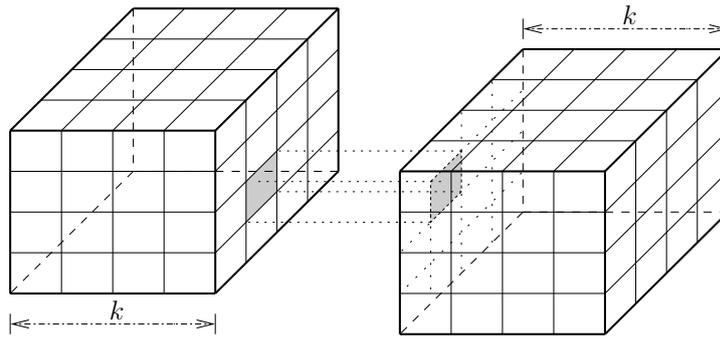
##### 3.1.2 Upper bound

► **Theorem 10.** *There exist pairs of  $d$ -dimensional polycubes, of total size  $N$ , that have  $O(2^d d(N/2)^{1-1/d})$  compositions.*

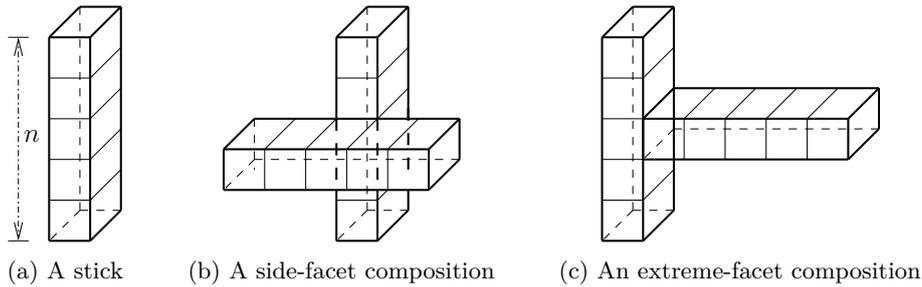
**Proof.** Let us first assume that  $N$  is of the form  $N = 2k^d$ . In this case, we compose two copies of a polycube  $P$  that is a cube made of  $N$  cells (see Figure 7). The two copies of  $P$  can slide towards each other in  $2d$  directions (two directions in each dimension) until they touch. Once we decide which facets of the hypercube touch each other, this can be done in  $(2k-1)^{d-1}$  ways. Indeed, in each of the  $d-1$  dimensions orthogonal to the sliding direction, there are  $2k-1$  possible offsets of one hypercube relative to the other. (This can be visualized easily in two and three dimensions.) Overall, the total number of compositions is

$$(2d)(2k-1)^{d-1} = 2d(2(N/2)^{1/d} - 1)^{d-1} = \Theta(2^d d(N/2)^{1-1/d}).$$

If  $N$  is not of the form  $N = 2k^d$ , let  $k = \lfloor (N/2)^{1/d} \rfloor$ . We form two polycubes  $P_1$  and  $P_2$  that contain the cube  $[0, k]^d$  of side length  $k$ , and that are contained in the cube  $[0, k+1]^d$  of side length  $k+1$ , in such a way that the cells along any axis-parallel line form a connected



■ **Figure 7** A composition of two hypercubes.



■ **Figure 8** Compositions of two “sticks.”

interval. (This can be achieved, for example, by starting with the smaller cube and adding extra cells of the larger cube  $[0, k + 1]^d$  in lexicographic order.) Arguing as above, we conclude that the number of compositions is at least  $(2d)(2k - 1)^{d-1}$  and at most  $(2d)(2k + 1)^{d-1}$ . ◀

### 3.2 Maximum number of compositions in $d \geq 3$ dimensions

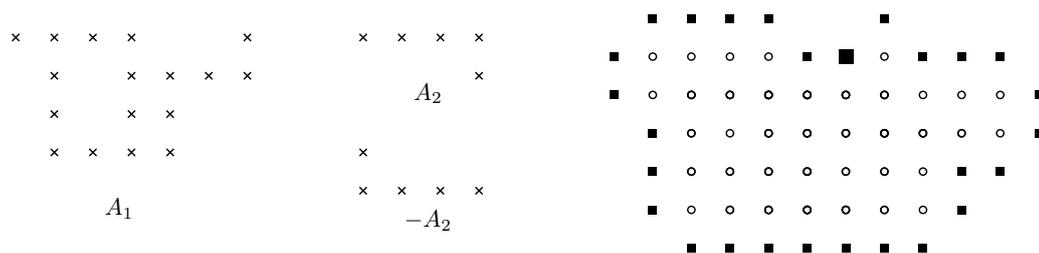
► **Theorem 11.** *Let  $d \geq 3$ . Any two  $d$ -dimensional polycubes of total size  $N = 2n$  have  $O(dn^2)$  compositions. The upper bound is attainable: There are two  $d$ -dimensional polycubes of total size  $2n$  with  $\Omega(dn^2)$  compositions.*

**Proof.** Similarly to two dimensions, any two polycubes  $P_1, P_2$  of total size  $2n$  have  $O(dn^2)$  compositions. Indeed, let  $n_1, n_2$  denote the sizes of  $P_1$  and  $P_2$ , respectively, where  $n_1 + n_2 = 2n$ . Then, every cell of  $P_1$  can touch every cell of  $P_2$  in at most  $2d$  ways, yielding  $2dn_1n_2 \leq 2dn^2$  as a trivial upper bound on the number of compositions.

The lower bound is attained asymptotically, for example, by two nonparallel “sticks” of size  $n$ , as shown in Figure 8(a). Each stick has two *extreme*  $(d-1)$ -dimensional facets (orthogonal to the direction along which the stick is aligned), plus  $2(d-1)n$  many  $(d-1)$ -dimensional *side* facets. The number of compositions that involve only side facets is  $2(d-2)n^2 = \Omega(dn^2)$ , see Figure 8(b): Indeed, for each of the  $d-2$  coordinate directions that are not parallel to any of the two directions of the sticks, there are  $2n^2$  different choices for letting two side facets of the sticks touch. The compositions that involve an extreme facet can be neglected since there are only  $4n$  of them, see Figure 8(c). ◀

Note the difference, for the maximum number of compositions, between the cases  $d = 2$  and  $d > 2$ . If  $d > 2$ , the dimensions along which the sticks are aligned, restrict the compositions of the sticks, but the existence of more dimensions allows every pair of cells,

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■ **Figure 9** The sets  $A_1$  and  $A_2$  of cell centers of the polyominoes  $P_1$  and  $P_2$ , respectively, from Figure 1, the Minkowski difference  $F = A_1 \oplus (-A_2)$  (circles), and the set of valid composition vectors (squares).  $P_1$  and  $P_2$  have 27 compositions. The composition from Figure 1 is highlighted.

one of each polycube, to have compositions through this pair only. This is not the case in two dimensions, a fact that makes the proof of Theorem 4 much more complicated.

4 Compositions and the Minkowski sum

As a preparation for the algorithm that determines (or counts) all compositions, we discuss an elementary connection between compositions of two polyominoes and the Minkowski sum, the element-wise sum of two sets of vectors  $A$  and  $B$ :

$$A \oplus B := \{ a + b \mid a \in A, b \in B \}.$$

In this connection, it is better to regard a polyomino as a discrete set  $A$  of *points*, namely the centers of the grid squares of which it is composed. The polyomino itself can then be obtained as the Minkowski sum of  $A$  with a unit square  $U$  centered at the origin:  $A \oplus U$ .

For two polyominoes  $P_1, P_2$ , we call an integer vector  $t \in \mathbb{Z}^d$  a *valid composition vector*, or simply a *valid composition* of  $P_1$  and  $P_2$ , if  $P_1$  and  $P_2 + t$  form a valid composition, *i.e.*, they do not overlap, but share at least one common edge.

► **Observation 12.** Let  $P_1, P_2$  be polyominoes and let  $A_1, A_2$  be their sets of centerpoints.

1. The set of (integer) translations  $t$  for which  $P_1$  and  $P_2 + t$  overlap is the Minkowski difference

$$F := A_1 \oplus (-A_2) := \{ c_1 - c_2 \mid c_1 \in A_1, c_2 \in B \}.$$

We call  $F$  the forbidden set.

2. The set of valid composition vectors for  $P_1$  and  $P_2$  is the set of neighbors of  $F$ : those integer vectors that have distance 1 from a point of  $F$  but that do not themselves belong to  $F$ .

See Figure 9 for an example.

**Proof.** The first statement is obvious: A vector  $t$  is of the form  $t = c_1 - c_2$  for some  $c_1 \in A_1$  and  $c_2 \in A_2$  if and only if the cells  $c_1 \in A_1$  and  $c_2 + t \in A_2 + t$  coincide:  $t = c_1 - c_2 \iff c_1 = c_2 + t$ .

To see the second statement, let  $t \notin F$  be a vector and  $t' \in F$  an adjacent vector. Then,  $c_1 \in A_1$  and  $c_2 + t' \in A_2 + t'$  coincide. If we move  $A_2 + t'$  by one unit to  $A_2 + t$ , the cell  $c_2 + t' \in A_2 + t'$  is adjacent to  $c_2 + t' = c_1 \in A_1$ , but  $A_2 + t$  becomes disjoint from  $A_1$ , and hence  $t$  is a valid composition.

On the other hand, if  $t$  is a valid composition, then  $t \notin F$ , but there must be two adjacent cells  $c_2 + t \in A_2 + t$  and  $c_1 \in A_1$ . Moving  $A_2$  by one unit brings these two cells to coincide; hence, there is a vector  $t'$  adjacent to  $t$  such that  $c_2 + t' = c_1$ , or in other words,  $t' \in F$ . ◀

## 5 Counting compositions

We now describe an efficient algorithm for finding all compositions of two polyominoes or polycubes.<sup>4</sup> We assume the unit-cost model of computation, in which numbers in the range  $[-n, n]$  can be accessed and be subject to arithmetic operations in  $O(1)$  time, and up to  $O(n^2d)$  memory cells can be accessed by their address in  $O(1)$  time.

► **Theorem 13.** (i) *Given two polyominoes, each of size at most  $n$ , their number of compositions can be computed in  $O(n^2)$  time and  $O(n^2)$  space.*

(ii) *Given two  $d$ -dimensional polycubes, each of size at most  $n$ , their number of compositions can be computed in  $O(d^2n^2)$  time and  $O(dn^2)$  space.*

**Proof.** A straightforward approach would try all  $O(n^2)$  possibilities of moving a cell  $y \in P_2$  next to a cell  $c_1 \in P_1$ , in  $2d$  possible ways, and check whether the two translated polyominoes overlap. Testing for overlap can be done very naively in  $O(n^2)$  time, or with little effort in  $O(n)$  time, but even this leads to an overall runtime of  $O(n^3)$ .

However, we can do better, by using the connection to the Minkowski sum from Observation 12. Let us first deal with the situation in the plane ( $d = 2$  dimensions). To compute  $F$ , we can use a bitmap data structure  $T$ , which holds the status of all possible translations in a  $(2n + 3) \times (2n + 3)$  array, with indices in the range  $-n - 1 \leq t \leq n + 1$  in each direction. Initially, all entries of  $T$  are cleared. In a double loop over the pairs of cells  $c_1 \in P_1, c_2 \in P_2$ , we set the entry in  $T$  corresponding to the translation  $t = c_1 - c_2$ . This sets the bits of  $F$ .

Obviously, both the size and preparation time of  $T$  are  $O(n^2)$ . Finally, by scanning each cell of  $T$ , we can determine in constant time if it lies outside  $F$  but has a neighbor belonging to  $F$ , and hence, according to Observation 12, represents a valid composition. Overall, the entire process requires  $\Theta(n^2)$  time and space.

These bounds assume the worst case, in which size- $n$  polyominoes have an extent of  $\Theta(n)$  in each dimension. By contrast, typical polyominoes can be expected to be somewhat compact. However, we are not aware of any empirical evidence for this statement.

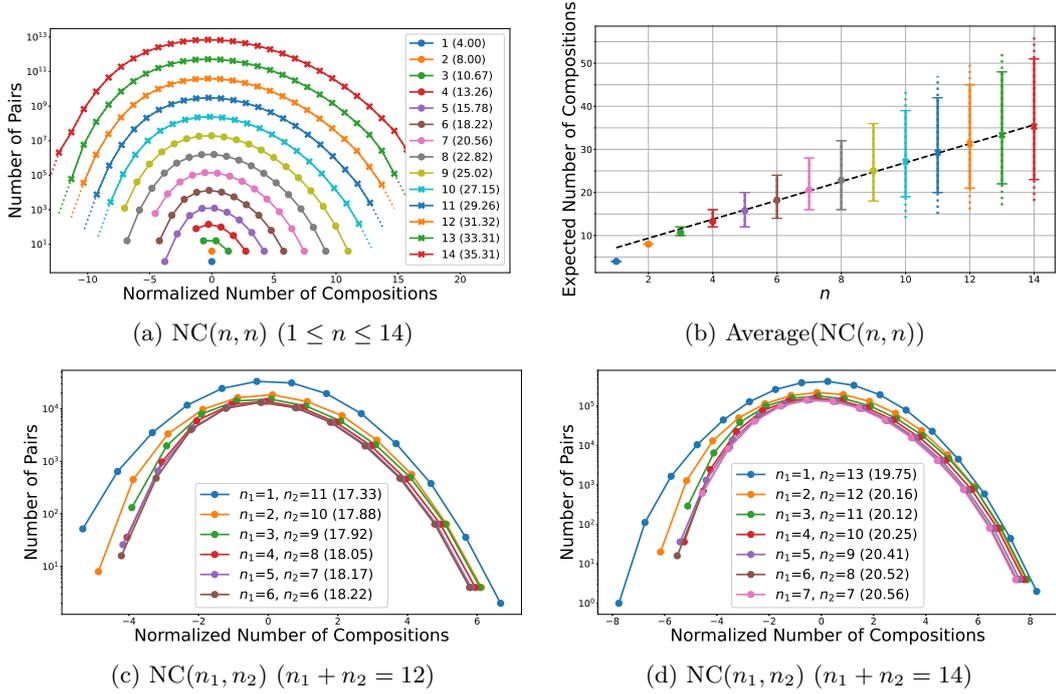
Finally, let us list the differences needed for following the same approach in  $d$  dimensions. Each cell now has  $d$  coordinates (instead of two), and so every cell or translation operation (*e.g.*, setting, comparing, checking, etc.) requires  $\Theta(d)$  instead of constant time. Instead of four neighboring cells, each polycube cell now has  $2d$  neighbors. The size of the input is  $\Theta(dn)$ . A bitmap would require space  $\Theta(n^d)$ , and we would like to avoid this exponential growth in  $d$ .

Instead, we will identify the cells of  $F$  by sorting. We generate the at most  $n^2$  elements of the Minkowski difference  $P_1 - P_2$ , one at a time, in  $O(n^2d)$  time, and store them in a list. Then we sort this list, using radix sort. Radix sort sorts the list in  $d$  passes over the data, each time assigning the elements to buckets according to one selected digit (coordinate). Each pass takes  $O(n^2)$  time (plus  $O(n)$  time for the range of values of the  $i$ th coordinate). Thus, in  $O(n^2d)$  time, we get the elements of  $F$  in sorted order, and then it is easy to eliminate duplicates.

In the second step, we generate  $2d$  neighbors of each element of  $F$ . These are  $O(n^2d)$  *candidates* for translations that may lead to valid compositions. We have to remove the candidates that belong to  $F$ , because they lead to collisions, and we have to eliminate

<sup>4</sup> For higher dimensions, the conference version of this paper [2, Thm. 7] provides three alternative algorithms which exhibit a trade-off between time and space. Our improved algorithm of Theorem 13(ii) dominates all of these algorithms both in time and space.

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■ **Figure 10** Distributions of the number of compositions of pairs of polyominoes of sizes  $n_1, n_2$ . Numbers in parentheses are values by which the curves are normalized (shifted horizontally to the left).

duplications. Again, we rely on radix-sort, but in order to save space, we use a special representation: Each neighbor of an element  $x$  of  $F$  is represented as a triplet  $(x, i, s)$ . The first component is a pointer to  $x$ . The index  $i$  lies in the range  $1 \leq i \leq d$  and indicates which coordinate is to be incremented ( $s = 1$ ) or decremented ( $s = -1$ ). This representation requires only constant space per candidate neighbor, and nevertheless, it is possible to access each coordinate in constant time.

In total, we need  $O(n^2d)$  space:  $O(d)$  space for each of the  $O(n^2)$  elements of  $F$ , which are represented explicitly; and  $O(1)$  space for each of the  $O(n^2d)$  candidates. We sort  $F$  plus the list of all candidates, using radix sort, in  $O(n^2d^2)$  time. This brings all elements with the same coordinates together, and allows us to eliminate duplicate or invalid candidates.<sup>5</sup> ◀

We mention that our algorithm actually *generates* all valid compositions within the same running time, in the sense that some procedure can *visit* every composition once, for example in order to collect some statistics. If one insists on producing an *explicit list* of all compositions, the storage requirement might increase to  $\Omega(d^2n^2)$ : By Theorem 11, there can be inputs with  $\Omega(dn^2)$  compositions, each requiring size  $\Theta(d)$  to write down.

## 6 Distribution and average in two dimensions

In this section, we present some empirical data concerning the interesting question of the *distribution* of  $\text{NC}(n_1, n_2)$ , the number of compositions of all pairs of polyominoes of sizes  $n_1, n_2$ .

Figure 10(a) shows with filled circles the distributions of the number of compositions of pairs of polyominoes of the same size. For each size up to  $n = 9$ , we took all pairs  $P_1, P_2$  of polyominoes of size  $n$  and counted the number of their compositions. For each number  $p$  of compositions, the graph shows the multiplicity with which  $p$  occurs, *i.e.*, the number of pairs  $(P_1, P_2)$  among the  $A(n)^2$  pairs that have  $p$  compositions, on a logarithmic scale. The points for a given size  $n$  are connected by a curve. In order to make the curves for different values of  $n$  comparable, we normalized the number  $p$  by subtracting the average number of compositions for size  $n$  (specified in the figure in parentheses). Thus, the horizontal axis is actually the deviation of  $p$  from the average. The averages are shown in Figure 10(b).

For polyominoes of size  $10 \leq n \leq 14$ , we sampled uniformly  $s = 5 \cdot 10^7$  out of all  $A(n)^2$  pairs because considering all pairs of polyominoes would be too time consuming. (The experiments reported here took about 10 days of CPU time.) The obtained results were multiplied by  $A(n)^2/s$  in order to get an estimate for the true multiplicities. These samples represent only a small fraction of all pairs: roughly  $1.7 \cdot 10^{-4}$  for  $n = 10$  and  $1.1 \cdot 10^{-8}$  for  $n = 14$ . Nevertheless, the estimates (shown with crosses in Figure 10(a)) appear visually consistent with the exact results, except that the sampling missed numbers of compositions with too few realizing pairs of polyominoes. The data were fitted to various discrete distributions, using the statistics module of the Python package `scipy`. The best fit was found with the negative-binomial distribution.

Figure 10(b) plots the average number of compositions of a pair of polyominoes of size  $n$ , as a function of  $n$ , and the vertical bars show the ranges of the numbers. The data suggest that the average value of  $\text{NC}(n, n)$  for two random polyominoes grows linearly with  $n$ . With the available data for  $3 \leq n \leq 14$  (considering the first two values as outliers), a linear regression gives the relation  $\text{NC}(n, n) \approx 2.19n + 4.97$ .

Similar patterns of distributions of the number of compositions are observed also for polyominoes of different sizes. In order not to clutter the figure, we show overlays of distributions of the number of compositions of pairs of polyominoes of the same total size. Figures 10(c–d) show the distributions of the number of compositions of pairs of polyominoes whose total size is 12 and 14, respectively. Again, each curve is normalized with respect to the average value which is specified in the figures in parentheses.

## 7 Conclusion

In this paper, we provide almost tight bounds on the minimum and maximum possible numbers of compositions of two polycubes in two and higher dimensions. While this goal is easy to achieve in three and higher dimensions, much more effort is needed in the two-dimensional case. We also provide an efficient algorithm for computing the number of compositions that two given polycubes have.

Future research directions include an estimation of the *average* number of composition

<sup>5</sup> In theory, one could combine the two phases, the generation of the elements of  $F$ , and of their neighbors, into one step without affecting the worst-case running time bound. In practice, however, eliminating duplications in  $F$  will reduce the number of elements that need to be considered in the second phase.

two polyominoes have. An efficient upper bound on this number may overcome the error in Ref. [3] and yield an upper bound on the growth constant of polyominoes.

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