On the Number of Compositions of Two Polycubes

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Abstract. We provide almost tight 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 $2n$, in two and higher dimensions. We also provide an efficient algorithm (with some trade-off between time and space) for computing the number of composition two given polyominoes (or polycubes) have.

Keywords: Lattice animals · Polyominoes · Polycubes · Compositions

1 Introduction

A d-dimensional *polycube* (*polyomino* if $d = 2$) is a connected set of cells on the cubical lattice $\mathbb{Z}^d$, where connectivity is through $(d-1)$-dimensional faces. Polycubes and "animals" of other lattices play for more than half a century an important role in enumerative combinatorics [4] as well as in statistical physics [3].

The *size* (volume, or area in the plane) of a polycube is the number of d-dimensional cells it contains. 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. The number of compositions of polycubes of certain sizes plays an important role in proving bounds on the growth constant of polycubes. For example, an incorrect upper

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bound on the maximum possible compositions of polyominoes [1] was used for claiming an erroneous upper bound on the growth constant of polyominoes. A corrected version of the argument [2] was used for obtaining an upper bound on the growth constant of polyiamonds (edge-connected sets of cells on the regular planar triangular lattice). The main question which we ask is:

Question 1: Given two polycubes **of total size $2n$**, how many different compositions (up to translations) do they have?

Alternatively, we can ask a similar question but in a more restricted setting:

Question 2: Given two polycubes, **each of size n**, how many different compositions (up to translations) do they have?

Obviously, the set of pairs of polycubes, each being of size n, is a subset of pairs of polycubes of total size $2n$. Hence, any lower (resp., upper) bound on the minimum (resp., maximum) number of compositions of polycubes in Question 1 also carries over to Question 2, and any upper (resp., lower) bound on the minimum (resp., maximum) number of compositions of polycubes 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. We summarize our results in Table 1.

Table 1. The number of compositions of two polycubes of total size $2n$.

Number of compositions	Two dimensions		$d \geq 3$ dimensions	
	Lower bound	Upper bound	Lower bound	Upper bound
Minimum	$\Theta(n^{1/2})$		$2n^{1-1/d}$	$O(2^d dn^{1-1/d})$
Maximum	$n^2/2^{O(\log^{1/2} n)}$	$O(n^2)$	$\Theta(dn^2)$	

We also provide an efficient algorithm for computing the number of composition two given polyominoes (or polycubes) have. A few possible implementations of the required data structures suggest a trade-off between the running time and the required memory.

2 Two Dimensions

2.1 Minimum Number of Compositions

Theorem 1
(i) Any pair of 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 ith 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. P_1 and P_2 can be composed in at most $2(2k_1 - 1 + 2k_2 - 1) = 4(2((n_1 + n_2)^{1/2} + 1) - 1) < 8(n_1 + n_2)^{1/2} + 4$ ways.

The following is a trivial corollary of Theorem 1.

Corollary 1. *Any pair of polyominoes of total size $2n$ 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 $\varepsilon > 0$.

Upper Bound

Observation 2. *Any pair of polyominoes of sizes n_1, n_2 has $O(n_1 n_2)$ compositions.*

Proof. Let n_1, n_2 be the sizes of polyominoes P_1, P_2, resp. Every cell of P_1 can touch every cell of P_2 in at most 4 ways, yielding $4n_1n_2$ as a trivial upper bound on the number of compositions.

Lower Bound

Theorem 3. *For every $n \geq 1$, there are two polyominoes, each of size at most n, that have at least $\frac{n^2}{2^{8 \cdot \sqrt{\log_2 n}}}$ compositions.*

The detailed proof of Theorem 3 is provided in the full version of the paper. In this extended abstract, we only note that the bound is obtained by a careful analysis of a construction of two "combs" whose first three levels are shown in Fig. 1.

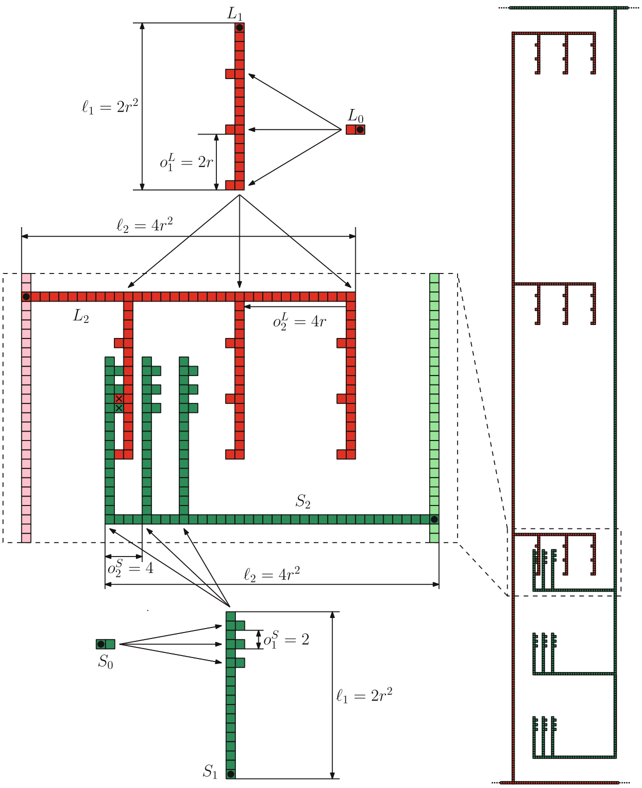

Fig. 1. A recursive construction of two "combs" for the proof of Theorem 3.

3 Higher Dimensions

3.1 Minimum Number of Compositions

Lower Bound

Theorem 4. *All pairs of d-dimensional polycubes of total size* $2n$ *have at least* $2n^{1-1/d}$ *compositions.*

Proof. The proof is similar to that of Theorem 1. Consider a pair of polycubes P_1, P_2 of total size $2n$. 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. Let V_i ($1 \leq i \leq d$) be the (d−1)-dimensional volume of the projection of P_1 orthogonal to the x_i axis. An isoperimetric inequality of Loomis and Whitney [5] ensures that $\prod_{i=1}^{d} V_i \geq n^{d-1}$. Let $V_k \geq n^{1-1/d}$ be largest among $V_1, \ldots, V_d$. Then, there are at least $2V_k \geq 2n^{1-1/d}$ different ways how P_2 may touch P_1. The polycube P_1 has V_k "columns" in the x_k direction. Pick one "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.

Upper Bound

Theorem 5. *There exist pairs of d-dimensional polycubes, of total size* $2n$*, that have* $O(2^d dn^{1-1/d})$ *compositions.*

Proof. Figure 2 shows a composition of two copies of a d-dimensional hypercube P of size $k \times k \times \ldots \times k$. The cube is made of n cells, hence, its sidelength is $k = n^{1/d}$. Two copies of P can slide towards each other in $2d$ directions until they touch. Obviously, there are no other compositions since no hypercube can penetrate into the bounding box of the other. 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. Overall, the total number of compositions in this example is $(2d)(2k-1)^{d-1} = 2d(2n^{1/d}-1)^{d-1} = \Theta(2^d dn^{1-1/d})$.

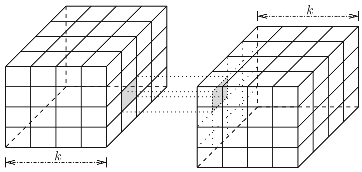

Fig. 2. A composition of two hypercubes

3.2 Maximum Number of Compositions in $d \geq 3$ Dimensions

Theorem 6. *Let* $d \geq 3$*. All pairs of d-dimensional polycubes of total size* $2n$ *have* $O(dn^2)$ *compositions. For* $d \geq 3$*, the upper bound is attainable: There exist pairs of 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 $n_1 = |P_1|$ and $n_2 = |P_2$, 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 an upper bound on the number of compositions.

The upper bound is attained asymptotically by two nonparallel "sticks" of size n, as shown in Fig. 3(a). Each stick has two *extreme* $(d-1)$-D facets (orthogonal to the direction of the stick), plus $2(d-1)n$ *middle* facets. The number of compositions that involve only middle facets is $2(d-2)n^2 = \Omega(dn^2)$, see Fig. 3(b): Indeed, for each of the $d-2$ directions which are not parallel to one of the sticks, there are $2n^2$ different choices for letting two middle facets of the sticks touch. We can ignore the $4n$ compositions that involve an extreme facet (see Fig. 3(c)).

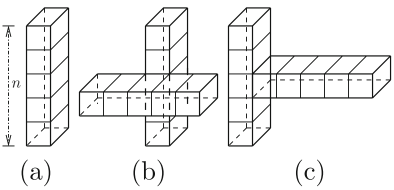

Fig. 3. Compositions of sticks

Note the difference, for the maximum number of compositions, between two and higher dimensions. In $d > 2$ dimensions, two of the dimensions (those along which the sticks in the proof of Theorem 6 are aligned) restrict the compositions of the sticks, but the existence of more dimensions allows every pair of cells, one of each polycube, to have compositions which manifest themselves through this pair only. This is not the case in two dimensions, a fact that makes the proof of Theorem 3 much more complicated.

4 Counting Compositions and Distribution Analysis

Finally, we refer to counting how many compositions a pair of polyominoes or polycubes have.

Theorem 7
(i) Given two polyominoes, each of size at most n, the number of compositions they have can be computed in $\Theta(n^2)$ time and $\Theta(n^2)$ space.
(ii) Given two d-dimensional polycubes, each of size at most n, the number of compositions they have can be computed in $O(d^2n^2)$ time and $O(dn^3)$ space, or $O(d^2n^2 \log n)$ time and $O(d^2n^2)$ space, or $O(d^2n^2)$ expected time and $O(d^2n^2)$ space.

We give the proof of Theorem 7 in the full version of the paper. The provided algorithms 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.

In the full version of the paper, we also present some empirical data concerning the *distribution* of $\text{NC}(n_1, n_2)$, the number of compositions of all pairs of polyominoes of sizes n_1, n_2. 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 $3 \leq n \leq 14$, a linear regression gives the relation $\text{NC}(n, n) \approx 2.19n + 4.97$. Available data of $\text{NC}(n_1, n_2)$, for several values of a constant $n_1 + n_2$, were fitted to various discrete distributions. The best fit was found with the negative-binomial distribution.

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