Automatic Proofs for Formulae Enumerating Proper Polycubes

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Abstract

This video describes a general framework for computing formulae enumerating polycubes of size n which are proper in $n-k$ dimensions (i.e., spanning all $n-k$ dimensions), for a fixed value of k. (Such formulae are central in the literature of statistical physics in the study of percolation processes and collapse of branched polymers.) The implemented software re-affirmed the already-proven formulae for $k \leq 3$, and proved rigorously, for the first time, the formula enumerating polycubes of size n that are proper in $n-4$ dimensions.

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1 Introduction

A d-dimensional polycube of size n is a connected set of n cubes in d dimensions, where connectivity is through $(d-1)$-dimensional faces. A polycube is said to be *proper* in d dimensions if the convex hull of the centers of its cubes is d-dimensional. Following Lunnon [8], let $\mathrm{DX}(n, d)$ denote the number of polycubes of size n that are proper in d dimensions.

Enumeration of polycubes and computing their asymptotic growth rate are important problems in combinatorics and discrete geometry, originating in statistical physics [5]. Polycubes (*polyominoes* in 2D) play a fundamental role in statistical physics in the analysis of percolation processes and collapse of branched polymers. To-date, no formula is known for $A_d(n)$, the number of polycubes of size n in d dimensions, for any value of d, let alone in the general case. The main interest in DX stems from the formula $A_d(n) = \sum_{i=0}^{d} \binom{d}{i} \mathrm{DX}(n, i)$ [8]. In a matrix listing the values of DX, the top-right triangular half and the main diagonal contain only 0s. This gives rise to the question of whether a pattern can be found in the sequences $\mathrm{DX}(n, n-k)$, where $k < n$ is the ordinal number of the diagonal.

Klarner [6] showed that the limit $\lambda_2 = \lim_{n\to\infty} \sqrt[n]{A_2(n)}$ exists. Much later Madras [10] proved the convergence of the sequence $(A_2(n+1)/A_2(n))_{n=1}^{\infty}$ to λ_2 (a similar claim holds in any dimension d). Thus, λ_2 is the *growth rate* limit of polyominoes. Its exact value has remained elusive till these days. The best known lower and upper bounds on λ_2 are roughly 4.0025 [2] and 4.6496 [7], respectively. Significant progress in estimating λ_d has been obtained in statistical physics, although the computations usually relied on unproven assumptions and on formulae for $\mathrm{DX}(n, n-k)$ interpolated empirically from known values of $A_d(n)$. Peard and Gaunt [12] predicted that for $k > 1$, the diagonal formula $\mathrm{DX}(n, n-k)$ has the pattern $2^{n-2k+1} n^{n-2k-1} (n-k) h_k(n)$, where $h_k(n)$ is a polynomial in n, and conjectured formulae for $h_k(n)$ for $k \leq 6$. Luther and Mertens [9] conjectured a formula for $k = 7$.

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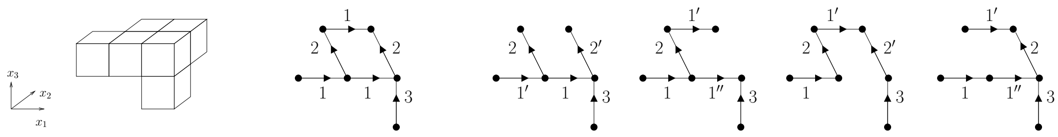

(a) Polycube (b) Adjacency graph (c) Four spanning trees

Figure 1 A polycube P, the corresponding graph $\gamma(P)$, and spanning trees of $\gamma(P)$.

It is easy to show that $\mathrm{DX}(n, n-1) = 2^{n-1}n^{n-3}$ (seq. A127670 in OEIS [11]). Barequet et al. [4] proved rigorously that $\mathrm{DX}(n, n-2) = 2^{n-3}n^{n-5}(n-2)(2n^2-6n+9)$ (seq. A171860). The proof uses a case analysis of the possible structures of spanning trees of the polycubes, and the various ways in which cycles can be formed in their cell-adjacency graphs. Similarly, Asinowski et al. [1] proved that $\mathrm{DX}(n, n-3) = 2^{n-6}n^{n-7}(n-3)(12n^5 - 104n^4 + 360n^3 - 679n^2 + 1122n - 1560)/3$, again, by counting spanning trees of polycubes, yet the reasoning and the calculations were significantly more involved. The inclusion-exclusion principle was applied in order to count correctly polycubes whose cell-adjacency graphs contained certain subgraphs, so-called “distinguished structures.” In comparison with $k = 2$, the number of such structures is substantially higher, and the ways in which they can appear in spanning trees are much more varied. The latter proof provided a better understanding of the difficulties that one would face in applying this technique to higher values of k. The number of distinguished structures grows rapidly, and their inclusion relations are much more complicated. As anticipated, it is impractical to achieve a similar proof manually for $k > 3$.

In this video we describe a theoretical set-up [3] for proving the formula for $\mathrm{DX}(n, n-k)$, for a fixed k. Using our implementation of this method, we could prove the following theorem.

▶ **Theorem 1.** $\mathrm{DX}(n, n-4) = 2^{n-7}n^{n-9}(n-4)(8n^8 - 128n^7 + 828n^6 - 2930n^5 + 7404n^4 - 17523n^3 + 41527n^2 - 114302n + 204960)/6$.

2 Method

Denote by $\mathcal{P}_n$ the set of polycubes of size n proper in $n-k$ dimensions. Let $P \in \mathcal{P}_n$, and let $\gamma(P)$ denote the directed edge-labeled graph that is constructed as follows: The vertices of $\gamma(P)$ correspond to the cells of P; two vertices of $\gamma(P)$ are connected by an edge if the corresponding cells of P are adjacent; and an edge has label i ($1 \leq i \leq n-k$) if the corresponding cells have different i-coordinate. The direction of the edge is from the lower to the higher cell (see Figure 1). Since $P \mapsto \gamma(P)$ is an injection, it suffices to count the graphs obtained from the members of $\mathcal{P}_n$ in this way. We count these graphs by counting their spanning trees. A spanning tree of $\gamma(P)$ has $n-1$ edges labeled by numbers from the set $\{1, 2, ..., n-k\}$; all these labels are present, otherwise the polycube is not proper in $n-k$ dimensions. Hence, $n-k$ edges of the spanning tree are labeled with the labels $1, 2, ..., n-k$, and the remaining $k-1$ edges are labeled with repeated labels from the same set. There is a bijection between the possibilities of repeated edge labels and the partitions of $k-1$. Specifically, each partition $p = \sum_{i=1}^{h} a_i \in \Pi(k-1)$ corresponds to h repeated labels in the spanning tree, such that the ith repeated label appears a_i+1 times. In such case, we say that the tree is *labeled according to p*. When we consider a spanning tree of $\gamma(P)$, we distinguish a repeated label i that appears r times by $i, i', ..., i'^{(r-1)}$. However, when considering $\gamma(P)$, repeated labels are assumed not to be distinguished. Every repeated label must occur an even number of times in any cycle of $\gamma(P)$. In addition, the number of cycles in $\gamma(P)$ and the length of each such cycle are bounded from above due to the limited multiplicity of labels.

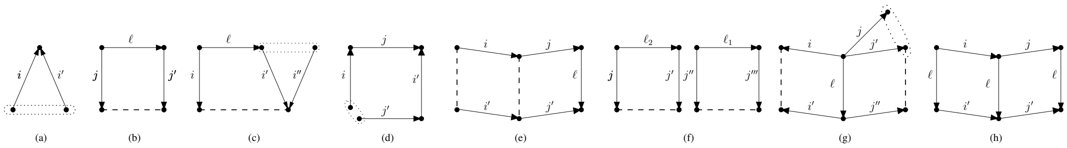

Figure 2 (a–g) A few distinguished structures for $k = 4$ (note that (f) is disconnected); (h) A cycle structure. A dotted line is drawn between every pair of neighboring cells and around every pair of coinciding cells.

In order to compute $|\mathcal{P}_n|$, we consider all possible directed edge-labeled trees of size n with edge labels as conjectured, and count only those that represent valid polycubes. In this process two things may happen:

(a) Cells may coincide (Figures 2(a,d)). A tree with overlapping cells is invalid; and (b) Two cells which are not connected by a tree edge may be adjacent (Figures 2(b,e)). Such a tree corresponds to a polycube P with cycles in $\gamma(P)$, hence, its spanning tree is not unique. In order to count correctly, we consider small structures (Figure 2), contained in these trees, which cause the problems above. The counting involves a delicate inclusion-exclusion analysis of the structures. See the video and [3] for more details.

3 The Video

The video illustrates the framework described above. First, it defines polycubes and explains what "proper polycubes" are. Then, it describes the importance of polycubes in combinatorics, discrete geometry, and statistical physics. The video then turns to defining DX$(n, n-k)$ and showing how it is computed automatically, using examples from the case $k = 4$. The video displays a few lemmas and formulas, defines *distinguished structures*, shows how they are generated, and explains the inclusion-exclusion graph built to obtain the sought formula. Finally, the video presents the results obtained by our program.

The video was produced on a 2.53GHz DELL 64 processor PC with 4GB of RAM. The animations were designed using the Autodesk Maya 2015 (student version) modeling software and Microsoft PowerPoint 2010. The video was constructed by Windows Live Movie Maker.

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