

Automatic Proofs for Formulae Enumerating Proper Polycubes

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Abstract

We develop a general framework for computing formulae enumerating polycubes of size n which are proper in $n-k$ dimensions (spanning all $n-k$ dimensions), for a fixed value of k . Besides the fundamental importance of knowing the number of these simple combinatorial objects, such formulae are central in the literature of statistical physics in the study of percolation processes and the collapse of branched polymers. We re-affirm the already-proven formulae for $k \leq 3$, and prove rigorously, for the first time, that the number of polycubes of size n that are proper in $n-4$ dimensions is $2^{n-7}n^{n-9}(n-4)(8n^8 - 128n^7 + 828n^6 - 2930n^5 + 7404n^4 - 17523n^3 + 41527n^2 - 114302n + 204960)/6$.

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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. Two *fixed* polycubes are considered distinct if they differ in their shapes or orientations. A polycube is called *proper* in d dimensions if the convex-hull of the centers of its cubes is d -dimensional. Following Lunnon [4], we let $DX(n, d)$ denote the number of fixed 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 [3], where they play a fundamental role in the analysis of percolation processes and the collapse of branched polymers. To-date, no formula is known for $A_d(n)$, the number of fixed polycubes of size n in d dimensions, for any fixed value of d . The main interest in DX stems from the fact that $A_d(n)$ can be easily computed using the formula $A_d(n) = \sum_{i=0}^d \binom{d}{i} DX(n, i)$ (Lunnon [4]). 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 $DX(n, n-k)$, where $k > 0$ is the ordinal number of the diagonal. Significant progress in estimating λ_d , the asymptotic growth rate of the number of polycubes in d dimensions, has been obtained in the literature of statistical physics, although the computations usually relied on unproven assumptions and on formulae for $DX(n, n-k)$ interpolated empirically from known values of $A_d(n)$. Peard and Gaunt [7] predicted that for $k > 1$, the diagonal formula $DX(n, n-k)$ 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 explicit formulae for $h_k(n)$ for $k \leq 6$. Luther and Mertens [5] conjectured a formula for $k = 7$.

It is easy to show that $DX(n, n-1) = 2^{n-1}n^{n-3}$ (seq. A127670 in [6]). Barequet et al. [2] proved for the first time that $DX(n, n-2) = 2^{n-3}n^{n-5}(n-2)(2n^2 - 6n + 9)$ (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 $DX(n, n-3) = 2^{n-6}n^{n-7}(n-3)(12n^5 - 104n^4 + 360n^3 - 679n^2 + 1122n - 1560)/3$, again, by counting spanning trees of polycubes, yet the reasoning and 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 the case $k=2$, the number of such structures is substantially higher, and the ways in which they can appear in spanning trees

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