Proper n-cell Polycubes in $n - k$ Dimensions

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Abstract

In this paper we develop a theoretical framework for computing the explicit formula enumerating polycubes with n cubes that span $n-k$ dimensions, for a fixed k and variable n. Besides the fundamental importance of knowing the number of these simple combinatorial objects, known as proper polycubes, such formulae are central in the literature of statistical physics in the study of percolation processes and collapse of branched polymers. We use this framework to prove the known, yet unproven conjecture about the general form of the formula for a varying k, and implement a computer program which reaffirmed the known formulae for $k = 2$ and $k = 3$, and proved rigorously, for the first time, the formulae for $k = 4$ and $k = 5$.

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 the same if one can be obtained by a translation of the other. We consider here only fixed polycubes, so we will omit this adjective throughout the paper. 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 [16], we let $\mathrm{DX}(n, d)$ denote the number of fixed polycubes of size n that are proper in d dimensions. Similarly, we denote by $\mathrm{DT}(n, d)$ the number of fixed *tree* polycubes (polycubes whose cell-adjacency graph is a tree) of size n which are proper in d dimensions. Despite the simplicity of their definition, computing the functions $\mathrm{DX}(n, d)$ and $\mathrm{DT}(n, d)$ has shown to be an extremely difficult task.

Enumeration of polycubes and computing their asymptotic growth rate are important problems in combinatorics and discrete geometry, originating in statistical physics [9]. While in the mathematical literature these objects are called polycubes (*polyominoes* in two dimensions), they are usually referred to as *lattice animals* in the literature of statistical physics, where they play a fundamental role in the analysis of percolation processes and 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, let alone in the general case. Counting polyominoes is a long-standing problem. The number of polyominoes, $A_2(n)$, is currently known up to $n = 56$ [12]. Tabulations of counts of polycubes in higher dimensions appear in the mathematics literature [1, 15, 16] as well as in the statistical-physics literature [10, 11, 19]. The main interest in the function DX stems from the fact that $A_d(n)$ can be easily computed using the formula

$$A_d(n) = \sum_{i=0}^{d} \binom{d}{i} \mathrm{DX}(n, i)$$

given originally by Lunnon [16]. The formula is proved by noting that every proper i-dimensional polycube can be embedded in the d-dimensional space in exactly $\binom{d}{i}$ different ways (according to the choice of dimensions for the polycube to occupy). Also, if $n \le d$, the polycube simply cannot occupy all the dimensions (since a polycube of size n can occupy at most $n - 1$ dimensions), and so $\mathrm{DX}(n, d) = 0$ in this case. Hence, 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. Obviously, if a simple formula is found for $\mathrm{DX}(n, n - k)$ for every k, this will yield a simple formula for $A_d(n)$ (using Lunnon's formula). Lunnon's formula has been widely used in the statistical-physics literature on lattice animals, and is called a "partition formula," where the partition is usually according to a few more parameters (attributes of the polycubes). The earliest references for this, that we are aware of, are from the 1960s.

The growth-rate limit of polycubes has also attracted much attention in the literature. Klarner [13] showed in a seminal work the existence of the limit $\lambda_2 = \lim_{n\to\infty} \sqrt[n]{A_2(n)}$. Only 32 years later, Madras [18] proved the

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convergence of the sequence $(A_2(n+1)/A_2(n))_{n=1}^{\infty}$ to λ_2, the *growth rate* limit of polyominoes (also known as *Kalrner's constant* or the *growth constant* of polyominoes). The exact value of λ_2 has remained elusive till these days. The currently best known lower and upper bounds on λ_2 are roughly 4.0025 [7] and 4.5685 [5], respectively. In fact, this leading decimal digit of λ was revealed [7] quite recently, after remaining illusive for over 50 years. In $d > 2$ dimensions, λ_d, the growth constant of the number of d-dimensional polycubes, also exists [18]. It was proven [8] that $\lambda_d = 2ed - o(d)$; moreover, λ_d was estimated $(2d-3)e + O(1/d)$. In [2] it was shown that λ_d^T, the growth constant of *tree* polycubes is also $2ed - o(d)$, and was estimated at $(2d - 3.5)e + O(1/d)$.

Significant progress in estimating λ_d has been obtained along the years in the literature of statistical physics, although the computations usually relied on unproven assumptions and on formulae for $\mathrm{DX}(n, n-k)$ which were interpolated empirically from known values of $A_d(n)$.

Peard and Gaunt [21] predicted that the diagonal formula $\mathrm{DX}(n, n-k)$ has the pattern $2^{n-2k+1}n^{n-2k-1}g_k(n)$ (for $k > 1$), where $g_k(n)$ is a polynomial in n. In fact, k has to be a root of $g_k(n)$ since $\mathrm{DX}(n, 0) = 0$ for $n > 1$. Therefore, the expected form is $2^{n-2k+1}n^{n-2k-1}(n-k)h_k(n)$, where $h_k(n)$ is a polynomial in n, and explicit formulae for $h_k(n)$ for $k \le 6$ were conjectured [21]. Luther and Mertens [17] later conjectured a formula for $k = 7$. After a careful inspection of the polynomials, which revealed that the leading coefficient of $h_k(n)$ has the form $2^{k-1}/(k-1)!$, Asinowski et. al. [3] refined the conjectured formula to

$$\mathrm{DX}(n, n-k) = \frac{2^{n-k}n^{n-2k-1}(n-k)}{(k-1)!}P_c(n),$$

where $P_c(n)$ is a monic polynomial in n. It has also been conjectured [8, 17] that the degree of $P_c(n)$ is $3k-4$. In this paper, we prove this refined conjecture rigorously.

Using Cayley trees, it can be shown (see, e.g. [8]) that

$$\mathrm{DX}(n, n-1) = 2^{n-1}n^{n-3}$$

(sequence A127670 in The Online Encyclopedia of Integer Sequences [20]). Barequet et al. [8] proved rigorously, for the first time, that

$$\mathrm{DX}(n, n-2) = 2^{n-3}n^{n-5}(n-2)(2n^2 - 6n + 9)$$

(sequence 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. [3] proved that

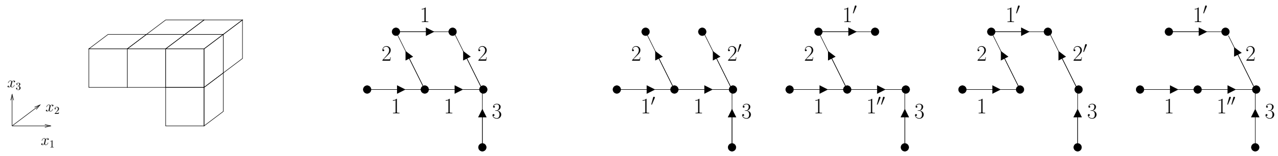
$$\mathrm{DX}(n, n-3) = 2^{n-6}n^{n-7}(n-3)(12n^5 - 104n^4 + 360n^3 - 679n^2 + 1122n - 1560)/3$$

again, by counting spanning trees of polycubes, yet the reasoning and the calculations were significantly more involved. The inclusion-exclusion principle was applied in the proof 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 for $k = 3$ 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, the inclusion relations between them are much more complicated, and the ways in which they will be connected by forests are much more varied. This will yield a large number of terms in the inclusion-exclusion analysis. As anticipated [3], carrying this approach beyond k=3 would create a case analysis beyond the patience of a human, making it totally impractical to manually achieve a similar proof for $k > 3$.

In this paper we create a theoretical set-up for proving the formula for $\mathrm{DX}(n, n-k)$, for a fixed value of k. Our method *fully automates* the manual method presented in [8, 3], allowing the case analysis to be made by a computer. For this nontrivial generalization we prove a few key observations about polycubes that are proper in $n-k$ dimensions. We also provide a general characterization of distinguished structures, and design algorithms that produce, analyze, and enumerate them automatically, even for complex structures, forests, and cycles that do not appear in the case k=3. Using our implementation of this method, we find the explicit formula (which has never been proven before) for $\mathrm{DT}(n, n-4)$, $\mathrm{DX}(n, n-4)$, $\mathrm{DT}(n, n-5)$ and $\mathrm{DX}(n, n-5)$, stated in the following theorems.

Theorem 1 $\mathrm{DT}(n, n-4) = 2^{n-7}n^{n-9}(n-4)(8n^8 - 140n^7 + 1010n^6 - 3913n^5 + 9201n^4 - 15662n^3 + 34500n^2 - 120552n + 221760)/6$.

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



(a) Polycube P (b) Adjacency graph $\gamma(P)$ (c) The spanning trees of $\gamma(P)$

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

Theorem 3 $\mathrm{DT}(n, n-5) = 2^{n-9}n^{n-11}(n-5)(240n^{11} - 6480n^{10} + 73640n^9 - 461232n^8 + 1778615n^7 - 4707195n^6 + 11632070n^5 - 41919528n^4 + 158857920n^3 - 483329520n^2 + 1481660640n - 2863123200)/360.$

Theorem 4 $\mathrm{DX}(n, n-5)2^{n-12}n^{n-11}(n-5)(240n^{11} - 6000n^{10} + 62240n^9 - 356232n^8 + 1335320n^7 - 4062240n^6 + 12397445n^5 - 42322743n^4 + 150403080n^3 - 535510740n^2 + 1923269040n - 3731495040)$

2 Definitions and Notations

Integer Partition. A partition of a positive integer m is a way of writing m as the sum of one or more positive integers, i.e., $m = \sum_i a_i$. Two sums that differ only in the order of their summands are considered the same, and so we choose the canonic representation of a partition to be the list of its summands in nondecreasing order. Let $\Pi(m)$ denote the set of all the partitions of the positive integer m. For example, there are two partitions of the integer 2 and three partitions of the integer 3: $\Pi(2) = \{1 + 1, 2\}$ and $\Pi(3) = \{1 + 1 + 1, 1 + 2, 3\}$. For a partition p, we denote by $|p|$ the number of summands in p, and by $p[i]$ the ith summand of p. Also, we let $p_{sum} = \sum_{i=1}^{|p|} p[i]$ denote the sum of the elements of p and $\pi(p)$ denote the number of essentially-different permutations of the summands of p. For example, $\pi(1, 1, 1) = 1$, and $\pi(1, 2) = 2$ (there are two different permutations of its summands: $1, 2$ and $2, 1$). When p_1 and p_2 are two partitions, we will say that p_1 contains p_2, denoting this relation by $p_2 \preceq p_1$, if there is a subpartition p_1^* of p_1 (an ordered subset of the elements of p_1), such that $|p_1^*| = |p_2|$ and $p_2[i] \leq p_1^*[i]$ for all $1 \leq i \leq |p_2|$. For example, $2 \preceq 1 + 2$, but $2 \not\preceq 1 + 1 + 1$.

Graph Isomorphism. Let $G = (V_G, E_G)$ and $H = (V_H, E_H)$ be two directed edge-labeled graphs with respective edge labels W_G and W_H, such that $|V_G| \leq |V_H|$. G is said to be *isomorphic* to H if there is a bijection $f : V_G \to V_H$ such that

- If for $u, v \in V_G$, $(u, v) \in E_G$, then $(f(u), f(v)) \in E_H$; and
- If for $e_1 = (u_1, v_1), e_2 = (u_2, v_2) \in E_G$, the labels of e_1 and e_2 are equal, then the labels of $(f(u_1), f(v_1))$ and $(f(u_2), f(v_2))$ are equal.

An automorphism of G is a form of symmetry in which G is mapped into itself while preserving the conditions above.

3 Overview of the Method

Denote by $\mathcal{P}_n$ the set of proper polycubes of size n in $n-k$ dimensions. (The value of k is fixed, therefore we omit it from the notation.) 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; an edge has label i $(1 \leq i \leq n - k)$ if the corresponding cells have different i-coordinate (their common $(d - 1)$-dimensional face is perpendicular to the x_i axis); The direction of the edge is from the lower to the higher cell. (with respect to the x_i direction.) See Figure 1 for an example.

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 shall 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 because the polycube is 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. Observation 6 characterizes all the different possibilities of repeated edge-labels in the spanning tree of a proper polycube.

Observation 5 *Let i be a positive integer, and let $p \in \Pi(i)$ be a partition of i. Let $p_r = i + |p|$. Then, $i+1 \le p_r \le 2i$. This follows from the fact that $1 \le |p| \le i$.*

Observation 6 *There is a bijection between the possibilities of repeated edge-labels and the partitions of the integer $k-1$. Specifically, each partition $p = \sum_{i=1}^{|p|} a_i \in \Pi(k-1)$ corresponds to the possibility of having $|p|$ different repeated labels in the spanning tree (and p_r repeated labels in total), such that the i^{th} repeated label appears a_i+1 times. In such case, we will say that the tree is* labeled according to p.

Observation 7 *Every label must occur an even number of times in any cycle of $\gamma(P)$.*

A clear consequence of Observation 6 is that a tree can have at most $2(k-1)$ repeated edge labels, in such case the repeated labels appear in $k-1$ pairs. 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.

In order to compute $|\mathcal{P}_n|$, we consider all the possible directed edge-labeled trees of size n with edge labels as observed, and count only those that represent valid polycubes. In the next section we characterize all substructures that are present in some of these trees due to the fact that the number of cells is greater than the number of dimensions. By analyzing these substructures, we will be able to compute how many of these trees actually represent polycubes. Then, we develop formulae for the numbers of all possible spanning trees of the polycubes, and then derive the actual number of polycubes.

3.1 Counting

Lemma 8 *[3, Lemma 7] [8, Lemma 2] The number of directed trees with n vertices and $n-1$ distinct edge labels $1, ..., n-1$ is $2^{n-1}n^{n-3}$, for $n \ge 2$.*

Our approach is to count polycubes by enumerating spanning trees of their adjacency graphs. In order to apply Lemma 8 to counting spanning trees of polycubes, we shall distinguished between the repeated labels in a tree. As explained in the previous chapter, a spanning tree T of $\gamma(P)$, for a polycube $P \in \mathcal{P}_n$, must be labeled according to some partition $p \in \Pi(k-1)$. Let us then denote by $\ell_1, \dots \ell_{|p|}$ the repeated labels of T such that ℓ_i appears $p[i]$ times in T. We will distinguish between the edges of T labeled with ℓ_i by relabeling them with the labels $\ell_i, \ell_i', ..., {\ell_i}'^{(p[i]-1)}$ (see, e.g. Figure 1 (c)). However, in $\gamma(P)$, the repeated labels are not distinguished. The trees that can be obtained by exchanging (permuting) $\ell_i, \ell_i', \dots, \ell_i'^{(p[i])}$ (for every ℓ_i), are, in fact, also spanning trees of $\gamma(P)$.

As a result, after enumerating all the spanning trees that correspond to valid polycubes, every polycubes will be represented by exactly $\prod_{j=1}^{|p|}(p[j]\,!)$ spanning trees. Therefore, dealing with the multiplicity in the counting caused by distinguishing the repeated labels will be straightforward.

Let, then, T_p denote the number of directed trees with n vertices that are labeled according to $p \in \Pi(k-1)$. Recall again that repeated labels in trees are distinguished.

Corollary 9 $T_p = \pi(p)\binom{n-k}{|p|}2^{n-1}n^{n-3}$.

3.2 Distinguished Structures

3.3 Generation

In the reasoning below we shall consider several small structures, which may be contained in the spanning trees that we count. These structures are interesting for the following reason. For each directed edge-labeled tree, we can attempt to build its corresponding polycube. Two things may happen:

(a) Cells may coincide (Figures 2(a,d)). A tree with overlapping cells is invalid and does not correspond to a valid polycube; 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 which has cycles in its cell-adjacency graph, and therefore, its spanning tree is not unique.

Similarly to Observation 7, for every label on the path between two vertices that correspond to coinciding cells, repetitions of this label occur an even number of times on this path, and a structure that leads to a non-existing adjacency results in an (even) cycle with one edge removed.

In order to count correctly, we will consider several small structures, contained in the trees we count, which cause the problems above. Following [3], we will refer to such structures as *distinguished structure*. A *distinguished*

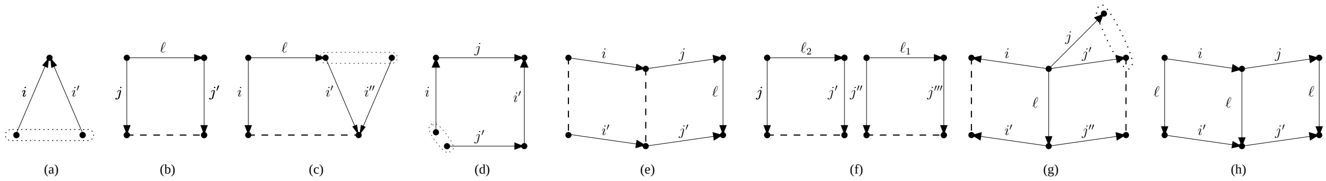


Figure 2: (a–f) A few distinguished structures for $k = 4$ (note that (f) is disconnected); (g) A cycle structure. A dotted line is drawn between every pair of neighboring cells and around every pair of coinciding cells.

structure is a subtree that is "responsible" for the presence of two coinciding or adjacent cells, as explained above. More precisely, a distinguished structure is the union of all paths (edges and incident vertices) that run between two coinciding or adjacent cells. Every such path uses up some repeated labels. Therefore, the number of their occurrences in the trees that we count is limited. The enumeration of the distinguished structures is, thus, a finite task.

Let $\mathcal{DS}_k$ denote the set of distinguished structures in $n{-}k$ dimensions. The above characterization of distinguished structures allows for the design of an algorithm for producing $\mathcal{DS}_k$. We hereafter refer to the *size* of a tree as the number of its vertices. The algorithm begins with generating all "free trees" (non-isomorphic trees) of size bound from above by $3k-2$, the value specified in Lemma **??** (In fact, this bound is only needed for the implementation in software in order to set a limit to the computation.) Then, it labels every free tree T of size t according to every partition $p \in \cup_{i=1}^{k-1}\Pi(i)$ so as to obtain a directed edge-labeled tree T'. and then checking whether T' contains coinciding or neighboring cells by a simple depth-first traversal that starts from an arbitrary node and assigns every other node its appropriate coordinate. If such cells are found, T' is added to $\mathcal{DS}_k$ if it is *not* isomorphic to any structure $\sigma \in \mathcal{DS}_k$ of size t, and at least one of the following conditions holds:

1. T' contains two coinciding or neighboring cells which are connected by a path of length $t{-}1$ (see, e.g., Figures 2(a,b,d,e));

2. T' is isomorphic to the union of $d_1, ..., d_m \in \mathcal{DS}_k$, such that the isomorphic copies of $d_1, ..., d_m$ in T' cover all its edges (see, e.g., Figures 2(c,g)).

It may happen that a distinguished structure is disconnected. Disconnected distinguished structures (see Fig. 2(f)) are generated by checking if every collection of edge-connected structures in $\mathcal{DS}_k$ yields a single disconnected structure labeled according to some $p \in \cup_{i=1}^{k-1}\Pi(i)$.

Lemma 10 *Let $\sigma^* \in \mathcal{DS}_k$ be a distinguished structure of size n^* that is composed of k^* connected components, and labeled according to $p^* \in \cup_{i=2}^{k-1}\Pi(i)$. Then, $p_r^* \le n^* - k^* \le p_r^* + p_{sum}^*$.*

Proof. The first inequality $n^* - k^* \ge p_r^*$ states that the number of edges in σ^* is at least the number of repeated labels implied by the partition p^*. In fact, this condition is necessary for p^* to label σ^*. The second inequality is true since it may happen that σ^* contain edges labeled with *unique* labels (labels each on which appears only once in σ^*), besides the p_r^* edges labeled with the p_r^* repeated labels. The number of unique labels in σ^* is bounded by p_{sum}^* because every repeated label ℓ_i (with repetition $p^*[i] + 1$) can add at most $p^*[i]$ unique edge labels to σ^*.

□

3.3.1 Enumeration

Let us now turn to the enumeration of occurrences (i.e. isomorphic copies) of distinguished structures in directed trees with edge labels as explained earlier.

Lemma 11 *Let σ be a distinguished structure composed of $k^* \ge 1$ trees $s_1, ..., s_{k^*}$ with a total of n^* vertices and distinct edge labels $1, ..., n^* - k^*$. The number of occurrences of σ in trees of size n with distinct edge labels $1, ..., n-1$ is*

$$F_n(\sigma) = (\textstyle\prod_{i=1}^{k^*} |s_i|)\frac{(n-n^*+k^*-1)!}{(n-n^*)!} n^{n-n^*+k^*-2}.$$

Proof. We proceed by double counting, enumerating in two ways the different sequences of directed edges that can be added to a graph composed of the union of $n{-}n^*$ vertices and the distinguished structure σ, so as to form a rooted tree with n vertices.

One way to count these sequences is to add the edges one by one, and to count the number of options available at each step. There are $\mathcal{N} = \prod_{i=1}^{k^*} |s_i|$ possibilities to choose a root for each component s_i of σ. In the beginning, we have a forest with $n{-}n^*{+}k^*$ rooted trees. After adding a collection of edges, forming a rooted forest with i trees, there are $n(i-1)$ choices for the next edge to add: Its starting vertex can be any one of the n vertices of the graph, and its ending vertex can be any one of the $i{-}1$ roots other than the root of the tree containing the starting vertex. Therefore, the total number of choices is

$$\mathcal{N} \prod_{i=2}^{n-n^*+k^*} n(i-1) = \mathcal{N} n^{n-n^*+k^*-1}(n-n^*+k^*-1)!. \tag{1}$$

An alternative way to count these edge sequences is to start with one of the $F_n(S)$ possible unrooted edge-labeled trees which contains σ, choose one of its n vertices as a root, and choose one of the $(n{-}n^*)!$ possible sequences, say, η, then label the $(n{-}n^*)$ vertices of the tree according to η (the vertices that do not belong to σ), and "shift" each vertex-label to the incident edge towards the root, producing an edge-labeled tree. The total number of sequences that can be formed this way is

$$nF_n(\sigma)(n-n^*)!. \tag{2}$$

Finally, we conclude from Equations (1) and (2) that the number of occurrences of σ in unrooted trees with edge labels $1, ..., n-1$ is

$$F_n(\sigma) = \mathcal{N}\frac{(n-n^*+k^*-1)!}{(n-n^*)!} n^{n-n^*+k^*-2}. \tag{3}$$

□

Let now $\mathcal{F}_n(\sigma)$ denote the number of occurrences of σ in *directed* edge-labeled trees of size n.

Corollary 12 $\mathcal{F}_n(\sigma) = 2^{n-n^*+k^*-1}F_n(\sigma)$.

Let $\sigma^* \in \mathcal{DS}_k$ be a distinguished structure labeled according to $p^* \in \cup_{i=1}^{k-1}\Pi(i)$. Let us denote by $\mathcal{O}_p(\sigma^*)$ the number of occurrences of σ^* in directed trees of size n that are labeled according to $p \in \Pi(k-1)$.

Observation 13 *If $p^* \not\preceq p$, then $O_p(\sigma^*) = 0$.*

There are .. steps to compute $\mathcal{O}_p(\sigma^*)$:

- Choosing the $|p|$ repeated labels of the tree out of the possible $n{-}k$ labels.
- Choosing the $|p^*|$ repeated labels of σ^* out of the $|p|$ repeated labels of the tree.
- Choosing the unique labels of σ^* (e.g. the label ℓ in structures (b,c,e,g) in Figure 2) if there are any.
- Calculate the number of essentially-different structures that can be produced out of all the $\prod_{j=1}^{|p^*|}(p^*[j]!)$ possible configurations of the repeated labels of σ^*. For example, for structure (a) in Figure 2, all the configurations yield the same structure, whereas for structure (b) (Figure 2), there are two essentially-different structures. In the first one, the label i is attached to the head of the edge labeled ℓ, and in the second one, i' is attached to its head. For structure (c) (Figure 2), there are six different structures, shown in Figure 3. This number can be obtained by computing the number of symmetries (automorphisms) of σ^*.
- Finally, multiplying by $\mathcal{F}_n(\sigma^*)$ completes the calculation of $\mathcal{O}_p(\sigma^*)$.

Two detailed examples are given in Appendix A.

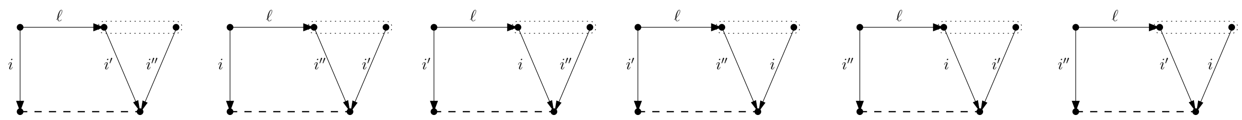


Figure 3: The six different configurations of structure (c).

4 Inclusion-Exclusion Graph

When counting the occurrences of a distinguished structure $\sigma \in \mathcal{DS}_k$, other distinguished structures which contain multiple occurrences of σ are counted multiple times. Obviously, if a distinguished structure σ_b contains c occurrences of a smaller structure σ_s, then when counting the occurrences of σ_s, σ_b is accounted for c times. The inclusion-exclusion principle is applied to eliminate this dependency between the different structures; In order to obtain the number of *trees* that contain σ as a subtree (using the quantity $\mathcal{O}_p(\sigma)$), we build an inclusion-exclusion graph $\mathrm{IE} = (\mathcal{V}, \mathcal{E})$. This graph contains a vertex corresponding to each structure $\sigma \in \mathcal{DS}_k$. There is an edge $e = \sigma_1 \to \sigma_2$ labeled with c if σ_1 contains c occurrences of σ_2. Hence, the roots $\mathcal{R} = \{v \in \mathcal{V} : I(v) = \emptyset\}$ of the IE graph are all the structures that are not contained in any other structure; in a sense, those are the "big" structures. Figure 4 shows a subgraph of the IE graph for $k = 4$.

Let $\ell(e)$ denote the label of the edge e, $h(\sigma)$ denote the length of the longest path from σ to a root of the IE graph, and $I(\sigma_2) = \{\sigma_1 \in \mathcal{V} : (\sigma_1, \sigma_2) \in \mathcal{E}\}$. Let us denote by $T_p(\sigma)$ the number of trees of size n labeled according to $p \in \Pi(k-1)$ that contain σ but no $\sigma' \in I(\sigma)$ as a subtree.

Lemma 14 $T_p(\sigma) = \mathcal{O}_p(\sigma) - \sum_{\sigma' \in I(\sigma)} \ell((\sigma', \sigma)) T_p(\sigma')$.

Proof. By Induction on $h(\sigma)$.

- The roots of the IE graph $\sigma \in \mathcal{R}$, for which $h(\sigma) = 0$, represent distinguished structures that are not contained in any other structure. Therefore, for any $p \in \Pi(k-1)$, the number of trees that contain σ as a subtree equals the number of occurrences of σ in directed trees labeled according to p. Thus, $T_p(\sigma) = \mathcal{O}_p(\sigma)$.
- Induction Hypothesis: Assume that the claim is correct for vertices of height $h < h_0$.
- Induction Step: Let $\sigma \in \mathcal{V}$ be at height h_0 ($h(\sigma) = h_0$). Let $\sigma' \in I(\sigma)$. The trees that contain σ' as a subtree are counted $\ell((\sigma', \sigma))T_p(\sigma')$ times in $\mathcal{O}_p(\sigma)$. Therefore, subtracting $\ell((\sigma', \sigma))T_p(\sigma')$ from $\mathcal{O}_p(\sigma)$ excludes all the trees that contain σ' as a subtree. Thus, $T_p(\sigma) = \mathcal{O}_p(\sigma) - \sum_{\sigma' \in I(\sigma)} \ell((\sigma', \sigma))T_p(\sigma')$.

□

A simple bottom-up procedure traverses the graph IE, implementing the equation in Lemma (14), and computes, for every structure $\sigma \in \mathcal{V}$, the number of directed edge-labeled trees that contain only $s(u)$ as a subtree.

5 Counting Polycubes

Proper tree polycubes are polycubes $P \in \mathcal{P}_n$ for which $\gamma(P)$ is a tree. The rest of the polycubes $P' \in \mathcal{P}_n$ are non-tree polycubes for which $\gamma(P')$ contains cycles.

5.1 Trees

Every tree polycube gives rise to a unique spanning tree. For every possibility of repeated labels $p \in \Pi(k-1)$, let $\mathrm{DT}_p(n)$ denote the number of proper tree polycubes such that the their corresponding (unique) spanning trees are labeled according to p. By Corollary 9, the total number of directed trees with n vertices that are labeled according to p is T_p. Every such tree corresponds to a tree polycube in $\mathcal{P}_n$ unless it contains a distinguished structure as a subtree. (Indeed, it can neither contain a distinguished structure that has coinciding cells because the latter is illegal, nor can it contain a distinguished structure that has neighboring cells since it is a tree). Therefore, all the trees that contain a distinguished structure as a subtree must be excluded. Hence, we have

$$\mathrm{DT}(n, n-k) = \sum_{p \in \Pi(k-1)} \mathrm{DT}_p(n) = \sum_{p \in \Pi(k-1)} \frac{T_p - \sum_{\sigma \in \mathcal{DS}_k} T_p(\sigma)}{\prod_{j=1}^{|p|} p[j]!} \tag{4}$$

The division by $\prod_{j=1}^{|p_i|}(p_i[j]!)$ is because each tree polycube is counted that many times, as discussed earlier.

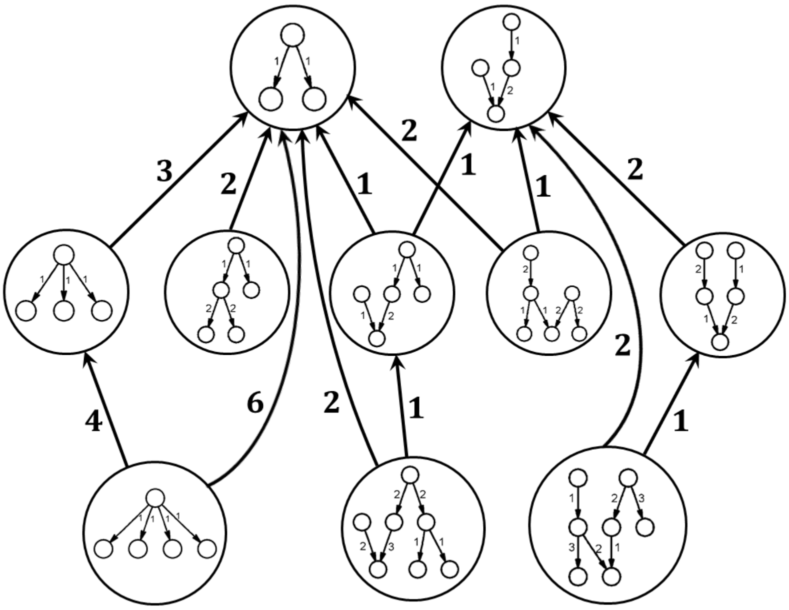


Figure 4: A snapshot of the IE graph for $k = 4$.

5.2 Nontrees

Let $\sigma \in \mathcal{DS}_k$ be a distinguished structure which contains only adjacent cells and no coinciding cells. Let σ_c denote the graph that is constructed by adding to σ all the missing cycle-edges between every pair of adjacent cells. σ_c is a *cycle structure*, or, in short, a *cycle*. For example, the distinguished structure shown in Figure 2(e) is a spanning tree of the cycle shown in Figure 2(h). Two cycle structures c_1 and c_2 are considered distinct if either c_1 is not isomorphic to c_2, or c_2 is not isomorphic to c_1. Let $\mathcal{C}$ denote the set of all cycle structures of polycubes in $\mathcal{P}_n$. $\mathcal{C}$ can be found using $\mathcal{DS}_k$ as described. Note that two different distinguished structures may be spanning trees of the same cycle structure. For every cycle structure $\mathcal{C}_i \in \mathcal{C}$, let $P_{\mathcal{C}_i}$ denote the number of polycubes $P \in \mathcal{P}_n$ that contain $\mathcal{C}_i$ in their cell-adjacency graph $\gamma(P)$. Suppose that a distinguished structure $\sigma \in \mathcal{DS}_k$ has c occurrences in $\mathcal{C}_i$. Then, we have that

$$P_{\mathcal{C}_i} = \sum_{p \in \Pi(k-1)} \frac{T_p(\sigma)}{c \prod_{j=1}^{|p|} p[j]!}. \tag{5}$$

This follows from the definition of $T_p(\sigma)$. Finally, we reach the desired formula.

$$\mathrm{DX}(n, n-k) = \mathrm{DT}(n, n-k) + \sum_{i=1}^{|\mathcal{C}|} P_{\mathcal{C}_i}. \tag{6}$$

Theorem 15 *The general pattern of* $\mathrm{DX}(n, n-k)$*, for a fixed* $k > 0$*, is* $\frac{2^{n-k}}{(k-1)!} n^{n-2k-1}(n-k)P_{3k-4}(n)$*, where* $P_c(n)$ *is a monic polynomial in* n *of order* c*.*

Proof. From the discussion in Sections 3 and 4 about the terms of the inclusion-exclusion formula and equations (4), (5) and (6), we conclude that for any $p \in \Pi(k-1)$, by corollary 9, the degree of T_p is at least $n-3$, and that the highest degree of n, namely, $n+k-4$, is contributed by $T_{(2,2,...,2)} = \binom{n-k}{k-1} n^{n-3} 2^{n-1}$: the case in which there are $k-1$ pairs of repeated edge-labels, corresponding to the partition $p = (1, 1, ..., 1) \in \Pi(k-1)$. The degrees of n contributed by $T_{p'}$ by all the other partitions $p' \in \Pi(k-1)$ are smaller than $n+k-4$.

Now let $\sigma^* \in \mathcal{DS}_k$ be a distinguished structure of size n^*, composed of k^* connected components, and labeled according to some partition $p^* \in \cup_{i=1}^{k-1} \Pi(i)$. Let u^* denote the number of unique labels in σ^*. We prove that the degree of n in $\mathcal{O}_p(\sigma^*)$, for any partition $p \in \Pi(k-1)$ for which $p^* \preceq p$, is bounded by $n-2k-1$ from bellow and by $n+k-5$ from above. As a result, since $T_p(\sigma^*)$ consists of linear combinations of $\mathcal{O}_p(\sigma^*)$ and $\mathcal{O}_p(\sigma')$ for other structures $\sigma' \in \mathcal{DS}_k$ (where the constants a_i of the linear combination are a function of k), the degree of n in $T_p(\sigma^*)$ is also bounded by $n-2k-1$ from bellow and by $n+k-5$ from above.

The degree of n in $\mathcal{O}_p(\sigma^*)$ is contributed by the following three factors:

- $\binom{n-k}{|p|}$: This factor corresponds to choosing $|p|$ repeated labels, and clearly contributes $|p|$ powers of n to $\mathcal{O}_p(\sigma^*)$.
- $\mathcal{F}_n(\sigma^*)$: The degree of n contributed by $\mathcal{F}_n(\sigma^*)$ is $n-n^*+2k^*-3$ (Equation (3)).
- u^*: These u^* unique labels must be different from the $|p^*|$ repeated labels in σ^*, and naturally, the degree of n contributed by their choice can be at most u^*.

Upper bound Therefore, the degree of n is bounded from above by the sum of the three factors above: $n-n^*+2k^*-3+u^*+|p|$. We now prove that $n-n^*+2k^*-3+u^*+|p| \leq n+k-5$:

1. By Lemma 10, $n^*-k^* \geq p_r^*$. Moreover, $n^*-k^* = p_r^*+u^*$, since clearly, the number of edges in σ^* (n^*-k^*) equals the total number of edge-labels in it $(p_r^*+u^*)$.
2. $|p| \leq k-1$.

Therefore, $n-n^*+2k^*-3+u^*+|p| \leq_2 n-n^*+2k^*+u^*+k-4$. To show that $n-n^*+2k^*+u^*+k-4 \leq n+k-5$, it is enough to show that $-n^*+2k^*+u^* \leq -1$. Multiplying this inequality by -1 we obtain $n^*-2k^*-u^* \geq 1$. $n^*-2k^*-u^* \geq_1 p_r^*+u^*-k^*-u^* = p_r^*-k^*$. We now claim that indeed $p_r^*-k^* \geq 1$. This is because every connected component in σ^* must have at least one pair of coinciding or neighboring cells, and to have such cells every connected component must have at least two repeated labels, implying that the difference between p_r^* (the total number of repeated labels in σ^*) and k^* (the number of connected components of σ^*), is bounded from bellow by 1.

Lower bound Now to show that the degree of n in $\mathcal{O}_p(\sigma^*)$ is bounded from bellow by $n-2k-1$, we prove that the degree contributed by the first two factors, namely, $|p|+n-n^*+2k^*-3$, is at least $n-2k-1$:

1. By Lemma 10, $n^*-k^* \leq |p^*|+2p_{sum}^*+1$.
2. Since $p^* \preceq p$, $|p^*|+2p_{sum}^* \leq |p|+2p_{sum} = |p|+2(k-1)$.

As a result, $n^*-k^* \leq_{1,2} |p|+2(k-1)+1$. Multiplying by -1 we get $|p|-n^*+k^* \geq -2k+1$. Therefore, $|p|+n-n^*+k^*-3 \geq n-2k-2$, and since $k^* \geq 1$, $|p|+n-n^*+2k^*-3 \geq n-2k-1$.

In Equation (4), $T_{(2,2,\ldots,2)}$ is divided by 2^{k-1} $(\prod_{j=1}^{|k-1|} 2)$. Thus, the coefficient of the highest order of n is $\frac{2^{n-k}}{(k-1)!}$. Hence, we obtain a global formula of the form $\frac{2^{n-k}}{(k-1)!}(n^{n+k-4}+\cdots+cn^{n-2k})$, where c is some integer coefficient. We can now factor out the quantity n^{n-2k-1} to obtain a formula of the form $\frac{2^{n-k}}{(k-1)!}n^{n-2k-1}P_{3k-3}(n)$. Finally, k must be a root of $\mathrm{DX}(n, n-k)$ since a polycube of size $n=k$ cannot span $n-k=0$ dimensions (unless $n=k=1$). Factoring out $n-k$ yields the claimed pattern. □

Note that $3k-3$ known values of $\mathrm{DX}(n, n-k)$ (for a specific value of k), including the two trivial values $\mathrm{DX}(k, 0)=0$ and $\mathrm{DX}(k+1, 1)=1$, suffice for interpolating uniquely $P_{3k-4}(n)$. However, a "physical" argument (see [17]) implies that as little as k values suffice for interpolating the polynomial. [1] In a nutshell, this argument is based on the unproven assumption that the "free energy" $(\log \mathrm{CX}(n,d))/n$ has a well-defined $1/d$-expansion whose coefficients depend on n and are bounded when n tends to infinity. Then, the powers of n in the terms of the expansion are tuned so as to avoid the explosion of the terms, therby imposing constraints which allow only k values of $\mathrm{DX}(n, n-k)$ to imply the general formula.

6 Results

The method outlined in the proceeding sections was implemented in a parallel C++ program, using *Wolfram Mathematica* to simplify the final formulae. All the calculations were performed on a supercomputer with 132 GB of RAM and 20 processors. [2] Our results, summarized in the tables bellow, agree completely with the formulae conjectured in the literature of statistical physics. The program produced data files which document the entire computation, serving as proofs of the formulae. This completes the proof of Theorems **??**.

[1]The cited reference actually claims that $k+1$ values are needed, not taking into account that k is a root of the polynomial (except in the first diagonal formula).

[2]The results reported in our EuroComb 2015 paper were obtained by running the program on a different computer, and thus the difference in the reported runtimes.

$k=3$	
$\lvert\mathcal{DS}_3\rvert$	147
$\lvert\mathcal{C}_3\rvert$	13
$\mathrm{DT}_{(2,2)}(n)$	$2^{n-6}n^{n-7}(n-3)(n-4)(4n^4-28n^3+97n^2-200n+300)$
$\mathrm{DT}_3(n)$	$2^{n-3}n^{n-7}(n-3)(2n^2-21n^3+106n^2-282n+360)/3$
$\mathrm{DT}(n,n-3)$	$2^{n-3}n^{n-7}(n-3)(2n^4-21n^3+106n^2-282n+360)/3$
$\sum_{i=1}^{13} P_{\mathcal{C}_i}$	$2^{n-6}n^{n-7}(n-3)(n-4)(4n^3-17n^2+11n+70)$
$\mathrm{DX}(n,n-3)$	$2^{n-6}n^{n-7}(n-3)(12n^5-104n^4+360n^3-679n^2+1122n-1560)/3$

$k=4$	
$\lvert\mathcal{DS}_4\rvert$	8397
$\lvert\mathcal{C}_4\rvert$	179
$\mathrm{DT}_{(2,2,2)}(n)$	$2^{n-7}n^{n-9}(n-4)(n-5)(n-6)(8n^6-84n^5+438n^4-1543n^3+4236n^2-9020n+19040)/6$
$\mathrm{DT}_{2,3}(n)$	$2^{n-4}n^{n-9}(n-4)(n-5)(4n^6-56n^5+383n^4-1654n^3+5106n^2-10920n+14112)/6$
$\mathrm{DT}_4(n)$	$2^{n-5}n^{n-9}(n-4)(4n^6-84n^5+851n^4-5191n^3+20190n^2-47552n+53760)/6$
$\mathrm{DT}(n,n-4)$	$2^{n-7}n^{n-9}(n-4)(8n^8-140n^7+1010n^6-3913n^5+9201n^4-15662n^3+34500n^2-120552n+221760)/6$
$\sum_{i=0}^{178} P_{\mathcal{C}_i}$	$2^{n-7}n^{n-9}(n-4)(n-5)(12n^6-122n^5+373n^4+68n^3-1521n^2-578n+3360)/6$
$\mathrm{DX}(n,n-4)$	$2^{n-7}n^{n-9}(n-4)(8n^8-128n^7+828n^6-2930n^5+7404n^4-17523n^3+41527n^2-114302n+204960)/6$

$k=5$	
$\lvert\mathcal{DS}_5\rvert$	652060
$\lvert\mathcal{C}_5\rvert$	3680
$\mathrm{DT}_{(2,2,2,2)}(n)$	$2^{n-12}n^{n-11}\prod_{i=5}^{8}(n-i)(16n^8-224n^7+1560n^6-7544n^5+29089n^4-98032n^3+319752n^2-819200n+2324880)/3$
$\mathrm{DT}_{(2,2,3)}(n)$	$2^{n-8}n^{n-11}\prod_{i=5}^{7}(n-i)(8n^8-140n^7+1206n^6-6917n^5+30322n^4-107966n^3+333720n^2-816696n+1321920)/3$
$\mathrm{DT}_{(3,3)}(n)$	$2^{n-7}n^{n-11}\prod_{i=5}^{6}(n-i)(8n^8-168n^7+1730n^6-11736n^5+59912n^4-238071n^3+722025n^2-1517688n+1814400)/9$
$\mathrm{DT}_{(2,4)}(n)$	$2^{n-8}n^{n-11}\prod_{i=5}^{6}(n-i)(8n^8-196n^7+2338n^6-17731n^5+95521n^4-384154n^3+1161728n^2-2462976n+2903040)/3$
$\mathrm{DT}_{(5)}(n)$	$2^{n-6}n^{n-11}(n-5)(4n^8-140n^7+2375n^6-25215n^5+183076n^4-932080n^3+3256940n^2-7149000n+7560000)/15$
$\mathrm{DT}(n,n-5)$	$2^{n-9}n^{n-11}(n-5)(240n^{11}-6480n^{10}+73640n^9-461232n^8+1778615n^7-4707195n^6+11632070n^5-41919528n^4+158857920n^3-483329520n^2+1481660640n-2863123200)/360$
$\sum_{i=0}^{3679} P_{\mathcal{C}_i}$	$2^{n-12}n^{n-11}(n-5)(n-6)(32n^9-568n^8+3592n^7-8001n^6-5009n^5+20971n^4+98945n^3+30014n^2-3298664n+9648576)/3$
$\mathrm{DX}(n,n-5)$	$2^{n-12}n^{n-11}(n-5)(240n^{11}-6000n^{10}+62240n^9-356232n^8+1335320n^7-4062240n^6+12397445n^5-42322743n^4+150403080n^3-535510740n^2+1923269040n-3731495040)$

Figure 5: Results for $k=3,4,5$.

7 Conclusion

In this paper we present a theoretical setup and an automatic tool for computing the diagonal formula $\mathrm{DX}(n, n-k)$ for any fixed $k > 0$. Using this setup, we prove the known conjecture about the form of $\mathrm{DX}(n, n-k)$ for a general constant k. As k grows, the number of distinguished structures grows, and the complexity of the calculations grows as well. We implemented the entire method so that the formulae are obtained completely automatically. As a byproduct, our software also provides a full *proof* of the formula: A complete listing of all structures, all the intermediate computation, a full description of the inclusion-exclusion relations between the structures, and a detailed account of all the calculations. We applied our method to the cases $k \leq 5$, reaffirming the known formulae for $k = 2, 3$ and proving rigorously the conjectured formulae for $\mathrm{DX}(n, n-4)$ and $\mathrm{DX}(n, n-5)$. Running the program for higher values of k is possible and might be part of future work. However, given that already for $k = 5$, the number of distinguished structures surpasses half a million, we do not believe that it will be feasible to go above $k = 7$.

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A Computing $\mathcal{O}_p(\sigma)$: Examples

We demonstrate the computation of $\mathcal{O}_p(\sigma)$ with two of the structures shown in Figure 2. The first structure, σ_1, is the one shown in Figure 2(c). The structure σ_1 is labeled according to $(3) \in \Pi(2)$. Therefore, it may appear in trees labeled according to $(2,3),(4) \in \Pi(3)$, but not according to $(2,2,2) \in \Pi(3)$ since $(3) \not\preceq (2,2,2)$. Let us detail the computation of $\mathcal{O}_{(2,3)}(\sigma_1)$. First, there are $\binom{n-4}{2}$ options to choose the two repeated (and distinguished) labels ℓ_1, ℓ_2 in the tree. We multiply by $\pi((2,3)) = 2$ (either $\ell_1, \ell_1', \ell_2, \ell_2', \ell_2''$ or $\ell_1, \ell_1', \ell_1'', \ell_2, \ell_2'$). The label i that is repeated three times in σ_1 is determined uniquely. Assume that i is assigned the label ℓ_1. There are $n-4$ options to choose the label ℓ; it is different from $\ell_1, \ell_1', \ell_1''$ but may be equal to ℓ_2 or ℓ_2'. There are three options to choose which label of $\ell_1, \ell_1', \ell_1''$ is attached to the head of ℓ, then two possibilities to choose the label that is attached to the tail of ℓ. This number is calculated from the number of automorphisms of σ_1. To complete the computation of $\mathcal{O}_{(2,3)}(\sigma_1)$, we multiply by $\mathcal{F}_n(\sigma_1)$. The second structure, σ_2, is the one shown in Figure 2(d). The structure σ_2 is labeled according to the partition $(2,2) \in \Pi(2)$. Hence, it may appear in trees labeled according to $(2,2,2)$, $(2,3) \in \Pi(3)$, but not according to $(4) \in \Pi(3)$ since $(2,2) \not\preceq (4)$. For computing $O_{(2,2,2)}(\sigma_2)$, there are $\binom{n-4}{3}$ options to choose the three repeated labels in the tree. This yields the labels $\ell_1, \ell_1', \ell_2, \ell_2', \ell_3, \ell_3'$ (note that $\pi((2,2,2)) = 1$). Then, there are $\binom{3}{2}$ options to choose the repeated labels i, j. Assume that the chosen labels are ℓ_1 and ℓ_2. Note the symmetry in this structure: It does not matter if i is assigned the label ℓ_1 and j is assigned the label ℓ_2, or vice versa, since the two options yield the same structure. Again, the number of symmetries of σ_2 is calculated from the number of its automorphisms and the computation is completed by multiplying by $\mathcal{F}_n(\sigma_2)$.