Enumeration and Asymptotic Formulas for Rectangular Partitions of the Hypercube

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Abstract

We study a two-parameter generalization of the Catalan numbers: $C_{d,p}(n)$ is the number of ways to subdivide the d-dimensional hypercube into n rectangular blocks using orthogonal partitions of fixed arity p. Bremner & Dotsenko [14] introduced $C_{d,p}(n)$ in their work on Boardman–Vogt tensor products of operads; they used homological algebra to prove a recursive formula and a functional equation. We express $C_{d,p}(n)$ as simple finite sums, and determine their growth rate and asymptotic behaviour. We give an elementary proof of the functional equation, using a bijection between hypercube decompositions and a family of full p-ary trees. Our results generalize the well-known correspondence between Catalan numbers and full binary trees.

1 Introduction

1.1 Catalan numbers

The (binary) Catalan numbers form a well-known and ubiquitous integer sequence[1]:

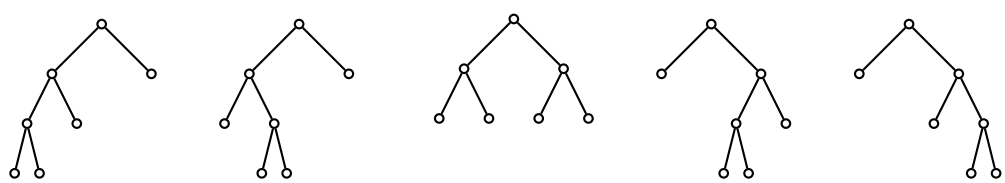
$$C(n) = \frac{1}{n}\binom{2n-2}{n-1} \qquad (n \geq 1).$$

These numbers have over 200 different combinatorial interpretations; see Stanley [47] and sequence A000108 from the Online Encyclopedia of Integer Sequences (OEIS) [45]. We focus on the following three:

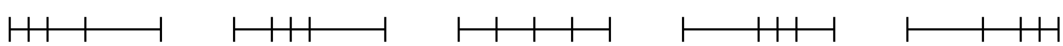
(i) Given a set with a binary operation, $C(n)$ counts the ways to parenthesize a sequence with $n-1$ operations and n factors. For example, the $C(4) = 5$ ways to parenthesize a product with 4 factors using 3 operations are as follows:

$$(((ab)c)d), \qquad ((a(bc))d), \qquad ((ab)(cd)), \qquad (a((bc)d)), \qquad (a(b(cd))).$$

(ii) $C(n)$ counts the plane rooted binary trees with $n-1$ internal nodes (including the root) and n leaves, assuming that every internal node has two children. For example, the $C(4) = 5$ rooted full binary trees with 4 leaves and 3 internal nodes are as follows:



(iii) $C(n)$ counts the dyadic partitions of the unit interval obtained by $n-1$ bisections into n subintervals [20, 21]. For example, the $C(4) = 5$ ways to partition the unit interval into 4 subintervals using 3 bisections are as follows:



If we write y for the generating function of $C(n)$,

$$y = \sum_{n\geq 1} C(n)x^n = x + x^2 + 2x^3 + 5x^4 + 14x^5 + 42x^6 + 132x^7 + 429x^8 + \cdots,$$

then one can check that y satisfies the functional equation

$$x + y^2 = y. \tag{1}$$

[1]We index these numbers starting at $n = 1$ rather than the more conventional $n = 0$ for reasons that will become apparent in the later sections.

1.2 Geometry of higher-dimensional Catalan numbers

We study a higher-dimensional generalization of the Catalan numbers, which we first describe in terms of subdividing the d-dimensional open unit hypercube using a sequence of p-ary partitions, generalizing interpretation (iii) for the ordinary Catalan numbers.

Definition 1. Fix a dimension $d \geq 1$. Consider an open d-rectangle in the open unit d-cube:

$$R = (a_1, b_1) \times \cdots \times (a_d, b_d) \subseteq (0,1)^d.$$

Fix an arity $p \geq 2$. For a fixed index $1 \leq i \leq d$, partition the i^{th} interval in the Cartesian product into p equal subintervals with endpoints

$$c_i(j) = a_i + \frac{j}{p}(b_i - a_i) \qquad (0 \leq j \leq p).$$

We define the *p-ary decomposition of R orthogonal to the i^{th} coordinate axis* to be

$$H_i(R) = \left\{ (a_1, b_1) \times \cdots \times \big(c_i(j-1), c_i(j)\big) \times \cdots \times (a_d, b_d) \mid 1 \leq j \leq p \right\}.$$

Fix an integer $m \geq 0$ and set $S_0 = \{(0,1)^d\}$. For $k = 1, \ldots, m$ perform these steps:

1. Choose an element $R \in S_{k-1}$.
2. Choose a direction $1 \leq i \leq d$.
3. Set $S_k = \big(S_{k-1} \setminus \{R\}\big) \cup H_i(R)$.

The result S_m is called a *(d,p,n)-decomposition*; by this we mean a p-ary decomposition of the unit d-cube into the disjoint union of n blocks (d-subrectangles) where $n = 1 + m(p-1)$. We define $C_{d,p}(n)$ to be the number of distinct (d,p,n)-decompositions.

Figure 1 illustrates all $(2,2,n)$-decompositions for $n \leq 4$. From the diagrams, we see that $C_{2,2}(n) = 1, 2, 8, 39$ for $n = 1, 2, 3, 4$ respectively.

For fixed d, p and n, the natural action of the d-dimensional hyperoctahedral group [7, 51] on the unit d-cube sends one (d,p,n)-decomposition to another; hence this group has a permutation representation on the set of all (d,p,n)-decompositions.

Observe that in the case of $d = 1$, $p = 2$ and $n \geq 1$, Definition 1 reduces to subdividing the unit interval into n subintervals using bisections. Thus, $C_{1,2}(n) = C(n)$ gives the ordinary Catalan numbers. More generally, $C_{1,p}(n)$ gives the p-ary Catalan numbers [6, 34]:

$$C_{1,p}(n) = \frac{1}{n} \binom{n-1}{\frac{n-1}{p-1}} \qquad (n \geq 1).$$

Thus $C_{d,p}(n)$ is a two-parameter generalization of the Catalan numbers, analogous in some ways to the Fuss–Catalan numbers (also known as Raney numbers). For several other higher-dimensional generalizations of the Catalan numbers, see [16, 30, 33, 36, 38].

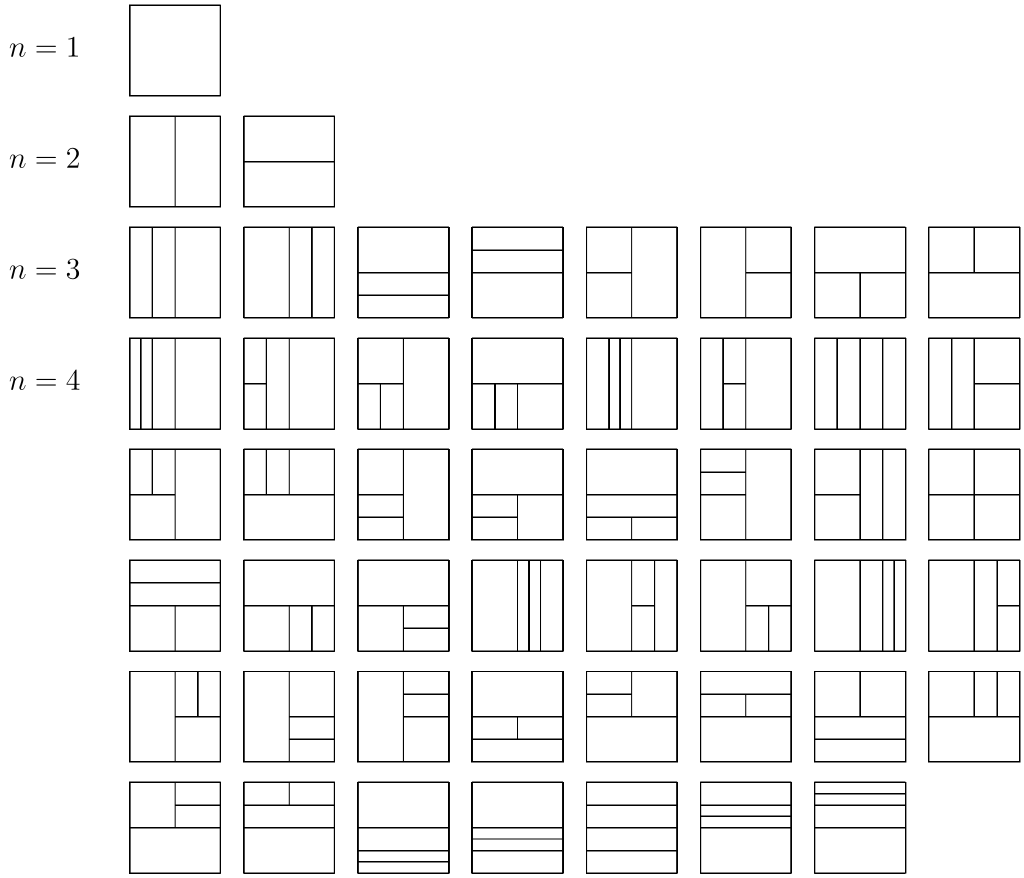


Figure 1: Partitions of the unit square into $n \leq 4$ subrectangles using bisections

1.3 Interchange laws for operations of higher arity

We provide another interpretation of $C_{d,p}(n)$ using d distinct p-ary operations (denoted by d operation symbols or by d types of parentheses), generalizing interpretation (i) of the ordinary Catalan numbers.

Definition 2. Fix integers $d \geq 1$ (*dimension*) and $p \geq 2$ (*arity*). Let S be a set and fix operations $f_1, \ldots, f_d \colon S^p \to S$. Let $A = (a_{ij})$ be a $p \times p$ array of elements of S. If f_k, f_ℓ are two of the operations, then we may either apply f_k to each row of A and then apply f_ℓ to the results, or apply f_ℓ to each column of A and then apply f_k to the results. If for every array A both ways produce the same element of S,

$$\begin{aligned} &f_\ell\big(f_k(a_{11}, \ldots, a_{1p}),\, f_k(a_{21}, \ldots, a_{2p}),\, \ldots,\, f_k(a_{p1}, \ldots, a_{pp}) \big) = \\ &f_k\big(f_\ell(a_{11}, \ldots, a_{p1}),\, f_\ell(a_{12}, \ldots, a_{p2}),\, \ldots,\, f_\ell(a_{1p}, \ldots, a_{pp}) \big), \end{aligned} \tag{2}$$

then we say that f_k and f_ℓ satisfy the *interchange law*. If equation (2) holds for every pair of distinct operations then we have an *interchange system* of arity p and dimension d.

In universal algebra (resp. algebraic operads), interchange systems were introduced in the early 1960s by Evans [27] (resp. in the early 1970s by Boardman and Vogt [12]). In the case of $d = p = 2$, two binary operations satisfying the interchange law first appeared in the late 1950s in Godement's *five rules of functorial calculus* [32, Appendix 1, (V)].

If we denote the two binary operations by $(--)$ and $\{--\}$, then the interchange law can be restated as

$$\{\,(a_{11}\,a_{12})\,(a_{21}\,a_{22})\,\} = (\,\{a_{11}\,a_{21}\}\,\{a_{12}\,a_{22}\}\,).$$

Observe that the operations trade places and the arguments a_{12}, a_{21} transpose. The interchange laws correspond naturally to the hypercube decompositions defined in Section 1.2: If we regard $(--)$ and $\{--\}$ respectively as vertical and horizontal bisections of rectangles in $\mathbb{R}^2$, then the interchange law expresses the equivalence of the two ways of partitioning a square into four equal subsquares:

$$\{\,(a_{11}\,a_{12})\,(a_{21}\,a_{22})\,\} \;=\; \begin{array}{|c|c|}\hline a_{11} & a_{12} \\ \hline \end{array} \atop \begin{array}{|c|c|}\hline a_{21} & a_{22} \\ \hline \end{array} \;=\; \begin{array}{|c|c|}\hline a_{11} & a_{12} \\ \hline a_{21} & a_{22} \\ \hline \end{array} \;=\; \begin{array}{|c|}\hline a_{11} \\ \hline a_{21} \\ \hline \end{array}\;\begin{array}{|c|}\hline a_{12} \\ \hline a_{22} \\ \hline \end{array} \;=\; (\,\{a_{11}\,a_{21}\}\,\{a_{12}\,a_{22}\}\,).$$

For further information on algebraic operads and higher categories, see [8, 9, 10, 15, 22, 37, 42, 43, 44, 48].

Using the Boardman–Vogt tensor product of operads, Bremner and Dotsenko [14] showed that this correspondence between interchange laws and hypercube partitions extends to arbitrary arity p and dimension d, in which case f_i $(i = 1, \ldots, d)$ corresponds to the H_i operation of Definition 1 (the dissection of a d-dimensional subrectangle into p equal parts by hyperplanes orthogonal to the i^{th} coordinate axis). They also proved the following result.

Theorem 3 ([14], §3.1)**.** *Define the generating function*

$$y = y_{d,p}(x) = \sum_{n \geq 0} C_{d,p}(n) x^n.$$

Then y satisfies this polynomial functional equation[2]*:*

$$\sum_{k=0}^{d} (-1)^k \binom{d}{k} y^{p^k} = x. \tag{3}$$

For $d = 1$ and $p = 2$, equation (3) reduces to equation (1), the functional equation for the ordinary Catalan numbers. One can derive from (3) this recursive formula:

$$C_{d,p}(n) = \sum_{k=1}^{d} \left((-1)^{k-1} \binom{d}{k} \sum_{\substack{n_1, \ldots, n_{p^k} \geq 1 \\ n_1 + \cdots + n_{p^k} = n}} \prod_{i=1}^{p^k} C_{d,p}(n_i) \right).$$

[2]The alternating sign was inadvertently omitted in [14].

One may also regard $C_{d,p}(n)$ as the number of association types [26] (or placements of parentheses and operation symbols) of degree n in higher-dimensional algebra [17, 18, 19] with d operations of arity p. Similar (but inequivalent) constructions in the literature include guillotine partitions, VLSI floorplans, and planar rectangulations [1, 2, 3, 4, 5, 23, 35, 41, 46].

1.4 Outline of this paper

In Section 2, we use Lagrange inversion to prove a simple closed formula (a finite sum) for $C_{d,p}(n)$ and then consider several special cases. In Section 3, we use analytic methods to determine the asymptotic behaviour of $C_{d,p}(n)$. In Section 4, we show that $C_{d,p}(n)$ counts a restricted set of p-ary trees, generalizing interpretation (ii) of the ordinary Catalan numbers. In particular, we establish a bijection between these trees and hypercube decompositions, and give a combinatorial proof (without homological algebra) that the generating function satisfies the functional equation (3); this provides a elementary proof of Theorem 3. In Section 5, we indicate how our results may also be understood from the point of view of Gröbner bases for shuffle operads. In Section 6, we briefly indicate some directions for further research.

2 Enumeration formulas

We first derive a summation formula for $C_{d,p}(n)$ and then discuss special cases for small values of d and p. We use the functional equation (3) to obtain our closed formula.

Theorem 4. *For all integers $d \geq 1$, $p \geq 2$, and $n \geq 1$ we have*

$$C_{d,p}(n) = \frac{1}{n} \sum_{t_1,\dots,t_d} \left[\binom{n-1+t_1+\cdots+t_d}{n-1,\, t_1,\, t_2,\, \dots,\, t_d} \prod_{k=1}^{d} \left((-1)^{t_k(k+1)} \binom{d}{k}^{t_k} \right) \right],$$

where the sum is over all integers $t_1, \dots, t_d \geq 0$ such that

$$\sum_{k=1}^{d} t_k(p^k - 1) = n-1.$$

Proof. We may rearrange the functional equation (3) to obtain $y = x\phi(y)$ where

$$\phi(y) = \left(\sum_{k=0}^{d} (-1)^k \binom{d}{k} y^{p^k-1} \right)^{-1}.$$

Since $\phi(y)$ can be expanded as a formal power series in y with nonzero constant term, we apply Lagrange inversion [31] to obtain

$$[x^n]y = \frac{1}{n}[y^{n-1}]\big(\phi(y)^n\big) = \frac{1}{n}[y^{n-1}] \left(\sum_{k=0}^{d} (-1)^k \binom{d}{k} y^{p^k-1} \right)^{-n},$$

where $[x^n]y$ denotes the coefficient of x^n in the power series y. If we expand the factor with the negative exponent and simplify the result then we obtain

$$\begin{aligned}
\phi(y)^n &= \sum_{j\geq 0}\binom{n-1+j}{j}\left(\sum_{k=1}^{d}(-1)^{k+1}\binom{d}{k}y^{p^k-1}\right)^j \\
&= \sum_{j\geq 0}\binom{n-1+j}{j}\sum_{\substack{t_1,\ldots,t_d\geq 0\\ t_1+\cdots+t_d=j}}\left[\binom{j}{t_1,t_2,\ldots,t_d}\prod_{k=1}^{d}\left((-1)^{t_k(k+1)}\binom{d}{k}^{t_k}y^{t_k(p^k-1)}\right)\right] \\
&= \sum_{t_1,\ldots,t_d\geq 0}\left[\binom{n-1+\sum_{i=1}^{d}t_i}{n-1,t_1,t_2,\ldots,t_d}\prod_{k=1}^{d}\left((-1)^{t_k(k+1)}\binom{d}{k}^{t_k}y^{t_k(p^k-1)}\right)\right].
\end{aligned}$$

In the last step we used the equation $\sum_{k=1}^{d} t_k = j$ to eliminate j, and then used the obvious combinatorial identity

$$\binom{n-1+j}{j}\binom{j}{t_1,\ldots,t_d} = \binom{n-1+j}{n-1,t_1,\ldots,t_d}.$$

The term of interest y^{n-1} occurs if and only if

$$\sum_{k=1}^{d} t_k(p^k-1) = n-1,$$

which completes the proof. ∎

Theorem 4 implies simple closed formulas for $C_{d,p}(n)$ for small d and p. We consider three specific instances: $(d,p) = (2,2), (3,2), (2,3)$.

Corollary 5. *The number of dyadic partitions of the unit square into n rectangles is*

$$C_{2,2}(n) = \frac{1}{n}\sum_{i=0}^{\lfloor\frac{n-1}{3}\rfloor}\binom{2(n-1-i)}{n-1,\ n-1-3i,\ i}(-1)^i\,2^{n-1-3i}.$$

Proof. For $d = p = 2$, Theorem 4 gives

$$C_{2,2}(n) = \frac{1}{n}\sum_{\substack{t_1,\,t_2\geq 0\\ t_1+3t_2=n-1}}\binom{n-1+t_1+t_2}{n-1,\ t_1,\ t_2}(-1)^{t_2}\,2^{t_1}. \tag{4}$$

If we set $t_2 = i$ then $t_1 = n-1-3i$, and the sum (4) is empty when $n-1-3i < 0 \iff i > \frac{n-1}{3}$. Hence (4) simplifies to the stated result. ∎

We believe this is the first explicit non-recursive formula for sequence A236339:

1, 2, 8, 39, 212, 1232, 7492, 47082, 303336, 1992826, 13299624, 89912992, ...

Remark 6. For $d = p = 2$, the functional equation (3) simplifies to the quartic polynomial $y^4 - 2y^2 + y = x$, to which one may apply Cardano's formula [49, §8.8] in order to solve explicitly for y as a function of x. Indeed, let ρ be a primitive cube root of unity and set

$$A^{\pm} = \sqrt[3]{72x - \tfrac{11}{2} \pm \tfrac{3}{2}\sqrt{768x^3 + 1536x^2 - 96x - 15}}\,,$$
$$\theta_1 = \tfrac{1}{3}(\,A^+ + A^-\,), \quad \theta_2 = \tfrac{1}{3}(\,\rho^2 A^+ + \rho A^-\,), \quad \theta_3 = \tfrac{1}{3}(\,\rho A^+ + \rho^2 A^-\,).$$

The four roots of the quartic polynomial may then be expressed as

$$y = \tfrac{1}{2}\Big(\delta\sqrt{-\theta_1} + \epsilon\sqrt{-\theta_2} + \delta\epsilon\sqrt{-\theta_3}\,\Big),$$

where $\delta, \epsilon \in \{\pm 1\}$. Only for $\delta = 1$, $\epsilon = -1$ does the power series expansion of y have constant term 1. However, computing the other coefficients of this power series seems rather difficult.

Corollary 7. *The number of dyadic partitions of the unit cube into n subrectangles is*

$$C_{3,2}(n) = \frac{1}{n}\sum_{j=0}^{\lfloor\frac{n-1}{7}\rfloor}\sum_{i=0}^{\lfloor\frac{n-1-7j}{3}\rfloor}\binom{2(n-1-i-3j)}{n-1,\, n-1-3i-7j,\, i,\, j}(-1)^i\, 3^{n-1-2i-7j}.$$

Proof. Similar to the proof of Corollary 5. For $d = 3$, $p = 2$ Theorem 4 gives

$$C_{3,2}(n) = \frac{1}{n}\sum_{\substack{t_1,t_2,t_3\geq 0\\ t_1+3t_2+7t_3=n-1}}\binom{n-1+t_1+t_2+t_3}{n-1,\ t_1,\ t_2,\ t_3}(-1)^{t_2}\, 3^{t_1+t_2}. \tag{5}$$

If we set $t_2 = i$, $t_3 = j$ then $t_1 = n-1-3i-7j$, and the sum (5) is empty for $n-1-3i-7j < 0$. Hence we may restrict the summation indices to $0 \leq j \leq \frac{n-1}{7}$ and $0 \leq i \leq \frac{n-1-7j}{3}$, and so (5) simplifies to the stated result. □

This gives an explicit non-recursive formula for the sequence A236342:

1, 3, 18, 132, 1080, 9450, 86544, 819154, 7949532, 78671736, 790930728, ...

For $p = 2$ and $4 \leq d \leq 10$ see sequences A237019 to A237025 and A237018.

Remark 8. For $d = 3$, $p = 2$, the functional equation (3) simplifies to the polynomial

$$y^8 - 3y^4 + 3y^2 - y + x = 0.$$

An open problem is to determine the solvability of the Galois group of this polynomial in y over a suitable field such as $\mathbb{C}(x)$ or its algebraic closure.

Corollary 9. *The number of triadic partitions of the unit square into n subrectangles is*

$$C_{2,3}(n) = \frac{1}{n}\sum_{i=0}^{\lfloor\frac{n-1}{8}\rfloor}\binom{3\left(\frac{n-1}{2}-i\right)}{n-1,\ \frac{n-1}{2}-4i,\ i}(-1)^i\, 2^{\frac{n-1}{2}-4i}.$$

Proof. For $d = 2$, $p = 3$, Theorem 4 gives

$$C_{2,3}(n) = \frac{1}{n} \sum_{\substack{t_1,t_2 \geq 0 \\ 2t_1+8t_2=n-1}} \binom{n-1+t_1+t_2}{n-1,\ t_1,\ t_2} (-1)^{t_2}\, 2^{t_1}. \tag{6}$$

If n is even then the above sum is empty, hence $C_{2,3}(n) = 0$. If n is odd then $t_1 + 4t_2 = \frac{n-1}{2}$. If we set $t_2 = i$ then $t_1 = \frac{n-1}{2} - 4i$, and the sum (6) is empty for $\frac{n-1}{2} - 4i < 0 \iff i > \frac{n-1}{8}$. Hence (6) simplifies to the stated result. ☐

This gives an explicit non-recursive formula for the sequence A322543:

$$1,\ 2,\ 12,\ 96,\ 879,\ 8712,\ 90972,\ 985728,\ 10979577,\ 124937892,\ 1446119664,\ \ldots.$$

Corollary 10. *The number of triadic partitions of the unit cube into n subrectangles is*

$$C_{3,3}(n) = \frac{1}{n} \sum_{j=0}^{\lfloor m/13 \rfloor} \sum_{i=0}^{\lfloor (m-13j)/4 \rfloor} \binom{3(m-i-4j)}{n-1,\ m-4i-13j,\ i,\ j} (-1)^i\, 3^{m-3i-13j},$$

where $m = \frac{n-1}{2}$.

Proof. Similar to Corollaries 5, 7, 9. ☐

At present this sequence (with 0s omitted) does not appear in the OEIS:

$$1,\ 3,\ 27,\ 324,\ 4452,\ 66231,\ 1038177,\ 16887528,\ 282394269,\ 4824324279,\ \ldots.$$

Explicit summation formulas for other values of d and p can be obtained similarly.

3 Asymptotic behaviour and growth rate

We now consider the asymptotic behaviour and growth rate of $C_{d,p}(n)$. Recall again the functional equation (3). If we define the polynomial

$$q_{d,p}(z) = \sum_{k=0}^{d} (-1)^k \binom{d}{k} z^{p^k},$$

then (3) can be restated simply as $q_{d,p}(y) = x$. We call this polynomial $q(z)$ when d, p are clear from the context.

Figure 2 shows the graph of $q(z)$ for small values of d and p.

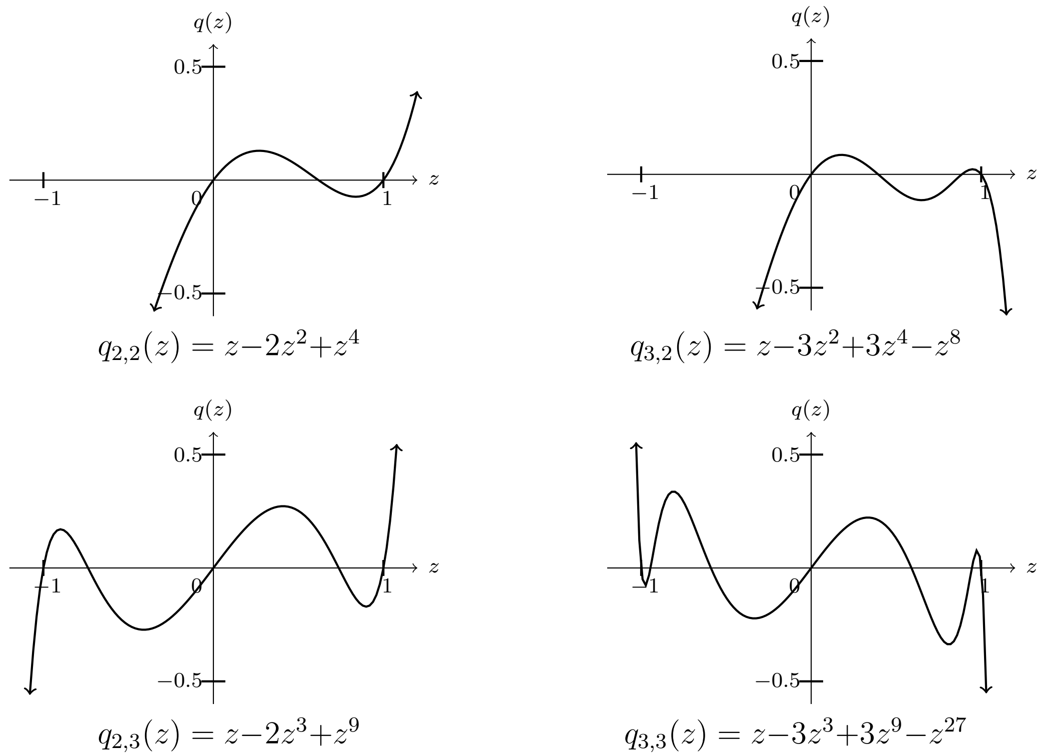


Figure 2: Graphs of the polynomials $q_{d,p}(z)$ for $(d, p) = (2, 2), (3, 2), (2, 3), (3, 3)$

3.1 Asymptotic behaviour

For $p = d = 2$, Kotěšovec gave this asymptotic formula (OEIS, sequence A236339):

$$C_{2,2}(n) \sim \frac{1}{\sqrt{-2\pi q''(s)}} n^{-3/2} q(s)^{1/2-n}.$$

Here $q(y) = y^4 - 2y^2 + y$, hence $q'(y) = 4y^3 - 4y + 1$ and $q''(y) = 12y^2 - 4$, and s is the smallest positive real number where $q'(s) = 0$. Kotěšovec's proof [39] relies on a theorem of Bender [11] that was later corrected and refined; see [28] and [29, Theorem VII.3]. We provide an asymptotic formula for $C_{d,p}(n)$ for all $d \geq 1$ and $p \geq 2$. An important property of the power series for $C_{d,p}(n)$ is its periodicity:

Definition 11. A power series ϕ in the variable z is k-*periodic* for some positive integer k if k is maximal subject to the condition that there exists a unique $l \in \{0, 1, \dots, k-1\}$ such that $[z^n]\phi(z) = 0$ for all $n \not\equiv l \pmod{k}$.

Then we have the following:

Lemma 12. *The power series* $y = \sum_{n\geq 1} C_{d,p}(n)x^n$ *is* $(p-1)$*-periodic.*

Proof. We have $C_{d,p}(1) = 1$ for all d and p, and each subsequent p-ary partition of a subrectangle increases the number of regions by $p-1$. Hence $C_{d,p}(n) = 0$ if $n \not\equiv 1 \pmod{p-1}$. ☐

The following result is a combination of Theorem VI.6 and [29, Note VI.17]:

Theorem 13. *Let y be a power series in x. Let $\phi\colon \mathbb{C} \to \mathbb{C}$ be a function such that:*

(i) ϕ is analytic at $z = 0$ and $\phi(0) > 0$;

(ii) $y = x\phi(y)$;

(iii) $[z^n]\phi(z) \geq 0$ for all $n \geq 0$, and $[z^n]\phi(z) \neq 0$ for some $n \geq 2$.

(iv) If r is the radius of convergence of ϕ then $\phi(s) = s\phi'(s)$ for a unique $s \in (0, r)$.

(v) The power series of ϕ is k-periodic.

Then for $n \equiv 1 \pmod{k}$,

$$[x^n]y \;\sim\; k\sqrt{\frac{\phi(s)}{2\pi\phi''(s)}}\, n^{-3/2}\, (\phi'(s))^n$$

Using Theorem 13, we obtain the following:

Theorem 14. *For all integers $d \geq 1$ and $p \geq 2$, define*

$$q(z) = \sum_{k=0}^{d} (-1)^k \binom{d}{k} z^{p^k}.$$

Let $s > 0$ be the smallest real number such that $q'(s) = 0$. Then for $n \equiv 1 \pmod{p-1}$,

$$C_{d,p}(n) \;\sim\; \frac{p-1}{\sqrt{-2\pi q''(s)}}\, n^{-3/2}\, q(s)^{\frac{1}{2}-n}.$$

Proof. Since $q(y) = x$, we have $y = x\phi(y)$ where

$$\phi(z) = \frac{z}{q(z)} = \frac{1}{\sum_{k=0}^{d}(-1)^k\binom{d}{k} z^{p^k-1}}. \tag{7}$$

We first show that $\phi(z)$ satisfies condition (v). The power series of ϕ has the form

$$\phi(z) = \sum_{n\geq 0} a_n z^n = \frac{1}{\sum_{k=0}^{d}(-1)^k\binom{d}{k} z^{p^k-1}} = \sum_{j\geq 0}\left(\sum_{k=1}^{d}(-1)^{k-1}\binom{d}{k} z^{p^k-1}\right)^j. \tag{8}$$

Since $p-1 \mid p^k-1$ for all $k \geq 1$, we see that $a_n = 0$ when $p-1 \nmid n$ and so ϕ is $(p-1)$-periodic.

Second, we show that $\phi(z)$ satisfies (iii). It is clear that $a_0 = 1$. We prove by induction on n that for all $d \geq 1$, $p \geq 2$, $n \geq p$ we have

$$a_n \geq (d-1)a_{n-(p-1)}.$$

For the basis, from (8) we see that $a_n = d^{n/(p-1)}$ for all $n < p^2 - 1$. For the inductive step, from (7) we see that a_n satisfies the recurrence relation

$$\begin{aligned} a_n &= \sum_{k=1}^{d} (-1)^{k-1} \binom{d}{k} a_{n-(p^k-1)} \\ &= (d-1)a_{n-(p-1)} + \underbrace{\left(a_{n-(p-1)} - \binom{d}{2} a_{n-(p^2-1)}\right)}_{\text{(I)}} + \underbrace{\sum_{k=3}^{d} (-1)^{k-1} \binom{d}{k} a_{n-(p^k-1)}}_{\text{(II)}}. \end{aligned}$$

To show that $a_n \geq (d-1)a_{n-(p-1)}$, we verify that the terms (I) and (II) are both nonnegative. By the inductive hypothesis, for all values of d and p we have

$$a_{n-(p-1)} \geq (d-1)^p a_{n-(p-1)-p(p-1)} = (d-1)^p a_{n-(p^2-1)} \geq \binom{d}{2} a_{n-(p^2-1)},$$

and so (I) is nonnegative. Furthermore, for $k \geq 3$ we have

$$\binom{d}{k} a_{n-(p^k-1)} \geq \binom{d}{k} (d-1) a_{n-(p^{k+1}-1)} \geq \binom{d}{k+1} a_{n-(p^{k+1}-1)}.$$

The first inequality follows from the inductive hypothesis, and the second from the fact that

$$\binom{d}{k}(d-1) \geq \binom{d}{k+1}$$

for all d, k. Thus, the term (II) is also nonnegative. Since $a_n \geq (d-1)a_{n-(p-1)}$, we hence conclude that $a_n \geq 0$ for all $n \geq 1$.

We now consider condition (iv). Clearly,

$$\phi'(z) = \frac{q(z) - zq'(z)}{q(z)^2}, \qquad \phi''(z) = \frac{-zq(z)q''(z) - 2q(z)q'(z) + 2z(q'(z))^2}{q(z)^3}. \tag{9}$$

Let r be the radius of convergence of ϕ at $z = 0$. Since $\phi(z) = z/q(z)$, we see that r is the smallest positive solution to $q(r) = 0$. We show there is unique $s \in (0, r)$ with $\phi(s) = s\phi'(s)$. Notice that

$$\phi(s) = s\phi'(s) \quad \Longrightarrow \quad \frac{s}{q(s)} = s\left(\frac{q(s) - sq'(s)}{q(s)^2}\right) \quad \Longrightarrow \quad sq'(s) = 0.$$

Since $q(0) = q(r) = 0$ and q is differentiable, it follows that $q'(s) = 0$ for some $s \in (0, r)$. This proves the existence of s. For uniqueness, since ϕ has nonnegative coefficients, it follows that ϕ'' is positive over $(0, r)$, and hence over $(0, r)$ we have

$$\frac{d}{dz}\big(\phi(z) - z\phi'(z)\big) = -z\phi''(z) < 0$$

Thus, $\phi(z) - z\phi'(z)$ is continuous and decreasing over $(0, r)$, and hence $\phi(z) - z\phi'(z) = 0$ cannot have distinct solutions over that interval.

Now that the analytic assumptions on $\phi(z)$ have been verified, we may establish the asymptotic formula. Since $q'(s) = 0$, the expression (9) simplifies to

$$\phi'(s) = \frac{1}{q(s)}, \qquad \phi''(s) = \frac{-sq''(s)}{q(s)^2}.$$

Therefore, when $n \equiv 1 \pmod{p-1}$ we have

$$\begin{aligned} C_{d,p}(n) = [x^n]y \;\sim\; & (p-1)\sqrt{\frac{\phi(s)}{2\pi\phi''(s)}}\, n^{-3/2}\, \phi'(s)^n \\ =\; & (p-1)\sqrt{\frac{s/q(s)}{2\pi\big(-sq''(s)/q(s)^2\big)}}\, n^{-3/2} \left(\frac{1}{q(s)}\right)^n \\ =\; & \frac{p-1}{\sqrt{-2\pi q''(s)}}\, n^{-3/2}\, q(s)^{1/2-n}, \end{aligned}$$

and this completes the proof. ☐

3.2 Growth rate

We define the growth rate of $C_{d,p}(n)$ as

$$\mathcal{G}_{d,p} = \lim_{m\to\infty} \frac{C_{d,p}\big((m+1)(p-1)+1\big)}{C_{d,p}\big(m(p-1)+1\big)}.$$

Then we have the following:

Corollary 15. *Given fixed integers $d \geq 1$ and $p \geq 2$,*

$$\mathcal{G}_{d,p} = \frac{1}{(q(s))^{p-1}},$$

where s is the smallest positive real number where $q'(s) = 0$.

Proof. This follows immediately from Theorem 14. ☐

We computed $\mathcal{G}_{d,p}$ for various d and p; see Figure 3. For $d = 1$ (the familiar p-ary Catalan numbers) we have

$$\mathcal{G}_{1,p} = \frac{p^p}{(p-1)^{p-1}},$$

which by Stirling's formula grows almost linearly in p since $\mathcal{G}_{1,p+1} - \mathcal{G}_{1,p} \approx e$ for $p \geq 1$. Figure 3 suggests that $\mathcal{G}_{d,p}$ also grows almost linearly in d for $d \geq 1$, and in fact $\mathcal{G}_{d,p} \approx d\,\mathcal{G}_{1,p}$.

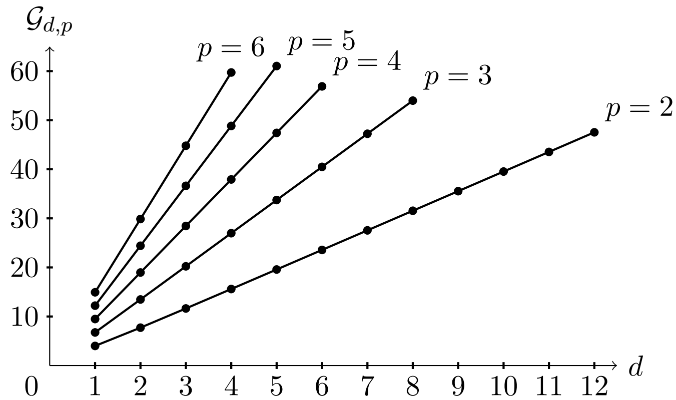


Figure 3: The growth rate $\mathcal{G}_{d,p}$ for various d, p.

4 Interpretation of $C_{d,p}(n)$ in terms of p-ary trees

Recall the three interpretations of the binary Catalan numbers from Section 1.1: (i) placements of parentheses, (ii) binary trees, and (iii) bisections of the unit interval. For the numbers $C_{d,p}(n)$, we saw in the previous sections that (i) generalizes to the number of ways to apply d distinct p-ary operations to n arguments while satisfying the interchange laws, and (iii) generalizes to the number of ways to divide the d-dimensional hypercube into n rectangular regions using p-ary partitions. In this section, we generalize interpretation (ii), and provide a combinatorial description of $C_{d,p}(n)$ in terms of certain p-ary trees by establishing a bijection between these trees and the set of (d, p, n)-decompositions.

4.1 Interchange maximal trees

Let $\mathcal{T}_{d,p,n}$ denote the set of full p-ary trees (every internal node has exactly p children) with n (unlabelled) leaves, such that each of the $m = \frac{n-1}{p-1}$ internal nodes is assigned a label from $\{1, \ldots, d\}$. Let $\mathcal{D}_{d,p,n}$ denote the set of (d, p, n)-decompositions (Definition 1).

We first describe a mapping from $\mathcal{T}_{d,p,n}$ to $\mathcal{D}_{d,p,n}$.

Definition 16. Define the function $f\colon \mathcal{T}_{d,p,n} \to \mathcal{D}_{d,p,n}$ recursively as follows:

- $(n = 1)$ f maps the exceptional tree with a single node to $\{(0,1)^d\}$, the decomposition with a single region, the entire unit hypercube.

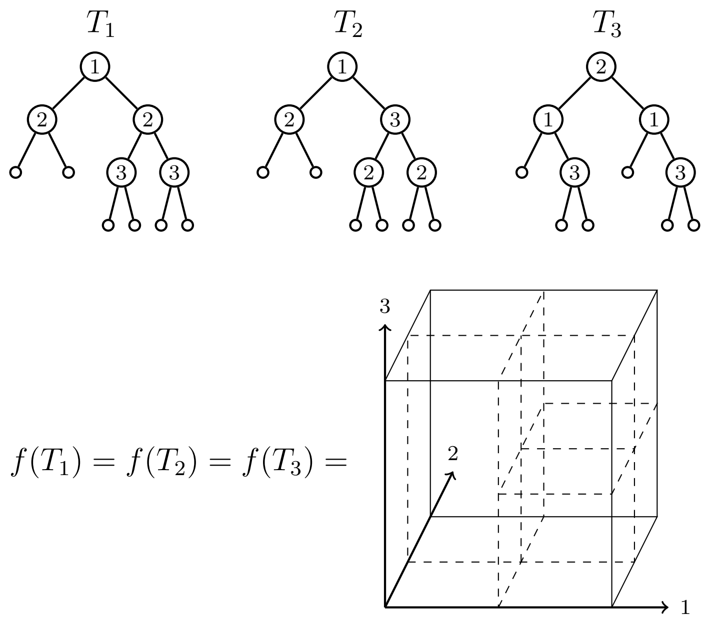


Figure 4: Example of the map f from trees to decompositions (Definition 16)

- ($n \geq 2$) Given $T \in \mathcal{T}_{d,p,n}$ with root labelled i and subtrees (from left to right) $T_1, \ldots, T_p$, for every $j \in \{1, \ldots, p\}$ place the decomposition $f(T_j)$ at

$$\left\{ \, x \in \mathbb{R}^d : x_i \in (j{-}1, j), \, x_k \in (0,1) \; \forall k \neq i \, \right\}.$$

Now that we have p hypercube decompositions lined up in a row along the i^{th} axis, we apply the linear transformation that compresses them along the i^{th} axis by a factor of p, and obtain a decomposition contained in $(0,1)^d$.

We define two trees T, T' to be *interchange equivalent* if $f(T) = f(T')$.

Figure 4 illustrates Definition 16: it displays three trees in $\mathcal{T}_{3,2,6}$ that are mapped by f to the same decomposition in $\mathcal{D}_{3,2,6}$, and hence shows that f is not one-to-one.

Figure 5 describes how to produce interchange equivalent trees. Suppose T is a tree with a subtree S whose root has label i and whose p children are internal nodes each with the same label $j \neq i$. Let $T_{11}, T_{12}, \ldots, T_{pp}$ denote the p^2 subtrees from left to right of the p nodes labelled j (top of Figure 5).

The interchange law implies that in the subtree S we may change the root label from i to j and simultaneously change the labels of the p children from j to i. The result is a new tree T' which is interchange equivalent to T. Notice that the three trees in Figure 4 can be transformed into each other using this "subtree swapping" process that preserves interchange equivalence.

Next, we consider a map that acts as an inverse of f by choosing a unique representative in each inverse image $f^{-1}(D)$ for $D \in \mathcal{D}_{d,p,n}$.

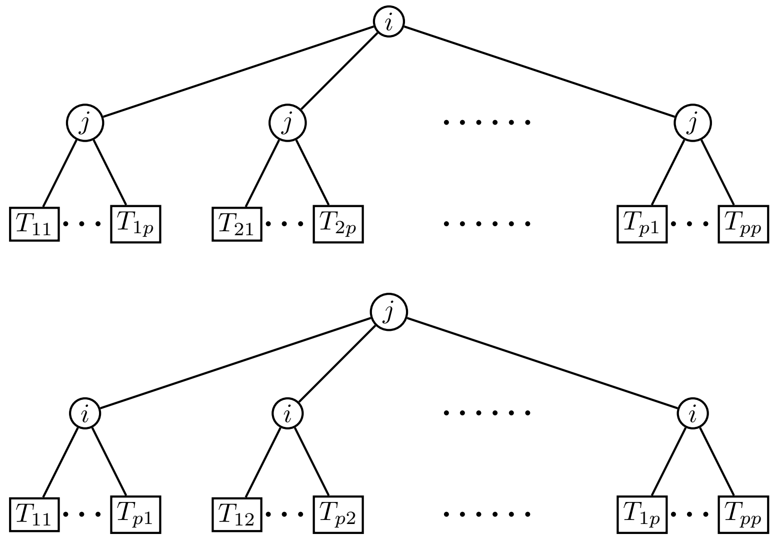


Figure 5: Two interchange equivalent subtrees

Definition 17. Define the function $g : \mathcal{D}_{d,p,n} \to \mathcal{T}_{d,p,n}$ recursively as follows:

- ($n = 1$) g maps the trivial decomposition $\left\{(0,1)^d\right\}$ to the tree with one node.
- ($n \geq 2$) Given indices $1 \leq i, j \leq p$, define the set

$$B_{i,j} = \left\{x \in (0,1)^d \mid (j-1)/p < x_i < j/p\right\}.$$

Then notice that $H_i\left((0,1)^d\right) = \{B_{i,j} \mid 1 \leq j \leq p\}$ (where H_i is as defined in Definition 1). Moreover, if we define the affine transformation $M_{i,j} : \mathbb{R}^d \to \mathbb{R}^d$ such that

$$[M_{i,j}(x)]_k = \begin{cases} x_k & \text{if } k \neq i; \\ px_k - (j-1) & \text{if } k = i, \end{cases}$$

then $M_{i,j}(B_{i,j}) = (0,1)^d$ for every i, j. Then given a decomposition $D \in \mathcal{D}_{d,p,n}$, we choose the largest index i such that every region in D is contained in $B_{i,j}$ for some j. Next, define $D_j = \{d \in D, d \subseteq B_{i,j}\}$ for every $j = 1, \ldots, p$. By the choice of i, $D_1, \ldots, D_p$ must partition D, and $M_{i,j}(D_j)$ is a decomposition of the unit hypercube in its own right.

We then define $g(D)$ to be the p-ary tree with root node labelled i, with subtrees $g\left(M_{i,j}(D_1)\right), \ldots, g\left(M_{i,j}(D_p)\right)$ from left to right.

Example 18. Let D be the decomposition in Figure 4, which has 6 regions:

$$D = \{\ (0,1/2) \times (0,1/2) \times (0,1), \qquad (0,1/2) \times (1/2,1) \times (0,1),$$

$$(1/2,1)\times(0,1/2)\times(0,1/2),\quad (1/2,1)\times(1/2,1)\times(0,1/2),$$
$$(1/2,1)\times(0,1/2)\times(1/2,1),\quad (1/2,1)\times(1/2,1)\times(1/2,1)\ \}.$$

Every region in D is contained in one of the sets

$$B_{1,1}=(0,1/2)\times(0,1)\times(0,1),\quad B_{1,2}=(1/2,1)\times(0,1)\times(0,1)..$$

However, the same can be said for

$$B_{2,1}=(0,1)\times(0,1/2)\times(0,1),\quad B_{2,2}=(0,1)\times(1/2,1)\times(0,1).$$

but *not* for the sets $B_{3,1}, B_{3,2}$. Thus, we choose the index $i = 2$, and so the root node of $g(D)$ has label 2. Continuing in this way, one finds that $g(D)$ is the tree T_3 in Figure 4.

By the construction of the functions f and g, it is clear that $f(g(D)) = D$ for every $D \in \mathcal{D}_{d,p,n}$. Hence f is onto, which implies that $C_{d,p}(n)$ counts the number of interchange equivalence classes in $\mathcal{T}_{d,p,n}$. In other words, $C_{d,p}(n)$ counts the number of trees in the image of g. We characterize these trees through the following definition:

Definition 19. A tree $T \in \mathcal{T}_{d,p,n}$ is *interchange maximal* if it has no subtree $\tilde{T}$ such that

1. $\tilde{T}$ has root labelled i;
2. there exists $\tilde{T}'$ with root labelled j where $j > i$ such that $f(\tilde{T}') = f(\tilde{T})$.

Example 20. In Figure 4, T_1 and T_2 are not interchange maximal since they both have root labelled $i = 1$, while there exists an interchange equivalent tree T_3 with root node labelled $j = 2$. One can check that T_3 is indeed interchange maximal.

Lemma 21. *Every tree output by g must be interchange maximal.*

Proof. This follows immediately from Definitions 17 and 19, as the function g always picks the largest possible node label when generating the tree from the top down. ☐

Remark 22. Condition 2. in Definition 19 is equivalent to

2′. There exists $j > i$ such that the path between the root of $\tilde{T}$ and every leaf of $\tilde{T}$ contains an internal node labelled j.

Condition 2′ characterizes interchange maximal trees without reference to hypercube decompositions. For instance, the tree T_2 in Figure 4 is not interchange maximal since it has root label 1, while the path from any leaf to the root contains a node labelled 2.

The reason we are interested in interchange maximal trees is the following:

Theorem 23. *For every $T \in \mathcal{T}_{d,p,n}$, there exists a unique $T' \in \mathcal{T}_{d,p,n}$ that is interchange maximal and satisfies $f(T') = f(T)$.*

Proof. First, we prove existence. Given a tree T, let $\alpha(T) = (\alpha_0, \alpha_1, \ldots,)$ be the sequence where α_k is the sum of the vertex labels of all level-k internal nodes of T. Now, if T is not interchange maximal, one can replace a subtree in T rooted at an i-node by a different subtree rooted at a j-node where $j > i$, and obtain a new tree T' where $f(T') = f(T)$.

Suppose the i-node in T is at level l. When we compare $\alpha(T) = (\alpha_0, \alpha_1, \ldots)$ and $\alpha(T') = (\alpha'_0, \alpha'_1, \ldots)$, we see that $\alpha'_k = \alpha_k$ for all $k < l$, and $\alpha'_l = \alpha_l + j - i > \alpha_l$. Thus, the sequence $\alpha(T')$ is strictly greater than $\alpha(T)$ in lexicographic order. If T' is not interchange maximal, we can repeat this process to find T'' where $\alpha(T'')$ is yet greater lexicographically. Since the label-sum sequence cannot increase indefinitely, we conclude that there exists an interchange maximal tree which is interchange equivalent to T.

Next, we prove uniqueness by contradiction. Suppose there are two distinct interchange maximal trees T, T' where $f(T) = f(T') = D$. Let l be the least level on which T, T' start to differ, and that at this level T has a node labelled i whereas the same node in T' has label j. Without loss of generality, we may assume that $j > i$. Let $\tilde{T}$ (resp. $\tilde{T}'$) be the subtree of T rooted at the i-node (resp. the subtree of T' rooted at the j-node).

Since the i-node in T and the j-node in T' have identical ancestors in their respective trees (by minimality of l), $\tilde{T}$ and $\tilde{T}'$ correspond to the same region in the decomposition D. Thus, when considered as trees in their own right, we must have $f(\tilde{T}) = f(\tilde{T}')$. If we now let T'' be the tree obtained from T by replacing the subtree $\tilde{T}$ by $\tilde{T}'$, we would have $f(T'') = f(T)$, showing that T is not interchange maximal, a contradiction. □

It follows from Theorem 23 that every class of interchange equivalent trees has exactly one interchange maximal representative. Thus, if we let $\mathcal{T}^+_{d,p,n} \subseteq \mathcal{T}_{d,p,n}$ denote the set of interchange maximal trees, then $|\mathcal{T}^+_{d,p,n}| = |\mathcal{D}_{d,p,n}| = C_{d,p}(n)$ for all $d \geq 1, p \geq 2, n \geq 1$. Moreover, if we restrict the domain of f to $\mathcal{T}^+_{d,p,n}$, then we obtain a bijection between the interchange maximal trees and the hypercube decompositions. Clearly, the inverse of this function is exactly g.

4.2 Deriving the functional equation (3) directly using trees

Having shown that $|\mathcal{T}^+_{d,p,n}| = C_{d,p}(n)$ by establishing a bijection between interchange maximal trees and hypercube decompositions, Theorem 3 can now be restated as follows:

Theorem 24. *Given fixed integers $d \geq 1, p \geq 2$, define the formal power series*

$$w = \sum_{n \geq 1} |\mathcal{T}^+_{d,p,n}| x^n.$$

Then w satisfies the functional equation

$$\sum_{i=0}^{d} (-1)^k \binom{d}{i} w^{p^i} = x. \tag{10}$$

In the rest of this section, we give a direct proof of Theorem 24, hence providing an alternative proof of Theorem 3 that is purely combinatorial (and, in our opinion, more elementary). First, we introduce some special families of trees.

Definition 25. Let $S = \{s_1, s_2, \dots, s_k\}$ where $1 \le s_1 < s_2 < \cdots < s_k \le d$ be a nonempty set of indices. Define $\mathcal{U}^S_{d,p,n} \subseteq \mathcal{T}_{d,p,n}$ to be the set of trees T for which

- T has root labelled s_1 and all p subtrees at the root s_1-node are interchange maximal.
- For all $j \ge 2$ there exists $T' \in \mathcal{T}_{d,p,n}$ such that T' has root labelled s_j and $f(T') = f(T)$.

Example 26. For the trees in Figure 4, we first see that $T_1 \notin \mathcal{U}^S_{3,2,6}$ for any S since the right subtree at the root node of T_1 is not interchange maximal. On the other hand, T_2 does have two interchange maximal subtrees at the root and so $T_2 \in \mathcal{U}^{\{1\}}_{3,2,6}$. Moreover, the existence of T_3 (which has root label 2 and is interchange equivalent to T_2) implies that $T_2 \in \mathcal{U}^{\{1,2\}}_{3,2,6}$ which is a subset of $\mathcal{U}^{\{1\}}_{3,2,6}$. Finally, $T_3 \in \mathcal{U}^{\{2\}}_{3,2,6}$, but T_3 is not an element of $\mathcal{U}^S_{3,2,6}$ for any other S.

More generally, an interchange maximal tree with root labelled i belongs to $\mathcal{U}^{\{i\}}_{d,p,n}$, but not $\mathcal{U}^S_{d,p,n}$ for any S with multiple indices. Thus, we obtain that

$$\mathcal{T}^+_{d,p,n} = \Bigg(\bigcup_{\substack{S\subseteq\{1,\dots,d\}\\|S|=1}} \mathcal{U}^S_{d,p,n} \Bigg) \setminus \Bigg(\bigcup_{\substack{S\subseteq\{1,\dots,d\}\\|S|=2}} \mathcal{U}^S_{d,p,n} \Bigg). \tag{11}$$

Note that (11) only applies for $n > 1$ (when the root of a tree is indeed an internal node). If $n = 1$ then $\mathcal{T}^+_{d,p,1}$ consists of only the tree with one node, thus $|\mathcal{T}^+_{d,p,1}| = 1$. While we can express the sets of interchange maximal trees in terms of the $\mathcal{U}^S_{d,p,n}$ with sets S of size $n \le 2$, it will be helpful to know the sizes of the $\mathcal{U}^S_{d,p,n}$ for all S. Thus, we have the following:

Lemma 27. *For every $d \ge 1, p \ge 2, n \ge 2$ and $S \subseteq \{1, \dots, d\}$ where $|S| = k$, we have*

$$|\mathcal{U}^S_{d,p,n}| = \sum_{n_1,\dots,n_{p^k}} \left(\prod_{j=1}^{p^k} |\mathcal{T}^+_{d,p,n_j}| \right),$$

where the summation is over all integers $n_1, \dots, n_{p^k} \ge 1$ with $\sum_{j=1}^{p^k} n_j = n$.

Proof. Instead of counting $|\mathcal{U}^S_{d,p,n}|$ directly, we first establish a bijection between $\mathcal{U}^S_{d,p,n}$ and another auxiliary set that has simpler structure.

Given $S = \{s_1, \dots, s_k\}$ where the indices are increasing, let $\mathcal{V}^S_{d,p,n} \subseteq \mathcal{T}_{d,p,n}$ be the collection of trees T such that

- For all $1 \le i \le k$, all p^{i-1} nodes at level $i-1$ of T are internal nodes with label s_i.
- All p^k subtrees of the p^{k-1} s_k-nodes at level $k-1$ are interchange maximal.

Using the trees from Figure 4 again, we have

$$T_1 \in \mathcal{V}^{\{1,2\}}_{3,2,6}, \qquad T_2 \in \mathcal{V}^{\{1\}}_{3,2,6}, \qquad T_3 \in \mathcal{V}^{\{2\}}_{3,2,6}.$$

Notice that if $|S| = 1$ then $\mathcal{U}^S_{d,p,n} = \mathcal{V}^S_{d,p,n}$ by definition. We now construct a bijection

$$h_S : \mathcal{U}^S_{d,p,n} \to \mathcal{V}^S_{d,p,n},$$

that applies to sets S of arbitrary size. First, given $T \in \mathcal{U}^S_{d,p,n}$, let $\tilde{D} \in \mathcal{D}_{d,p,p^k}$ denote the decomposition obtained by partitioning $(0,1)^d$ into p regions along the s_1-axis, then partitioning each of those regions into p regions along the s_2-axis (resulting in p^2 regions at this point), and so on, until finally we partition along the s_k-axis and obtain p^k total regions of the hypercube. The fact that T has root label s_1, and that there exist trees with root labels $s_2, \ldots, s_k$ that are interchange equivalent to T, implies that every region in the decomposition $f(T)$ is contained in one of the regions in $\tilde{D}$. Thus, we can consider $f(T)$ as consisting of p^k decompositions, one for each of the regions in $\tilde{D}$. Moreover, for each region, there exists a unique (see Theorem 23) interchange maximal tree representing this decomposition. We thus obtain p^k trees.

Next, define the tree $\tilde{T} \in \mathcal{T}_{d,p,p^k}$ such that for $1 \le i \le k$, all p^{i-1} vertices at level $i-1$ are internal nodes labelled s_i, followed by p^k leaves at level k. Obviously, $f(\tilde{T}) = \tilde{D}$. Now, define $h_S(T)$ to be the tree obtained by replacing the p^k leaves of $\tilde{T}$ by the corresponding p^k trees obtained from the previous paragraph. By construction, $f(h_S(T)) = f(T)$ and $h_S(T) \in \mathcal{V}^S_{d,p,n}$. For example, in Figure 4, we have $T_2 \in \mathcal{U}^{\{1,2\}}_{3,2,6}$ and $h_{\{1,2\}}(T_2) = T_1 \in \mathcal{V}^{\{1,2\}}_{3,2,6}$.

We now show that the mapping h_S is onto. Given $T \in \mathcal{V}^S_{d,p,n}$, note that T has root label s_1. Let $T_1, \ldots, T_p$ be the subtrees of T at the root. For every $i \in \{1, \ldots, p\}$, there exists a unique T'_i that is interchange maximal and satisfies $f(T_i) = f(T'_i)$. We replace the subtrees $T_1, \ldots, T_p$ in T by $T'_1, \ldots, T'_p$ respectively, and call the modified tree T'. By construction, $f(T) = f(T')$. We also see that $T' \in \mathcal{U}^S_{d,p,n}$, since it has s_1 as root label and p interchange maximal subtrees at the root. Moreover, for $1 \le i \le k$, since T has a level of internal nodes all of which have label s_i, we can use the subtree-swapping steps outlined in Figure 5 to obtain a tree which is interchange equivalent to T and has s_i as root label. By construction of T', we have $h_S(T') = T$. Thus, every tree $T \in \mathcal{V}^S_{d,p,n}$ is in the image of h_S.

It remains to show that h_S is one-to-one. Assume to the contrary that there exist distinct trees $T, T' \in \mathcal{U}^S_{d,p,n}$ with $h_S(T) = h_S(T')$. Both T and T' have root label s_1, so one of their subtrees at the root must differ. Suppose the i^{th} subtrees at the roots of T, T' are T_i, T'_i respectively and $T_i \ne T'_i$. Since both T_i, T'_i are interchange maximal, $f(T_i) \ne f(T'_i)$. This implies that $f(T) \ne f(T')$, since the i^{th} slice along the s_1-axis in the corresponding decompositions are not the same. However, we showed above that $h_S(T)$ is interchange equivalent to T, and hence $h_S(T) \ne h_S(T')$.

Thus, we have established that $|\mathcal{U}^S_{d,p,n}| = |\mathcal{V}^S_{d,p,n}|$. Finally, it is easy to see that there is a natural correspondence between $\mathcal{V}^S_{d,p,n}$ and ordered sets of p^k interchange maximal trees that have a total of n leaves. This completes the proof. ∎

We are now ready to prove the main result of this section.

Proof of Theorem 24. From equation (11), we obtain

$$|\mathcal{T}^{+}_{d,p,n}| = \left|\left(\bigcup_{\substack{S\subseteq\{1,\dots,d\}\\|S|=1}} \mathcal{U}^{S}_{d,p,n}\right) \setminus \left(\bigcup_{\substack{S\subseteq\{1,\dots,d\}\\|S|=2}} \mathcal{U}^{S}_{d,p,n}\right)\right| = \underbrace{\left|\bigcup_{\substack{S\subseteq\{1,\dots,d\}\\|S|=1}} \mathcal{U}^{S}_{d,p,n}\right|}_{\text{(I)}} - \underbrace{\left|\bigcup_{\substack{S\subseteq\{1,\dots,d\}\\|S|=2}} \mathcal{U}^{S}_{d,p,n}\right|}_{\text{(II)}}.$$

Since (II) is a subset of (I), the difference of the sizes of the sets equals the size of the difference of the sets. Since $\mathcal{U}^{\{i\}}_{d,p,n}$ and $\mathcal{U}^{\{j\}}_{d,p,n}$ are disjoint for distinct $i \neq j$, the size of (I) is simply

$$\sum_{i=1}^{d} \left|\mathcal{U}^{\{i\}}_{d,p,n}\right|.$$

For (II), observe that given two-index sets $S_1 = \{s_{11}, s_{12}\}, \dots, S_k = \{s_{k1}, s_{k2}\}$ such that $1 \leq s_{j1} < s_{j2} \leq d$ for all j, we have

$$\bigcap_{j=1}^{k} \mathcal{U}^{S_j}_{d,p,n} = \begin{cases} \mathcal{U}^{\left(\bigcup_{j=1}^{k} S_j\right)}_{d,p,n} & \text{if } s_{11} = s_{21} = \cdots = s_{k1}; \\ \emptyset & \text{if } s_{11}, s_{21}, \dots, s_{k1} \text{ are not identical.} \end{cases}$$

In the first case, observe that $\bigcup_{j=1}^{k} S_j = \{s_{11}, s_{12}, s_{22}, \dots, s_{k2}\}$ and has size $k+1$. Thus, by the principle of inclusion-exclusion, the size of (II) is

$$\left|\bigcup_{\substack{S\subseteq\{1,\dots,d\}\\|S|=2}} \mathcal{U}^{S}_{d,p,n}\right| = \sum_{i=2}^{d} \left((-1)^{i-1} \sum_{\substack{S\subseteq\{1,\dots,d\}\\|S|=i}} \left|\mathcal{U}^{S}_{d,p,n}\right|\right).$$

Putting this all together, we see that for all $n > 1$, we have

$$\begin{aligned} |\mathcal{T}^{+}_{d,p,n}| &= |(\mathrm{I})| - |(\mathrm{II})| \\ &= \sum_{i=1}^{d} \left|\mathcal{U}^{\{i\}}_{d,p,n}\right| - \sum_{i=2}^{d} \left((-1)^{i-1} \sum_{\substack{S\subseteq\{1,\dots,d\}\\|S|=i}} \left|\mathcal{U}^{S}_{d,p,n}\right|\right) \\ &= \sum_{i=1}^{d} \left((-1)^{i} \sum_{\substack{S\subseteq\{1,\dots,d\}\\|S|=i}} \left|\mathcal{U}^{S}_{d,p,n}\right|\right) \\ &= \sum_{i=1}^{d} \left((-1)^{i} \binom{d}{i} \sum_{n_1,\dots,n_{p^i}} \left(\prod_{j=1}^{p^i} |\mathcal{T}^{+}_{d,p,n_j}|\right)\right), \end{aligned}$$

where we applied Lemma 27 to obtain the last equality. If we take the above equation, multiply both sides by x^n, and sum over for $n \geq 1$, we obtain

$$w = x + \sum_{i=1}^{d} (-1)^i \binom{d}{i} w^{p^i},$$

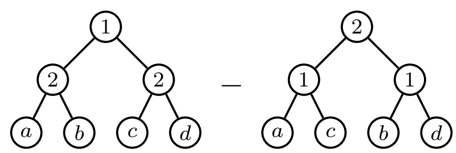
which rearranges to give (10), and this completes the proof. $\square$

5 Gröbner bases for shuffle operads

Recall that the original motivation for this paper came from combinatorial aspects of the work by the third author and Dotsenko [14] on Boardman–Vogt tensor products of operads. In this section we give an operadic explanation of the fact that the three distinct trees in Figure 4 give rise to the same rectangular decomposition of the cube. This discussion is based on the theory and algorithms of Gröbner bases for shuffle operads developed originally by Dotsenko and Khoroshkin [24]; we follow the notation of [13].

5.1 Dimension 2

For completeness we begin with dimension 2. When $d = 2$ and $p = 2$ we have two operations $\bullet_1$ and $\bullet_2$ satisfying the interchange law represented by this tree polynomial:

$\alpha \;=$ 

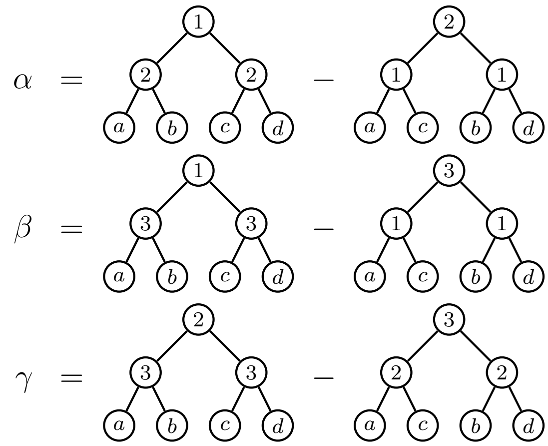
Node labels 1 and 2 correspond to operations $\bullet_1$ and $\bullet_2$. The leading term of α does not have any small common multiple with itself, so there are no S-polynomials and the Gröbner basis of this shuffle operad consists simply of α.

5.2 Dimension 3

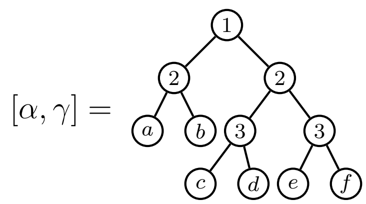
When $d = 3$ and $p = 2$, we have three operations $\bullet_1$, $\bullet_2$, $\bullet_3$ that satisfy three interchange laws represented by these tree polynomials:

$$(a \bullet_2 b) \bullet_1 (c \bullet_2 d) = (a \bullet_1 c) \bullet_2 (b \bullet_1 d),$$
$$(a \bullet_3 b) \bullet_1 (c \bullet_3 d) = (a \bullet_1 c) \bullet_3 (b \bullet_1 d),$$
$$(a \bullet_3 b) \bullet_2 (c \bullet_3 d) = (a \bullet_2 c) \bullet_3 (b \bullet_2 d).$$

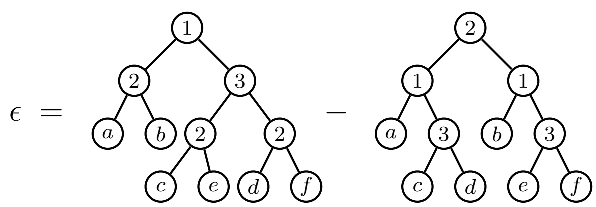
The operation order $\bullet_1 \prec \bullet_2 \prec \bullet_3$ extends in the usual way to a monomial order on the shuffle operad generated by these three operations satisfying these three relations. The three interchange laws are represented by the following three tree polynomials; in each case the leftmost tree is the leading monomial with respect to the monomials order:



The least common multiple of the leading terms of α and γ is this tree:



The corresponding S-polynomial obtained from α and γ is as follows:



The tree polynomial ϵ is the first element in the Gröbner basis of this shuffle operad (beyond the tree polynomials α, β, γ). The two terms in ϵ correspond to the two trees T_2 and T_3 in Figure 4. This gives an operadic explanation of the fact that T_2 and T_3 produce the same decomposition of the cube. It remains an open problem to compute a complete Gröbner basis for this shuffle operad.

6 Future research

This paper has developed a more complete understanding of the numbers $C_{d,p}(n)$ and established a connection between (i) hypercube decompositions, (ii) interchange maximal trees, and (iii) algebraic operads. It is an important open problem to determine if a similar theory can be developed for other well-known variations on the Catalan numbers. In particular, we consider the Wedderburn–Etherington numbers [25, 50]; see also OEIS A001190. In this case we have a binary operation that is commutative but not associative; we let $W(n)$ denote the number of ways to interpret x^n under this operation. For instance, for x^4 we have

$$((xx)x)x = (x(xx))x = x(x(xx)) = x((xx)x),$$

but all of these are distinct from $(xx)(xx)$. Thus there are only two distinct interpretations of x^4, and so $W(4) = 2$. The following table lists the distinct n^{th} powers for $n \leq 5$.

n	n^{th} commutative nonassociative powers	$W(n)$
1	x	1
2	xx	1
3	$(xx)x$	1
4	$((xx)x)x$, $(xx)(xx)$	2
5	$((xx)x)x)x$, $((xx)xx))x$, $((xx)x)(xx)$	3

While the growth rate of $W(n)$ has been determined [40], it is an open problem to determine a non-recursive formula for these numbers. It would be interesting to investigate higher-dimensional analogues of the Wedderburn–Etherington numbers involving d distinct p-ary operations satisfying various generalizations of commutativity.

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