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# Sequence positivity through numeric analytic continuation: uniqueness of the Canham model for biomembranes

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**Abstract**. We prove solution uniqueness for the genus one Canham variational problem arising in the shape prediction of biomembranes. The proof builds on a result of Yu and Chen that reduces the variational problem to proving positivity of a sequence defined by a linear recurrence relation with polynomial coefficients. We combine rigorous numeric analytic continuation of D-finite functions with classic bounds from singularity analysis to derive an effective index where the asymptotic behaviour of the sequence, which is positive, dominates the sequence behaviour. Positivity of the finite number of remaining terms is then checked separately.

**Keywords.** Analytic combinatorics, D-finite, P-recursive, positivity, Canham model **Mathematics Subject Classifications.** 05A16, 68Q40, 30B40

### **1. Introduction**

An influential biological model of Canham [Can70] predicts the preferred shapes of biomembranes, such as blood cells, by solving a variational problem involving mean curvature. For a fixed genus<sup>1</sup> g and constants  $a_0$  and  $v_0$  determined by physical details, such as ambient temper-

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<sup>&</sup>lt;sup>1</sup>The model fixes a genus as experimental observations have found no topological changes in surfaces whose external systems evolve, at accessible time-scales. Although genus zero biomembranes are more commonly observed in living organisms, genus one membranes can be observed under the microscope in laboratory settings [MB95, Sect. 4].

ature, the model of Canham asks one to find, among all orientable closed surfaces of genus g of prescribed area  $a_0$  and volume  $v_0$ , a surface S minimizing the *Willmore energy* 

$$W(S) = \int_{S} H^2 dA, \qquad (1.1)$$

where H is the mean curvature. Because W(S) is scaling invariant, prescribing the area A(S) and volume V(S) of the surface turns out to be equivalent to prescribing the *isoperimetric ratio* 

$$\iota(S) = \pi^{1/6} \frac{\sqrt[3]{6V(S)}}{\sqrt{A(S)}} = \iota_0.$$

The *isoperimetric inequality* states that  $\iota(S) \in (0, 1]$ , with  $\iota(S) = 1$  achieved uniquely for the sphere.

The existence of a solution to the Canham model in genus g = 0 and any  $\iota_0 \in (0, 1]$  was shown by Schygulla [Sch12], while Keller et al. [KMR14] proved existence of solutions for higher genus and some values of  $\iota_0$  between zero and one. Marques and Neves [MN14] solved a long-standing conjecture of Willmore [Wil65] by establishing that the stereographic images in  $\mathbb{R}^3$  of  $\{ [\cos u, \sin u, \cos v, \sin v]/\sqrt{2} : u, v \in [0, 2\pi] \}$ , known as *Clifford tori*, minimize the Willmore energy among all embedded closed surfaces of genus at least one. The Marques–Neves theorem establishes solution existence in genus one for values of  $\iota_0 \in [\tau, 1)$  where  $\tau = \frac{3}{25/4\sqrt{\pi}}$ .

Due to the apparent uniqueness of biomembrane shapes observed in experimental settings, it is natural to ask whether such a prediction model admits a unique solution. Computational investigations of solution existence and uniqueness for the Canham model have been carried out in Seifert [Sei97] and Chen et al. [CYB<sup>+</sup>19]. Recent work of Yu and Chen [YC22] further investigates the uniqueness problem, with a focus on the genus one case<sup>2</sup>.

**Conjecture 1.1** (Yu and Chen [YC22]). Up to homothety, a *Clifford torus* is uniquely determined by its isoperimetric ratio. Consequently, the Canham model in genus g = 1 has a unique solution when  $\iota_0 \in [\tau, 1)$  where  $\tau = \frac{3}{2^{5/4}\sqrt{\pi}}$ .

Yu and Chen reduce proving Conjecture 1.1 to showing that a certain sequence of rational numbers has positive terms. More specifically, let  $(d_n)$  be the unique sequence with initial terms  $(d_0, \ldots, d_6) = (72, 1932, 31248, \frac{790101}{2}, \frac{17208645}{4}, \frac{338898609}{8}, \frac{1551478257}{4})$  satisfying the explicit order seven linear recurrence relation

$$\sum_{i=0}^{7} r_i(n) d_{n+i} = 0, \qquad r_i(n) \in \mathbb{Z}[n]$$
(1.2)

whose coefficients  $r_i$  are defined in the appendix.

**Conjecture 1.2** (Yu and Chen [YC22]). All terms of the sequence  $(d_n)$  are positive.

<sup>&</sup>lt;sup>2</sup>Conjecture 1.1 was labeled Conjecture 1.1 in the original draft of [YC22], and then upgraded to Theorem 1.1 after those authors were informed that the present work proves their conjecture.

# **Proposition 1.3** (Yu and Chen [YC22]). *If all terms of the sequence* $(d_n)$ *are positive then Conjecture 1.1 holds.*

The main result of this paper is to prove Conjecture 1.2, thus completing the uniqueness proof for the Clifford torus in the Canham model.

#### **Theorem 1.4.** All terms of the sequence $(d_n)$ defined by (1.2) are positive.

Our proof aims to illustrate a general method to obtain asymptotic approximations with error bounds of sequences defined by recurrence relations of the type (1.2), based on analytic combinatorics and rigorous numerics. The method is implicit in the work of Flajolet and collaborators [FP86, FO90, FS09], however, to the best of our knowledge, it has never been detailed or used in published work. We also aim to illustrate the computational tools available to compute these bounds on practical applications. A Sage notebook containing our calculations can be found online in static<sup>3</sup> and interactive<sup>4</sup> versions.

A more direct proof of Conjecture 1.1 is also possible. Indeed, the argument of Yu and Chen shows that it follows from the fact that a certain function denoted lso is bijective, which itself follows from the positivity of the sum  $\sum_{n\geq 0} d_n z^n$  for all  $z \in (0, 3 - 2\sqrt{2})$ . As outlined in Section 4.2, this weaker result can be established using variants of our arguments for Theorem 1.4, without going through a full proof of positivity of the coefficient sequence.

Since the completion of the first version of this paper, Bostan and Yurkevich [BY22] gave an alternative proof of the positivity of lso based on an explicit expression in terms of Gauss hypergeometric functions.

#### 1.1. Related work

Our approach to sequence positivity can be applied to problems well beyond the current application. The study of positivity for recursively defined sequences has a long history; a full accounting of works on the topic would be more than enough to fill a survey paper, so we aim only to highlight some specific problems close to our results and approach.

One of the oldest outstanding problems in this area is the so-called Skolem problem for *C*finite sequences satisfying linear recurrence relations with constant coefficients. Skolem's problem asks one to decide, given a C-finite sequence encoded by a linear recurrence with constant coefficients and a sufficient number of initial terms, whether some term in the sequence is zero. Because the term-wise product  $(a_nb_n)$  of any two C-finite sequences  $(a_n)$  and  $(b_n)$  is also Cfinite, Skolem's problem for a real sequence  $(a_n)$  can be reduced to deciding when the C-finite sequence  $(a_n^2)$  has only positive terms. Although the general term of a C-finite sequence can be algorithmically represented as an explicit finite sum involving powers of algebraic numbers, decidability of positivity has essentially been open since Skolem's work [Sko34] characterizing zero index sets of C-finite sequences in the 1930s. Skolem's problem has received great attention in the theoretical computer science literature, as the counting sequences of regular languages are always C-finite. See Kenison et al. [KLOW20] for an overview of the topic, together with some recent progress.

<sup>&</sup>lt;sup>3</sup>https://doi.org/10.5281/zenodo.4274504

<sup>&</sup>lt;sup>4</sup>https://mybinder.org/v2/zenodo/10.5281/zenodo.4274504/?filepath=Positivity.ipynb

For more general recurrence relations, Gerhold and Kauers [GK05] introduced a computer algebra procedure that tries to find an inductive proof of positivity using algorithms for cylindrical algebraic decomposition. The special case of linear recurrence relations with *polynomial* coefficients—like (1.2)—was further studied by Kauers and Pillwein [KP10, Pil13], who gave extensions of the basic technique and sufficient conditions for termination<sup>5</sup>. Another computer algebra method of Cha [Cha14] sometimes allows one to express solution sequences as sums of squares. The present paper indirectly builds on a different family of algorithms, going back to Cauchy [Cau42], that provide *upper* bounds on the magnitude of coefficients of power series solutions to various kinds of functional equations. Singularity analysis allows us, in a sense, to "turn upper bounds into two-sided ones" and use them to derive positivity results. Further references can be found in [Mez19, Sec. 2.1].

Finally, we mention that positivity of power series coefficients has long been of interest to analysts (in contexts not so different from the variation problem at the heart of Canham's model). For instance, during their 1920s work on solution convergence for finite difference approximations to the wave equation, Friedrichs and Lewy attempted to prove positivity of a three-dimensional sequence defined as the power series coefficients of a trivariate rational function; positivity was shown by Szegö [Sze33] using properties of Bessel functions. Askey and Gasper [AG72] detail this problem and additional ones in a similar vein.

#### 2. Singular behaviour and eventual positivity

We study  $(d_n)$  by encoding it by its generating function,

$$f(z) = \sum_{n \ge 0} d_n z^n.$$

Because  $(d_n)$  satisfies a linear recurrence relation with polynomial coefficients, f satisfies a linear differential equation with polynomial coefficients, and such a differential equation can be determined automatically: see [FS09, Sect. VII. 9] or [BCG<sup>+</sup>17, Ch. 14] for details. In this case, f(z) satisfies a third-order differential equation

$$c_3(z)F'''(z) + c_2(z)F''(z) + c_1(z)F'(z) + c_0(z)F(z) = 0, \qquad c_j(z) \in \mathbb{Z}[z]$$
(2.1)

whose coefficients are given explicitly in the appendix.

Because (2.1) is a linear homogeneous differential equation its formal power series solutions form a complex vector space of dimension at most three. Our particular generating function solution F(z) = f(z) can be uniquely specified among the formal power series solutions of (2.1) by a finite number of initial conditions  $F(0) = d_0, F'(0) = d_1, \ldots$  Although we do not use a closed form expression of f(z), we can leverage its representation as a solution of (2.1) to

<sup>&</sup>lt;sup>5</sup>Thomas Yu informed us that the method described by Kauers and Pillwein fails in practice to prove positivity of our sequence  $d_n$ , though it does apply to simpler sequences used in intermediary computations by Yu and Chen [YC22].

compute enough information to prove positivity of  $(d_n)$ . Our computations are carried out in the Sage<sup>6</sup> ore\_algebra<sup>7</sup> package [KJJ15, Mez16].

**Example 2.1.** The ore\_algebra package represents linear differential equations such as (2.1) as *Ore polynomials*: essentially, polynomials in two non-commuting variables which encode linear differential operators. For instance, to load the package and encode the equation (2.1) one can enter

```
sage: from ore_algebra import *
sage: Pols.<z> = PolynomialRing(QQ); Diff.<Dz> = OreAlgebra(Pols)
sage: deq = ((25165779*z^15 - ... - 25165779*z^2)*Dz^3 + ...
....: + (6341776308*z^12 - ... + 2701126946))
```

where each ... represents explicit input which is truncated here for readability. A term of the form  $Dz^k$  represents an operator mapping f(z) to its kth derivative.

We prove positivity of  $d_n$  through comparison with its asymptotic behaviour. We will soon see that the power series f(z) is convergent, and hence defines an analytic function, in a neighbourhood of zero in the complex plane; we also denote this analytic function by f(z). Dominant asymptotics are calculated using the transfer method of Flajolet and Odlyzko [FO90], which shows how the asymptotic behaviour of  $d_n$  is linked to the singular behaviour of the analytic function f(z). In particular, to determine asymptotic behaviour of  $d_n$  it is enough to identify the singularity of f(z) with minimal modulus (in this case there is only one), compute a singular expansion of f(z) in a region near this singularity, then transfer information from the dominant terms of this singular expansion directly into dominant asymptotic behaviour of  $d_n$ .

The singular behaviour of f(z) is constrained by the fact that it satisfies (2.1). The classical Cauchy existence theorem for analytic differential equations implies that analytic solutions of (2.1) can be analytically continued to any simply connected domain  $\Omega \subseteq \mathbb{C}$  where the leading coefficient

$$c_3(z) = z^2(z+1)^2(z-1)^3(z^2-6z+1)^2(3z^4-164z^3+370z^2-164z+3)$$

of (2.1) does not vanish. In fact, only a subset of these zeroes will be singularities of the solutions to (2.1).

#### **Lemma 2.2.** If $\zeta \in \mathbb{C}$ is a singularity of a solution to (2.1) then $\zeta$ lies in the set

$$\Xi = \{0, 1, 3 \pm 2\sqrt{2}\}.$$

*Proof.* Following the Sage code from Example 2.1, the command deq.desingularize() returns an order 7 linear differential operator, with leading coefficient  $C(z) = (z-1)^2 z^2 (z^2 - 6z + 1)^2$ , which can be checked to be divisible on the right by the operator deq encoding the differential equation (2.1). The order 7 operator thus annihilates all solutions of (2.1), and hence any singularity of one of these solutions must be a root of C, that is, an element of  $\Xi$ . (See, *e.g.*, [CKS16] for more on desingularization.)

<sup>&</sup>lt;sup>6</sup>Available at http://sagemath.org/. We use version 9.1 (doi:10.5281/zenodo.4066866, Software Heritage persistent identifier swh:1:rel:5e11f7bf8344447a93ae043b915f3b25e62b7ed6).

<sup>&</sup>lt;sup>7</sup>Available at https://github.com/mkauers/ore\_algebra/. We use git revision 2d71b5 (Software Heritage persistent identifier swh:1:rev:2d71b50ebad81e62432482facfe3f78cc4961c4f).

For a given  $\zeta \in \Xi$  some solutions of the differential equation (2.1) may admit convergent power series expansions, while others may admit  $\zeta$  as a singularity. In the present case, for each  $\zeta \in \Xi$  the Fuchs criterion [Poo36, §15] shows that  $\zeta$  is a *regular singular point* of the equation, meaning that the equation admits a full basis of formal solutions of the form

$$g(z) = z^{\nu} \sum_{n=0}^{\infty} \left( \sum_{k=0}^{\kappa} C_{n,k} \log^{k} \frac{1}{1 - z/\zeta} \right) (z - \zeta)^{n}, \qquad (2.2)$$

where  $\nu \in \overline{\mathbb{Q}}$  (the field of algebraic numbers),  $\kappa \in \mathbb{N}$ , and each  $C_{n,k} \in \mathbb{C}$ . In addition, the power series  $\sum_{n=0}^{\infty} C_{n,k}(z-\zeta)^n$  all converge in a disk centered at  $\zeta$  and extending at least up to the closest other singular point. Thus, the expression (2.2) defines an analytic function on a *slit disk*  $\Delta_{\zeta}$  around  $\zeta$  (a disk with a line segment from the center of the disk to the boundary removed).

*Remark* 2.3. We always take  $\log$  to mean the principal branch of the complex logarithm, defined by

$$\log(re^{i\theta}) = \log r + i\theta \quad \text{for } r > 0 \text{ and } -\pi < \theta \leqslant \pi.$$
(2.3)

The cut in  $\Delta_{\zeta}$  then points to the left, and any solution defined in a sector with apex at  $\zeta$  that does not intersect  $\zeta + \mathbb{R}_{<0}$  has a singular expansion as a finite sum of terms of the form (2.2), possibly with different  $\nu$ .

Methods dating back to Frobenius allow one to compute local series expansions of this type to any order for a basis of solutions (see [Poo36, Ch. V] for details).

**Example 2.4.** The point z = 0 is a regular singular point and lies in  $\Xi$ , so solutions of (2.1) may have singularities at the origin but still admit convergent expansions of the type (2.2). The command deq.local\_basis\_expansions(0, order=3) returns truncated expansions

$$A_1(z) = z^{-1} \log z - 9(\log z)^2 + 141 \log z + z \left(\frac{475}{12} - \frac{483}{2} \log^2 z + 3471 \log z\right) + \cdots$$
$$A_2(z) = z^{-1} - 18 \log z + z \left(\frac{625}{2} - 483z \log z\right) + \cdots$$
$$A_3(z) = 1 + \frac{161}{6}z + \cdots$$

for series converging in  $\Delta_0 = \{z : |z| < 3 - 2\sqrt{2}, z \notin \mathbb{R}_{\leq 0}\}$  which form a basis to the solution space of the differential equation. Because the formal series f(z) satisfies (2.1), it converges in  $\Delta_0$  and can be written as a  $\mathbb{C}$ -linear combination of the  $A_j$ . Since f, by definition, involves no logarithmic terms, and  $f(0) = d_0 = 72$ , we can write

$$f(z) = 0 \cdot A_1(z) + 0 \cdot A_2(z) + 72 \cdot A_3(z).$$

As stated above, we wish to find the singularity of f(z) of minimal modulus, so we let  $\rho = 3 - 2\sqrt{2}$  be the non-zero element of  $\Xi$  with minimal modulus.

Example 2.5. The commands

```
sage: rho = QQbar(3-2*sqrt(2))
sage: deq.local_basis_expansions(rho, order=3)
```

return truncated expansions

$$B_{1}(z) = (z - \rho)^{-4} \log(z - \rho) - (z - \rho)^{-3} \left(\frac{5\sqrt{2}}{8} + 1 + \frac{1}{2}\log(z - \rho)\right) + \cdots$$
  

$$B_{2}(z) = (z - \rho)^{-4} - \frac{1}{2}(z - \rho)^{-3} + \cdots$$
  

$$B_{3}(z) = 1 - \left(\frac{5}{\sqrt{2}} + \frac{9}{2}\right)(z - \rho) + \cdots$$
  
(2.4)

for a basis of formal solutions at  $z = \rho$  of (2.1). These formal series converge in a disk around  $z = \rho$  slit along the half-line  $(-\infty, \rho]$ . The general theory of solutions at regular singular points [Poo36, §16] also yields an expansion order past which the degree in  $\log(z - \rho)$  of truncated solutions can no longer increase. Recomputing the expansions up to this bound (which can be done by omitting the order parameter in the above commands) reveals that the terms not displayed here involve  $\log(z - \rho)^2$  factors, but no higher powers of  $\log(z - \rho)$  can appear. In other words, we have  $\kappa = 2$  in the notation of (2.2).

*Remark* 2.6. The ore\_algebra package returns singular expansions which are linear combinations of powers of  $(z-\zeta)$  and  $\log(z-\zeta)$ . For singularity analysis, however, it is convenient to represent these expansions as linear combinations of powers of  $(z - \zeta)$  and  $\log(1/(1 - z/\zeta))$ , so as to obtain expressions that are analytic in a slit neighbourhood of  $\zeta$  with the cut pointing away from 0. As we use the principal branch described in (2.3), we may write  $\log((1 - z/\rho)^{-1}) = \log(-\rho) - \log(z-\rho) + L$  with L = 0 when  $\Im(z) \ge 0$  and  $L = -2\pi i$  when  $\Im(z) < 0$ .

The transfer theorems of Flajolet and Odlyzko [FO90] show how dominant asymptotics of  $d_n$  can be immediately deduced from the singular expansion of f near  $z = \rho$ . The transfer theorems apply because, by Lemma 2.2, the function f extends analytically to the domain

$$\Delta = \{ z : |z| < 1 \} \setminus [\rho, 1].$$
(2.5)

The functions  $\tilde{B}_1, \tilde{B}_2, \tilde{B}_3$  obtained by replacing  $\log(z - \rho)$  by  $\log((1 - z/\rho)^{-1})$  in (2.4) form a basis of the solution space of (2.1) in a neighbourhood of  $\rho$  in  $\Delta$ , and to determine asymptotics it is sufficient to represent f in the  $\tilde{B}_j$  basis. Example 2.4, which expressed f in the  $A_j$  basis, crucially relied on our knowledge of f(z) near the origin, supplied by its power series coefficients  $d_n$ . This argument does not apply at any non-zero point, however it is possible to compute the change of basis matrix between the  $A_j$  and the  $\tilde{B}_j$  when viewed as solutions of (2.1) on the same domain contained in  $\Delta$  using rigorous numeric analytic continuation along a path. By Remark 2.6 each  $\tilde{B}_j$  coincides with  $B_j$  in the upper half-plane, so for practical reasons we compute the change of basis matrix between the  $A_j$  and  $B_j$  bases.

The ore\_algebra package uses numeric approximations of real numbers certified to lie in intervals, as implemented in the Arb library [Joh17]. In what follows, any expression of the form  $[x \pm \varepsilon]$  for  $x \in \mathbb{R}$  and  $\varepsilon \ge 0$  refers to an exact constant which is known to lie in the interval  $[x - \varepsilon, x + \varepsilon]$ . The values displayed in the text are low-precision over-approximations of the intervals used in the actual computation.

**Example 2.7.** We select an analytic continuation path that goes from 0 to  $\rho$  without leaving the domain  $\Delta$ , and, because of the relation between  $B_j$  and  $\tilde{B}_j$ , that arrives at  $\rho$  from the upper half-plane. Using the polygonal path  $\gamma = (0, i, \rho)$  for the required analytic continuation, the commands

sage: M = deq.numerical\_transition\_matrix(path=[0, I, rho], eps=1e-20)
sage: [lambda1, lambda2, lambda3] = M \* vector([0, 0, 72])

compute the change of basis M from the  $A_j$  to the  $B_j$  basis, then determine rigorous approximations  $\lambda_1 = [-0.042 \pm 4 \cdot 10^{-5}] + [\pm 2 \cdot 10^{-14}] i$ ,  $\lambda_2 = [-0.0141 \pm 4 \cdot 10^{-5}] + [0.132 \pm 2 \cdot 10^{-4}] i$ ,  $\lambda_3 = [-12.5 \pm 0.05] + [26.8 \pm 0.02] i$  to the constants  $\lambda_1, \lambda_2, \lambda_3$  such that

$$f(z) = \lambda_1 B_1(z) + \lambda_2 B_2(z) + \lambda_3 B_3(z) = \lambda_1 \tilde{B}_1(z) + \lambda_2 \tilde{B}_2(z) + \lambda_3 \tilde{B}_3(z),$$

where all functions are implicitly extended by analytic continuation along  $\gamma$ .

The expansions (2.4) from Example 2.5 then give the initial terms of a singular expansion

$$f(z) = \left( \left[ 0.0598 \pm 4.79 \cdot 10^{-5} \right] + \left[ \pm 9.21 \cdot 10^{-14} \right] i \right) (z - \rho)^{-4} + \left( \left[ 0.0420 \pm 3.14 \cdot 10^{-5} \right] + \left[ \pm 1.21 \cdot 10^{-14} \right] i \right) (z - \rho)^{-4} \log \frac{1}{1 - z/\rho} + \cdots \right)$$

where '...' hides terms with factors  $(z - \rho)^{\alpha} \log(z - \rho)^{\beta}$  where  $\alpha \ge -3$  and  $\beta \le 2$ . Since f is a real function the imaginary parts appearing in the coefficients are exactly zero, and

$$f(z) = C_1(z-\rho)^{-4} + C_2(z-\rho)^{-4}\log\frac{1}{1-z/\rho} + \cdots$$
(2.6)

for constants  $C_1 = [0.0598 \pm 4.79 \cdot 10^{-5}]$  and  $C_2 = [0.0420 \pm 3.14 \cdot 10^{-5}]$ . The fact that the computed intervals containing  $C_1$  and  $C_2$  do not contain zero confirms that the analytic function f is singular at  $\rho$ .

Corollary 5 of Flajolet and Odlyzko [FO90] gives an explicit formula for the dominant asymptotics of  $d_n$  in terms of the constants in the singular expansion (2.6), leading to dominant asymptotic behaviour

$$d_n = \rho^{n-4} \frac{n^3}{6} \left( C_1 + C_2 (\log n - \gamma - 11/6) \right) + O\left(\rho^{-n} n^2 \log^2 n\right)$$
  
=  $[8.07 \pm 2 \cdot 10^{-3}] \rho^{-n} n^3 \log n + [1.37 \pm 2 \cdot 10^{-3}] \rho^{-n} n^3 + O\left(\rho^{-n} n^2 \log^2 n\right),$  (2.7)

where  $\gamma = [0.58 \pm 4 \cdot 10^{-3}]$  is the Euler–Mascheroni constant. The leading term of the expansion (2.7) is also given in Yu and Chen's article [YC22, (4.8)], albeit without proof or explicit lower bound on the numeric constant. Although we have not computed the constants in closed form, this expansion shows that  $d_n$  is *eventually* positive.

#### **Proposition 2.8.** There exists $N \in \mathbb{N}$ such that $d_n > 0$ for all n > N.

Because Conjecture 1.1 asks us to prove that *all* terms of  $d_n$  are positive, we must delve deeper. We will now show that the positive leading asymptotic term dominates the error in the asymptotic approximation for all n > 1000 (so that one can take N = 1000 above), then computationally check the finite number of remaining values.

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#### **3.** Complete positivity

Our proof mirrors the constructive proofs of transfer theorems for asymptotic behaviour of sequences by Flajolet and Odlyzko [FO90]. The starting point is the Cauchy integral formula. Since f is analytic on the domain  $\Delta$  defined in Equation (2.5), the Cauchy integral formula gives the representation

$$d_n = \frac{1}{2\pi i} \int_{|z|=\delta} \frac{f(z)}{z^{n+1}} dz$$

for any  $0 < \delta < \rho$  and all  $n \ge 0$ . Asymptotic behaviour is determined by manipulating the domain of integration  $\{|z| = \delta\}$  without crossing the singularities of the integrand, so that the integral over part of the domain of integration is negligible while integration over the remaining part can be approximated by replacing f(z) by its singular expansion at its singularity  $z = \rho$  closest to the origin.

Towards our explicit asymptotic bounds, let  $\ell(z)$  denote the leading term in the singular expansion (2.6) of f(z) at  $z = \rho$ , meaning

$$\ell(z) = C_1(z-\rho)^{-4} + C_2(z-\rho)^{-4} \log \frac{1}{1-z/\rho}$$

for the constants  $C_1$  and  $C_2$  in the singular expansion (2.6). This expansion implies the existence of functions  $h_0(z)$ ,  $h_1(z)$ , and  $h_2(z)$ , analytic at  $z = \rho$ , such that

$$f(z) = \ell(z) + \underbrace{(z-\rho)^{-3} \left( h_0(z) + h_1(z) \log \frac{1}{1-z/\rho} + h_2(z) \log^2 \frac{1}{1-z/\rho} \right)}_{g(z)}.$$
 (3.1)

Series expansions of the  $h_j$  at  $z = \rho$  can be computed to arbitrary order with coefficients rigorously approximated to any precision using series expansions of the  $B_j$  basis at  $z = \rho$  and the change of basis matrix M from above.

*Remark* 3.1. Since the origin is the closest element of  $\Xi$  to  $\rho$ , the functions  $h_0, h_1$ , and  $h_2$  appearing in (3.1) are analytic on the disk  $|z - \rho| < \rho$ . Because f and  $\ell$  are both analytic on  $\Delta$ , so is  $g = f - \ell$ .

Write

$$d_n = \frac{1}{2\pi i} \int_{|z|=\delta} \frac{\ell(z)}{z^{n+1}} dz + \frac{1}{2\pi i} \int_{|z|=\delta} \frac{g(z)}{z^{n+1}} dz$$

Behaviour of the first integral, which equals the *n*th power series coefficient of  $\ell(z)$ , is easily lower-bounded using standard generating function manipulations.

**Proposition 3.2.** *For all*  $n \in \mathbb{N}$ *,* 

$$\frac{1}{2\pi i} \int_{|z|=\delta} \frac{\ell(z)}{z^{n+1}} dz \ge \rho^{-n} n^3 \ (8.07 \ \log n + 1.37).$$

*Proof.* Proposition 3.2 is proven in Section 3.1.

After lower-bounding the integral of the leading term  $\ell(z)$ , which is positive for all n, we turn to upper-bounding the integral of the remainder g(z).

**Proposition 3.3.** For all integers  $n \ge 1000$ ,

$$\left|\frac{1}{2\pi i} \int_{|z|=\delta} \frac{g(z)}{z^{n+1}} dz\right| \leqslant 1196 \,\rho^{-n} n^2 \log^2 n.$$

*Proof.* Proposition 3.3 follows from Propositions 3.7, 3.8 (in the limit  $\varphi \to 0$ ), and 3.9 in Section 3.2.

This immediately gives an explicit bound where asymptotic behaviour implies sequence positivity.

**Corollary 3.4.** One has  $d_n > 0$  for all  $n \in \mathbb{N}$ .

*Proof.* Propositions 3.2 and 3.3 imply that

$$d_n \ge \rho^{-n} n^2 \log^2 n \left( 8.07 \frac{n}{\log n} + 1.37 \frac{n}{\log^2 n} - 1196 \right)$$

for all  $n \ge 1000$ . The final factor is increasing for  $n \ge 8$  and positive at n = 1000, hence  $d_n > 0$  for  $n \ge 1000$ . One can explicitly check that  $d_n > 0$  for  $0 \le n < 1000$ .

#### 3.1. Lower-bounding the leading term

If a(z) is a complex-valued function analytic at the origin, we write  $[z^n] a(z)$  for the *n*th term in the power series expansion of a(z) centered at z = 0.

*Proof of Proposition 3.2.* Differentiating the geometric series  $(1-z)^{-1} = \sum_{n \ge 0} z^n$  three times with respect to z implies

$$[z^n] (1-z)^{-4} = \frac{(n+1)(n+2)(n+3)}{6} \ge \frac{n^3}{6}$$

while the identity

$$(1-z)^{-4}\log\frac{1}{1-z} = \frac{d^3}{dz^3} \left(\frac{\log(1/(1-z))}{6(1-z)} - \frac{11}{36(1-z)}\right)$$

implies

$$[z^{n}](1-z)^{-4}\log\frac{1}{1-z} = \frac{(n+1)(n+2)(n+3)}{6}\left(H_{n+3} - \frac{11}{6}\right)$$

where  $H_n = \sum_{k=1}^n 1/k$  is the *n*th harmonic number. Since  $H_n \ge \log n + \gamma$ ,

$$[z^{n}]\ell(z) = [z^{n}]C_{1}(z-\rho)^{-4} + [z^{n}]C_{2}(z-\rho)^{-4}\log\frac{1}{1-z/\rho}$$
$$= C_{1}\rho^{-n-4}[z^{n}](1-z)^{-4} + C_{2}\rho^{-n-4}[z^{n}](1-z)^{-4}\log\frac{1}{1-z}$$
$$\geqslant \left(\frac{C_{1}+(\gamma-11/6)C_{2}}{6\rho^{4}}\right)n^{3}\rho^{-n} + \frac{C_{2}}{6\rho^{4}}n^{3}\rho^{-n}\log n.$$

Note that this lower bound matches the leading asymptotic behaviour (2.7).

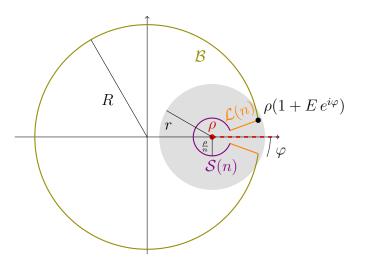


Figure 3.1: The integration path is deformed into the union of a big arc  $\mathcal{B}$ , a small arc  $\mathcal{S}(n)$ , and two line segments  $\mathcal{L}(n)$ . The series expansions of the basis (2.4) are defined on the disk  $|z - \rho| < r$  with a segment removed.

#### 3.2. Upper-bounding the remainder

Following Flajolet and Odlyzko [FO90], to upper-bound the integral of g(z) we deform the domain of integration  $|z| = \delta$ , without crossing any singularities of the integrand, into

- An arc  $\mathcal{B}$  of a 'big' circle of radius  $R > \rho$ ,
- An arc S(n) of a 'small' circle of radius  $\rho/n$ ,
- Two line segments L(n) connecting the arcs of the big and small circles, supported by lines passing through ρ at small angles ±φ with the positive real axis.

See Figure 3.1 for an illustration.

To exploit the series expansions of the  $h_j$  at  $z = \rho$  we select R so that, for large enough n and small enough  $\varphi$ , the paths S(n) and  $\mathcal{L}(n)$  lie within the disk of convergence of these expansions. By Remark 3.1, any  $R < 2\rho$  satisfies this constraint. For our computations it is convenient to pick a radius r such that the punctured disk  $0 < |z - \rho| < r$  does not contain any root of the leading polynomial of the differential equation (2.1) and then choose R with  $\rho < R < \rho + r$ . With this in mind, we take  $r = 1/8 \approx 0.73\rho$  and R just smaller than  $\rho + r$ .

#### 3.2.1 Bounding the Integrals Near the Singularity

The first step towards our desired bounds is to upper-bound  $h_0, h_1$ , and  $h_2$  on the disk  $|z - \rho| < r$ .

**Lemma 3.5.** If  $h_0, h_1, h_2$  are the functions defined in (3.1) then there exist constants

$$b_0 = [6.86 \pm 2.71 \cdot 10^{-4}], \ b_1 = [2.85 \pm 3.20 \cdot 10^{-3}], \ b_2 = [0.309 \pm 2.78 \cdot 10^{-4}]$$
 (3.2)

such that  $|h_j(z)| \leq b_j$  for all  $0 \leq j \leq 2$  and  $|z - \rho| < r$ .

*Proof.* The bounds are computed using the implementation in ore\_algebra of the algorithm described in [Mez19], and full details can be found in the accompanying Sage notebook.

We write the singular expansion of f at  $\rho$  in the form

$$f(\rho+w) = \ell(\rho+w) + w^{-4}\left(u_0(w) + u_1(w)\log w + u_2(w)\frac{\log^2 w}{2}\right), \quad \Im w > 0.$$

Note that the factors  $\log^j(w)$  differ from the  $\log^j(1/(1-z/\rho)) = (\log(-\rho) - \log w)^j$  appearing in the definition (2.6) of the  $h_j$ , and that the polar part  $(z-\rho)^{-3}$  has become  $w^{-4}$ , so that  $u_j(0) =$ 0 for all j. We compute regions containing the coefficients of the truncations  $\tilde{u}_j(w) = c_{j,1}w +$  $\cdots + c_{j,49}w^{49}$  of the  $u_j$  to order 50, and set  $m_0 = \sum_{k=1}^{49} \max_j |c_{j,k}| r^{k-1}$  so that  $|w^{-1}\tilde{u}_j(w)| \leq m_0$  for  $|w| \leq r$ .

Then, to bound the "tails"  $u_j(w) - \tilde{u}_j(w)$ , we change z to  $\rho + w$  in (2.1), and apply [Mez19, Algorithm 6.11] with  $\lambda = -4$ , N = 50, and

$$u_{-4+k} = c_{0,k} + c_{1,k} \log w + (c_{2,k}/2) \log^2 w, \quad k = 49, 48, \dots$$

This yields a *majorant*  $\hat{u}(w)$  with a power series expansion of the form  $\hat{u}(w) = \hat{c}_{50}w^{50} + \hat{c}_{51}w^{51} + \cdots$  whose coefficients satisfy  $|c_{j,k}| \leq \hat{c}_k$  for j = 0, 1, 2 and  $k \geq 50$  [Mez19, Proposition 6.12]. Using [Mez19, Algorithm 8.1], we evaluate  $w^{-1}\hat{u}(w)$  at w = r and obtain a bound  $m_1$  such that  $|w^{-1}(u_j(w) - \tilde{u}_j(w))| \leq m_1$  for  $|w| \leq r$ .

We add these bounds to conclude  $|w^{-1}u_j(w)| \leq m_0 + m_1$  for  $|w| \leq r$ . Finally, if  $a = \log(-\rho)$  the expressions of the  $h_j$  in terms of the  $u_j$  read

$$h_0(z) = w^{-1}\left(u_0 + au_1 + \frac{a^2u_2}{2}\right), \quad h_1(z) = w^{-1}\left(-u_1 - au_2\right), \quad h_2(z) = w^{-1}\frac{u_2}{2},$$

so we may take  $b_j = d_j (m_0 + m_1)$  where  $d_0 = (|a| + |a|^2/2), d_1 = (1 + |a|), \text{ and } d_2 = 1/2.$ 

**Definition 3.6.** Let *B* be the quadratic polynomial  $B(z) = b_0 + b_1 z + b_2 z^2$ , where  $b_0$ ,  $b_1$ , and  $b_2$  are the constants in (3.2).

The bounds on the  $h_j(z)$  in Lemma 3.5 allow us to bound the integrals of g(z) over S(n) and  $\mathcal{L}(n)$ .

**Proposition 3.7.** For all integers  $n \ge 5$ ,

$$\left|\frac{1}{2\pi i} \int_{\mathcal{S}(n)} \frac{g(z)}{z^{n+1}} dz\right| \leqslant \rho^{-n} n^2 \frac{4}{\rho^3} B(\pi + \log n)$$

*Proof.* Let  $n \ge 5$ . Parametrizing  $|z - \rho| = \rho/n$  by  $z = \rho + \rho e^{i\theta}/n$  we have  $|z| \ge \rho(1 - 1/n)$  and

$$\left|\log\frac{1}{1-z/\rho}\right| = \left|\log\left(e^{-i\theta}\right) - \log n\right| \leqslant \pi + \log n,$$

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so, using the fact that  $\rho/n < r$ ,

$$\left| \frac{1}{2\pi i} \int_{\mathcal{S}(n)} \frac{g(z)}{z^{n+1}} dz \right| \leq \frac{\operatorname{length}(\mathcal{S}(n)) \ (n/\rho)^3}{2\pi \rho^{n+1} (1-1/n)^{n+1}} \cdot \max_{z \in \mathcal{S}(n)} \left| h_0(z) + h_1(z) \log \frac{1}{1-z/\rho} + h_2(z) \log^2 \frac{1}{1-z/\rho} \right| \\ \leq \rho^{-n-3} n^2 (1-1/n)^{-n-1} \left( b_0 + b_1(\pi + \log n) + b_2(\pi + \log n)^2 \right).$$

The factor  $(1 - 1/n)^{-n-1}$  is decreasing, and less than 4 for n = 5.

**Proposition 3.8.** For all integers  $n \ge 2$  and all small enough  $\varphi$ ,

$$\left|\frac{1}{2\pi i}\int_{\mathcal{L}(n)}\frac{g(z)}{z^{n+1}}dz\right|\leqslant\rho^{-n}n^2\cdot\frac{B(\pi+\log n)}{\pi\rho^3\cos\varphi}.$$

*Proof.* Fix  $n \ge 2$ . The integral over the upper part of  $\mathcal{L}(n)$  equals

$$L_{+}(n) = \frac{1}{2\pi i} \int_{\rho(1+e^{i\varphi/n})}^{\rho(1+E\,e^{i\varphi/n})} \frac{g(z)}{z^{n+1}} dz = \frac{1}{2\pi i} \sum_{j=0}^{2} \int_{\rho(1+e^{i\varphi/n})}^{\rho(1+E\,e^{i\varphi/n})} \frac{h_{j}(z)\log^{j}\frac{1}{1-z/\rho}}{(z-\rho)^{3}z^{n+1}} dz$$

for some  $E \ge r$  (depending on  $\varphi$  but not on n). The substitution  $z = \rho(1 + e^{i\varphi}t/n)$  yields

$$L_{+}(n) = \frac{1}{2\pi} \sum_{j=0}^{2} \int_{1}^{E_{n}} \frac{h_{j} \left(\rho(1 + e^{i\varphi}t/n)\right) \log^{j}(-e^{i\varphi}n/t)}{(\rho e^{i\varphi}t/n)^{3} \rho^{n+1} (1 + e^{i\varphi}t/n)^{n+1}} \frac{\rho e^{i\varphi}}{n} dt.$$

When  $\varphi > 0$  is small enough, one has  $\log(-e^{i\varphi}n/t) = i(\varphi - \pi) + \log(n/t)$ , and the integration segment is contained in the disk  $|z - \rho| \leq r$ , so that  $|h_j(z)| \leq b_j$  in the integrand. Therefore the modulus of the integral satisfies

$$|L_{+}(n)| \leq \rho^{-n} n^{2} \cdot \frac{B(\pi + \log n)}{2\pi\rho^{3}} \cdot \int_{1}^{\infty} t^{-3} \left(1 + \frac{t\cos\varphi}{n}\right)^{-n-1} dt$$

where

$$\int_{1}^{\infty} t^{-3} \left( 1 + \frac{t \cos \varphi}{n} \right)^{-n-1} dt \leqslant \int_{1}^{\infty} \left( 1 + \frac{t \cos \varphi}{n} \right)^{-n-1} dt = \frac{1}{\cos \varphi} \left( 1 + \frac{\cos \varphi}{n} \right)^{-n}$$

The right-hand side is decreasing, and is bounded by  $1/\cos\varphi$  as soon as  $n \ge 2$  and  $\varphi < \pi/3$ . The same reasoning applies to the integral over the other part of  $\mathcal{L}(n)$ , with the sole difference that  $\varphi$  is replaced by  $-\varphi$ , so that the logarithmic factor in the integrand becomes  $i(-\varphi + \pi) + \log(n/t)$ .

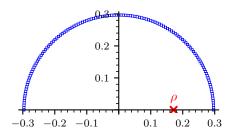


Figure 3.2: The overlapping rectangles used to establish Proposition 3.9.

#### 3.2.2 Bounding the Integral on the Big Circle

Finally, we can bound the integral over the big circle.

**Proposition 3.9.** *For all*  $n \in \mathbb{N}$ *,* 

$$\left|\frac{1}{2\pi i} \int_{\mathcal{B}} \frac{g(z)}{z^{n+1}} dz\right| \leqslant 1753.15 \, R^{-n}$$

Proof. Standard integral bounds imply

$$\left|\frac{1}{2\pi i} \int_{\mathcal{B}} \frac{g(z)}{z^{n+1}} dz\right| \leqslant R^{-n} \cdot \max_{z \in \mathcal{B}} |g(z)| = R^{-n} \cdot \max_{z \in \mathcal{B}} |f(z) - \ell(z)|.$$

Since we know  $\ell(z)$  in closed form, the stated upper bound follows bounding f(z) on the circle |z| = R. In fact, because  $\overline{f(z)} = f(\overline{z})$  it is sufficient to upper bound  $f(z) - \ell(z)$  on the upper half of |z| = R. This is accomplished by covering this half-circle by overlapping rectangles with rational coordinates, displayed in Figure 3.2, then rigorously computing bounds for f(z) and  $\ell(z)$  on these rectangles.

Numeric regions containing the image by f of each rectangle are computed in Sage using the numerical\_solution() method of differential operators to solve the differential equation (2.1) in interval arithmetic. This method implements a strategy very similar to the one we employed to bound the functions  $h_j$  in the proof of Lemma 3.5—but limited to the simpler case where the function to be evaluated is a solution of the differential equation over a domain free of singularities, as opposed to a function obtained starting from a solution by factoring out a singular part.

## 4. Final remarks

#### 4.1. Multivariate techniques

Yu and Chen [YC22] give the sequence  $(d_n)$  as a nested sequence of binomial sums, and such a sequence can be automatically written as the diagonal of the power series expansion of a multi-variate rational function using algorithms of Bostan et al. [BLS17]. The field of analytic combinatorics in several variables [PW13, Mel21] aims to determine the asymptotics of such rational

diagonals by expressing them as an integer sum of multivariate saddle-point integrals. Determining the integer coefficients in this decomposition is an open problem in general, and the domains of integration for these saddle-point integrals are only defined explicitly in some cases (in general, they are defined using gradient flows on algebraic varieties). More practically, when we ran the Maple implementation of Bostan et al. [BLS17] on the binomial sum expressions in Yu and Chen [YC22] the computation did not terminate (we ran the program for more than an hour on a modern laptop). Thus, although it is theoretically possible to approach Theorem 1.4 and similar results through explicit bounds for multivariate saddle-point integrals, multivariate techniques have several severe drawbacks compared to our univariate approach. On the other hand, when the techniques of analytic combinatorics in several variables succeed they give explicit constants (instead of certified intervals) for leading asymptotic terms. Baryshnikov et al. [BMP21] detail an example combining the analysis of a D-finite function with multivariate techniques to explicitly determine leading asymptotic coefficients. Such a hybrid strategy could be extended with our present approach to additionally bound sub-dominant terms.

#### 4.2. A more direct proof of Conjecture 1.1

While the proof of Conjecture 1.2 is interesting in its own right, Yu and Chen's uniqueness result only requires that the function f(z) take positive values on the real interval  $z \in (0, \rho)$ [YC22, Sec. 1.3, III and Sec. 4.5]<sup>8</sup>. This weaker statement is easier to prove using rigorous numerics than the positivity of the coefficient sequence. The idea is to split the interval  $[\varepsilon, \rho - \varepsilon]$ into subintervals over which we can evaluate f accurately enough to check that it is positive, handling the limits  $z \to 0$  and  $z \to \rho$  as in the proof of Lemma 3.5.

The presence in the interior of the interval of a root  $z_0 = 0.019...$  of the leading coefficient  $c_3(z)$  of the differential equation (2.1) with  $z_0 \notin \Xi$  (an *apparent singularity* of the differential equation) causes a small complication, for numerical\_solution() currently does not support evaluation on (non-point) intervals containing singular points. One way around the issue would be to treat this singularity like 0 and  $\rho$ . As a quicker alternative, we perform a *partial desingularization* of (2.1), yielding a new differential equation satisfied by f that does not have  $z_0$  as a singularity while not being as large and difficult to solve numerically as the fully desingularized equation of Lemma 2.2.

Using this new equation, no additional subinterval besides the neighborhoods of 0 and  $\rho$  turns out to be necessary. Indeed, one can show that the tail  $\sum_{n=58}^{\infty} d_n z^n$  of the series expansion of fat the origin is bounded by 1.71 for  $|z| \leq r_0 = 0.0675$ . As  $d_0 = 72$  and  $d_n > 0$  for all  $n \leq 1000$ , this implies that f(z) > 0 for  $0 < z < r_0$ . Then, reusing the results of the computations done for the proof of Lemma 3.5 and its notation, one has  $|u(w) - \tilde{u}(w)| \leq \hat{u}(\rho - r_0) \leq m = 7.82 \cdot 10^{-9}$ for  $w \leq \rho - r_0$ . We rewrite the local expansion of f in terms of  $-w = \rho - z$  and  $-\log(-w)$ , both positive for  $r_0 < z < \rho$ , and subtract  $m (1 - \log(\rho - z) - (1/2) \log^2(\rho - z))$  from its explicitly computed order-50 truncation to obtain a lower bound on f(z). This lower bound is an explicit polynomial in w and  $\log(-w)$  that can be verified to take positive values for  $r_0 - \rho < w < 0$ . Details of the calculations can be found in the accompanying Sage notebook.

<sup>&</sup>lt;sup>8</sup>Our f(z) is equal to  $\overline{D}(z)$  in Yu and Chen's notation, so that  $D(z) = 2zf(z^2)$ , and we have  $\rho = (\sqrt{2} - 1)^2$ .

#### 4.3. Possible extensions and limitations

The method employed here to study the sequence  $(d_n)$  can be used, more generally, to produce approximations with error bounds

$$u_n = \rho^{-n} n^{\alpha} \sum_{k=0}^{K} \sum_{j=0}^{J} [c_{k,j} \pm \varepsilon_{k,j}] \frac{\log^j n}{n^k}, \qquad n \ge n_0,$$

of sequences  $u_n$  whose generating series satisfy linear differential equations with polynomial coefficients and regular dominant singularities.

However, it does not produce *arbitrarily tight* asymptotic enclosures for every sequence, and the best enclosure one obtains for a given positive sequence may be too coarse to prove its positivity. For example:

- The proof presented in this article relies on the existence of an asymptotic expansion whose leading term is asymptotically positive. The C-finite, positive sequence u<sub>n</sub> = 2 + (−1)<sup>n</sup> admits no such expansion, but the approach easily adapts to show that u<sub>n</sub> = [2 ± ε] + [1 ± ε](−1)<sup>n</sup> ≥ 0. In the case of v<sub>n</sub> = 1.1 + (−1)<sup>n</sup> + cos(nπ/2), however, additional arguments are necessary (cf. [vdH97]).
- The sequence w<sub>n</sub> = J<sub>n</sub>(1)/n!, where J<sub>n</sub> is the Bessel function of the first kind, satisfies (n + 1)(n + 2)w<sub>n+2</sub> 2(n + 1)<sup>2</sup>w<sub>n+1</sub> + w<sub>n</sub> = 0. One has w<sub>n</sub> ~ 1/(2<sup>n</sup>n!<sup>2</sup>), hence w<sub>n</sub> is asymptotically positive. The minimal differential equation annihilating the generating series f(z) = ∑<sub>n≥0</sub> w<sub>n</sub>z<sup>n</sup> is (2z 1)f''(z)+2f'(z)-1 = 0. This equation has a (genuine, regular) singular point at z = 1/2, so that the best our numeric approach can prove is that w<sub>n</sub> = [0±ε] t<sub>n</sub> for some explicit t<sub>n</sub> with t<sub>n</sub> = 2<sup>n</sup> n<sup>O(1)</sup> and any given ε > 0. This is related to the fact that (w<sub>n</sub>) is a minimal solution of the corresponding recurrence; the enclosure would have the correct order of magnitude for any solution not collinear with w<sub>n</sub>.
- According to Ouaknine and Worrell [OW14], an algorithm capable of deciding in full generality whether a *C-finite* sequence of order 6 is *ultimately* positive would imply a major breakthrough in Diophantine approximation. Besides, it is classical that the positivity problem for C-finite sequences is at least as hard as the Skolem problem: proving that (u<sup>2</sup><sub>n</sub>) contains only positive terms is equivalent to proving u<sub>n</sub> ≠ 0 for all n. The crucial open case for decidability of the Skolem problem [OW12] concerns order 5 sequences (u<sub>n</sub>) of the form u<sub>n</sub> = a(λ<sup>n</sup><sub>1</sub> + λ<sup>n</sup><sub>1</sub>) + b(λ<sup>n</sup><sub>2</sub> + λ<sup>n</sup><sub>2</sub>) + cρ<sup>n</sup> where |λ<sub>1</sub>| = |λ<sub>2</sub>| > |ρ| with a, b, c real algebraic numbers and |a| ≠ |b|.

Although there are major decidability issues related to the positivity of C-finite sequences, in naturally occurring combinatorial examples these pathological issues typically do not arise<sup>9</sup> and

<sup>&</sup>lt;sup>9</sup>For instance, in her address to the 2006 ICM, Bousquet-Mélou [BM06] stated that she "never met a counting problem that would yield a rational, but not  $\mathbb{N}$ -rational GF."  $\mathbb{N}$ -rational functions are a proper sub-class of rational functions defined as the smallest set that contains 1 and a variable x and is closed under addition, multiplication, and *pseudo-inverse*  $f \mapsto 1/(1-xf)$ . The singularities of an  $\mathbb{N}$ -rational function that are closest to the origin differ by multiples of roots of unity [Ber71], leading to predicable periodic behaviour.

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one can easily determine positivity using classical asymptotic results. In contrast, the increased complexity of P-recursive sequences means that even in the "easy" case when a sequence has positive asymptotic behaviour it is not easy to prove complete positivity of the sequence. Inspired by a real-world application brought to our attention by non-combinatorialists, we have provided a method to close this gap between positivity proofs for C-finite and P-recursive sequences. We leave it for future work to understand exactly how general it can be made, and how to turn it into a practical algorithm that would automatically choose judicious values for all parameters.

# Acknowledgments

The authors thank Thomas Yu for bringing the uniqueness of the Canham model, and its connection to integer sequence positivity, to our attention, Joris van der Hoeven for pointing out the possible connection to [vdH97], Alin Bostan for interesting comments on [KLOW20], and the anonymous referees for their careful reading.

## References

[AG72]	Richard Askey and George Gasper. Certain rational functions whose power series have positive coefficients. <i>Amer. Math. Monthly</i> , 79:327–341, 1972.					
[BCG <sup>+</sup> 17]	Alin Bostan, Frédéric Chyzak, Marc Giusti, Romain Lebreton, Grégoire Lecerf, Bruno Salvy, and Éric Schost. <i>Algorithmes Efficaces en Calcul Formel</i> . Frédéric Chyzak (self-pub.), Palaiseau, 2017. URL: https://hal.archives-ouvertes. fr/AECF/.					
[Ber71]	Jean Berstel. Sur les pôles et le quotient de Hadamard de séries N-rationnelles. <i>C. R. Acad. Sci. Paris Sér. A-B</i> , 272:A1079–A1081, 1971.					
[BLS17]	Alin Bostan, Pierre Lairez, and Bruno Salvy. Multiple binomial sums. J. Symbolic Comput., 80(2):351–386, 2017. doi:10.1016/j.jsc.2016.04.002.					
[BM06]	Mireille Bousquet-Mélou. Rational and algebraic series in combinatorial enumer- ation. In <i>International Congress of Mathematicians</i> . <i>Vol. III</i> , pages 789–826. Eur. Math. Soc., Zürich, 2006.					
[BMP21]	Y. Baryshnikov, S. Melczer, and R. Pemantle. Stationary points at infinity for analytic combinatorics. <i>Foundations of Computational Mathematics</i> , 2021.					
[BY22]	Alin Bostan and Sergey Yurkevich. A hypergeometric proof that lso is bijec- tive. <i>Proceedings of the American Mathematical Society</i> , 150:2131–2136, 2022. URL: https://hal.archives-ouvertes.fr/hal-03426008, doi:10.1090/ proc/15836.					
[Can70]	P. B. Canham. The minimum energy of bending as a possible explanation of the biconcave shape of the human red blood cell. <i>J. Theor. Biol.</i> , 26(1):61–81, Jan 1970.					

- [Cau42] Augustin Cauchy. Mémoire sur l'emploi du nouveau calcul, appelé calcul des limites, dans l'intégration d'un système d'équations différentielles. *Comptes-rendus de l'Académie des Sciences*, 15:14, July 1842.
- [Cha14] Yongjae Cha. Closed form solutions of linear difference equations in terms of symmetric products. *Journal of Symbolic Computation*, 60:62–77, 2014. doi: 10.1016/j.jsc.2013.10.002.
- [CKS16] Shaoshi Chen, Manuel Kauers, and Michael F. Singer. Desingularization of Ore operators. *Journal of Symbolic Computation*, 74:617–626, May 2016. doi:10. 1016/j.jsc.2015.11.001.
- [CYB<sup>+</sup>19] J. Chen, T. P.-Y. Yu, Kusner. R. Brogan, P., Y. Yang, and A. Zigerelli. Numerical methods for biomembranes: conforming subdivision versus non-conforming PL methods. 2019. arXiv:1901.09990.
- [FO90] Philippe Flajolet and Andrew Odlyzko. Singularity analysis of generating functions. *SIAM J. Discrete Math.*, 3(2):216–240, 1990. doi:10.1137/0403019.
- [FP86] Philippe Flajolet and Claude Puech. Partial match retrieval of multidimensional data. Journal of the ACM, 33(2):371–407, 1986. URL: http://algo.inria.fr/ flajolet/Publications/FlPu86.pdf.
- [FS09] Philippe Flajolet and Robert Sedgewick. *Analytic combinatorics*. Cambridge University Press, Cambridge, 2009. doi:10.1017/CB09780511801655.
- [GK05] Stefan Gerhold and Manuel Kauers. A procedure for proving special function inequalities involving a discrete parameter. In *Proceedings of the 2005 International Symposium on Symbolic and Algebraic Computation*, ISSAC '05, pages 156–162, New York, NY, USA, July 2005. Association for Computing Machinery. doi:10.1145/1073884.1073907.
- [Joh17] Fredrik Johansson. Arb: Efficient arbitrary-precision midpoint-radius interval arithmetic. *IEEE Transactions on Computers*, 66(8):1281–1292, 2017. arXiv: 1611.02831, doi:10.1109/TC.2017.2690633.
- [KJJ15] Manuel Kauers, Maximilian Jaroschek, and Fredrik Johansson. Ore polynomials in Sage. In Computer algebra and polynomials, volume 8942 of Lecture Notes in Comput. Sci., pages 105–125. Springer, Cham, 2015. doi:10.1007/ 978-3-319-15081-9\_6.
- [KLOW20] George Kenison, Richard Lipton, Joël Ouaknine, and James Worrell. On the Skolem problem and prime powers. In *Proceedings of the 45th International Symposium on Symbolic and Algebraic Computation*, ISSAC '20, pages 289–296, New York, NY, USA, 2020. Association for Computing Machinery.
- [KMR14] Laura Gioia Andrea Keller, Andrea Mondino, and Tristan Rivière. Embedded surfaces of arbitrary genus minimizing the Willmore energy under isoperimetric constraint. *Arch. Ration. Mech. Anal.*, 212(2):645–682, 2014.
- [KP10] Manuel Kauers and Veronika Pillwein. When can we detect that a P-finite sequence is positive? In *ISSAC 2010—Proceedings of the 2010 International Symposium*

on Symbolic and Algebraic Computation, pages 195–201. ACM, New York, 2010. doi:10.1145/1837934.1837974.

- [MB95] Xavier Michalet and David Bensimon. Vesicles of toroidal topology: Observed morphology and shape transformations. *Journal de Physique II*, 5(2):263–287, February 1995.
- [Mel21] Stephen Melczer. An Invitation to Analytic Combinatorics: From One to Several Variables. Texts and Monographs in Symbolic Computation. Springer International Publishing, 2021.
- [Mez16] Marc Mezzarobba. Rigorous multiple-precision evaluation of D-finite functions in SageMath. Extended abstract of a talk at the 5th International Congress on Mathematical Software, 2016. arXiv:1607.01967.
- [Mez19] Marc Mezzarobba. Truncation bounds for differentially finite series. Ann. H. Lebesgue, 2:99–148, 2019. doi:10.5802/ahl.17.
- [MN14] Fernando C. Marques and André Neves. Min-max theory and the Willmore conjecture. *Annals of Mathematics*, pages 683–782, 2014. doi:10.4007/annals. 2014.179.2.6.
- [OW12] Joël Ouaknine and James Worrell. Decision problems for linear recurrence sequences. In Alain Finkel, Jérôme Leroux, and Igor Potapov, editors, *Reachability Problems*, Lecture Notes in Computer Science, pages 21–28, Berlin, Heidelberg, 2012. Springer. doi:10.1007/978-3-642-33512-9\_3.
- [OW14] Joël Ouaknine and James Worrell. Positivity problems for low-order linear recurrence sequences. In *Proceedings of the Twenty-Fifth Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 366–379. Society for Industrial and Applied Mathematics, 2014. doi:10.1137/1.9781611973402.27.
- [Pil13] Veronika Pillwein. Termination conditions for positivity proving procedures. In Proceedings of the 38th International Symposium on Symbolic and Algebraic Computation, ISSAC '13, pages 315–322, New York, NY, USA, 2013. Association for Computing Machinery. doi:10.1145/2465506.2465945.
- [Poo36] Edgar Girard Croker Poole. *Introduction to the theory of linear differential equations.* Clarendon Press, New York, 1936.
- [PW13] Robin Pemantle and Mark C. Wilson. Analytic combinatorics in several variables, volume 140 of Cambridge Studies in Advanced Mathematics. Cambridge University Press, Cambridge, 2013. doi:10.1017/CB09781139381864.
- [Sch12] Johannes Schygulla. Willmore minimizers with prescribed isoperimetric ratio. *Arch. Ration. Mech. Anal.*, 203(3):901–941, 2012.
- [Sei97] Udo Seifert. Configurations of fluid membranes and vesicles. *Adv. Phys.*, 46(1):13–137, 1997.
- [Sko34] T. Skolem. Ein Verfahren zur Behandlung gewisser exponentialer Gleichungen und diophantischer Gleichungen. In 8. Skand. Mat. Kongr., pages 163–188, Stockholmn, 1934.

[Sze33]	G. Szegö. Über gewisse Potenzreihen mit lauter positiven Koeffizienten. Math. Z.,
	37(1):674–688, 1933.

- [vdH97] Joris van der Hoeven. On the computation of limsups. Journal of Pure and Applied Algebra, 117:381–394, 1997. URL: https://hal.archives-ouvertes. fr/hal-03209583.
- [Wil65] Thomas J. Willmore. Note on embedded surfaces. Analele ştiinţifice ale Universităţii "Alexandru Ioan Cuza" din Iaşi. Matematică (Serie nouă), 11(493-496):18, 1965.
- [YC22] Thomas Yu and Jingmin Chen. Uniqueness of Clifford torus with prescribed isoperimetric ratio. *Proceedings of the American Mathematical Society*, 150:1749–1765, 2022. doi:10.1090/proc/15750.

## **Appendix:** The recurrence and differential equation coefficients

The sequence  $(d_n)$  satisfies the recurrence (1.2) with coefficients  $r_j(n)$  determined by the matrix equation  $(r_0, \ldots, r_7)^T = M(1, n, \ldots, n^7)^T$  where M equals

$\begin{pmatrix} -13041659232\\ 145756088208\\ -647595717744\\ 1390493835900\\ -1472211879228\\ 709311266388\\ -119236161300\\ 6546653568 \end{pmatrix}$	$\begin{array}{c} -12704294700\\ 149564708370\\ -677411701022\\ 1451619424860\\ -1524577250976\\ 732023855346\\ -125550276502\\ 7041743904 \end{array}$	$\begin{array}{r} -5284701480\\ 65315724828\\ -301814933466\\ 645518710454\\ -672459054524\\ 321841622840\\ -56351691266\\ 3234766134\end{array}$	$\begin{array}{c} -1216898711\\ 15735207287\\ -74228837833\\ 158457515673\\ -163720428321\\ 78121412337\\ -13970430847\\ 822460415\end{array}$	$\begin{array}{r} -167529251\\ 2258693435\\ -10882115811\\ 23184921987\\ -23758375953\\ 11304865929\\ -2065443305\\ 124982969\end{array}$	$\begin{array}{c} -13789578\\ 193221622\\ -950915746\\ 2021855198\\ -2054897438\\ 975235426\\ -182059702\\ 11350218\end{array}$	$\begin{array}{r} -628408\\ 9123400\\ -45861816\\ 97303624\\ -98090344\\ 46440856\\ -8857640\\ 570328\end{array}$	$\begin{array}{c} -12232\\ 183480\\ -941864\\ 1993816\\ -1993816\\ 941864\\ -183480\\ 12232 \end{array} \right)$
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and its generating function f(z) satisfies the differential equation (2.1) where

$$\begin{split} c_3 &= z^2 \cdot (z+1)^2 \cdot (z-1)^3 \cdot (z^2-6z+1)^2 \cdot (3z^4-164z^3+370z^2-164z+3), \\ c_2 &= z \cdot (z+1) \cdot (z-1)^2 \cdot (z^2-6z+1) \\ &\quad \cdot (66z^8-3943z^7+18981z^6-16759z^5-30383z^4+47123z^3-17577z^2+971z-15), \\ c_1 &= 2 \cdot (z-1) \cdot (210z^{12}-13761z^{11}+101088z^{10}-178437z^9-248334z^8+930590z^7-446064z^6 \\ &\quad - 694834z^5+794998z^4-267421z^3+24144z^2-649z+6), \\ c_0 &= 2 \cdot (378z^{12}-25452z^{11}+145173z^{10}-143106z^9-639207z^8+1565968z^7-506446z^6 \\ &\quad - 1822124z^5+2348092z^4-1142836z^3+228041z^2-10178z+161). \end{split}$$