SEQUENCE POSITIVITY THROUGH NUMERIC ANALYTIC CONTINUATION: UNIQUENESS OF THE CANHAM MODEL FOR BIOMEMBRANES

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 non-negativity 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 computationally.

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[1] g and constants a_0 and v_0 determined by physical details, such as ambient temperature, 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*

$$W(S) = \int_S H^2 \, dA, \tag{1}$$

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 ι_0 between zero and one. In genus one, Keller et al. [KMR14] show solution existence for values of $\iota_0 \in [\tau, 1)$ with $\tau = \frac{3}{2^{5/4}\sqrt{\pi}}$. 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

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[1] 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].

and uniqueness for the Canham model have been carried out in Seifert [Sei97] and Chen et al. [CYB+19]. Recent work of Yu and Chen [YC20] further investigates the uniqueness problem, with a focus on the genus one case[2].

Conjecture 1.1 (Yu and Chen [YC20])**.** Up to homothety, the *Clifford torus* defined by a stereographic image in $\mathbb{R}^3$ of $\{[\cos u, \sin u, \cos v, \sin v]/\sqrt{2} : u, v \in [0, 2\pi]\}$ is uniquely determined by its isoperimetric ratio. The Clifford torus is the unique solution of the Canham model in genus $g = 1$ when $\iota_0 \in [\tau, 1)$.

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 $(d_0, \ldots, d_6) = \big(72, 1932, 31248, \frac{790101}{2}, \frac{17208645}{4}, \frac{338898609}{8}, \frac{1551478257}{4}\big)$ satisfying the explicit order seven linear recurrence relation

$$\sum_{i=0}^{7} r_i(n) d_{n+i} = 0, \qquad r_j(n) \in \mathbb{Z}[n] \tag{2}$$

whose coefficients r_j are defined in the appendix.

Conjecture 1.2 (Yu and Chen [YC20])**.** All terms of the sequence (d_n) are positive.

Proposition 1.3 (Yu and Chen [YC20])**.** *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 (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 (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[3].

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

1.1. Related work.

Our approach to sequence postivity 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

[2] Conjecture 1.1 was labeled Conjecture 1.1 in the original draft of [YC20], and then upgraded to Theorem 1.1 after those authors were informed that the present work proves their conjecture.

[3] https://mybinder.org/v2/zenodo/10.5281/zenodo.4274505/?filepath=Positivity.ipynb

by a linear recurrence with constant coefficients and a sufficient number of initial terms, whether any term in the sequence is zero. Because the term-wise product $(a_n b_n)$ of any two C-finite sequences (a_n) and (b_n) is also C-finite, 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.

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 (2)—was further studied by Kauers and Pillwein [KP10, Pil13], who gave extensions of the basic technique and sufficient conditions for termination[4]. 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*,

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

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$^+$17, Ch. 14] for details. In this case, $f(z)$ satisfies a third-order differential equation

$$c_3(z)F'''(z) + c_2F''(z) + c_1F'(z) + c_0F(z) = 0, \qquad c_j(z) \in \mathbb{Z}[z] \tag{3}$$

whose coefficients are given explicitly in the appendix.

[4]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 [YC20].

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Because (3) is a *linear* 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 (3) by a finite number of initial conditions $F(0) = d_0, F'(0) = d_1, \ldots$. Although $f(z)$ cannot be easily expressed in closed form, we can leverage its representation as a solution of (3) to compute enough information to prove positivity of (d_n). Our computations are carried out in the Sage[5] ore_algebra[6] package [KJJ15, Mez16].

Example 2.1. The ore_algebra package represents linear differential equations such as (3) 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 (3) 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 taking $f(z)$ 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 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 (3). The classical Cauchy existence theorem for analytic differential equations implies that analytic solutions of (3) can be analytically continued to any simply connected domain $\Omega \subseteq \mathbb{C}$ where the leading coefficient

$$c_3(z) = 8388593z^2(z+1)^2(z-1)^3(z^2-6z+1)^2(3z^4-164z^3+370z^2-164z+3)$$

of (3) does not vanish. In fact, only a subset of these zeroes will be singularities of the solutions to (3).

Lemma 2.2. *If $\zeta \in \mathbb{C}$ is a singularity of a solution to* (3) *then ζ lies in the set*

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

Proof. Following the Sage code above, the command `desing_deq.desingularize()` returns an order 7 linear differential equation, satisfied by all solutions of (3), whose leading coefficient polynomial is $C(z) = (z-1)^2 z^2 (z^2 - 6z + 1)^2$. The stated

[5] Available at http://sagemath.org/. We use version 9.1 (doi:10.5281/zenodo.4066866, Software Heritage persistent identifier swh:1:rel:5e11f7bf8344447a93ae043b915f3b25e62b7ed6).

[6] Available at https://github.com/mkauers/ore_algebra/. We use git revision 2d71b5 (Software Heritage persistent identifier swh:1:rev:2d71b50ebad81e62432482facfe3f78cc4961c4f).

conclusion then follows from the Cauchy existence theorem applied to this differential equation, as the roots of C form the set Ξ. □

For a given $\zeta \in \Xi$ some solutions of the differential equation (3) may admit convergent power series expansions, while others may admit ζ as a singularity. In the present case, for each $\zeta \in \Xi$ the Fuchs criterion [Poo36, §55] shows that ζ is a *regular singular point* of the equation, meaning the equation admits a full basis of formal solutions of the form

$$g(z) = z^{\nu} \sum_{n=0}^{\infty} \left(\sum_{k=0}^{\kappa} C_{n,k} \log^k \frac{1}{1 - z/\zeta} \right) (z-\zeta)^n \,, \tag{4}$$

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 ζ and extending at least up to the closest other singular point. Thus, the expression (4) defines an analytic function on a *slit disk* Δ_ζ around ζ (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

$$\log(re^{i\theta}) = \log r + i\theta \quad \text{for } r > 0 \text{ and } -\pi < \theta \leq \pi. \tag{5}$$

The cut in Δ_ζ then points to the left, and any solution defined in a sector with apex at ζ that does not intersect $\zeta + \mathbb{R}_{<0}$ has a singular expansion as a finite sum of terms of the form (4), possibly with different ν.

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 $z = 0$ lies in Ξ, so solutions of (3) may have singularities at the origin. The command `deq.local_basis_expansions(0, order=3)` returns truncated expansions

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

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

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

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 Ξ 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

$$
\begin{aligned}
&B_1(z) = (z-\rho)^{-4}\log(z-\rho) - (z-\rho)^{-3}\left(\tfrac{5\sqrt{2}}{8} + 1 + \tfrac{1}{2}\log(z-\rho)\right) + \cdots \\
(6)\qquad &B_2(z) = (z-\rho)^{-4} - \tfrac{1}{2}(z-\rho)^{-3} + \cdots \\
&B_3(z) = 1 - \left(\tfrac{5}{\sqrt{2}} + \tfrac{9}{2}\right)(z-\rho) + \cdots
\end{aligned}
$$

for a basis of formal solutions at $z = \rho$ of (3). These formal series converge in a disk around $z = \rho$ slit along the half-line $(-\infty, \rho]$. Running the same command without the `order` parameter reveals that the terms not displayed here also involve $\log(z-\rho)^2$ and shows that no higher powers of $\log(z-\rho)$ can appear; i.e., in the notation of (4) we have $\kappa = 2$. ◁

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 $\log\big(1/(1-z/\zeta)\big)$, so as to obtain expressions that are analytic in a slit neighbourhood of ζ with the cut pointing away from 0. As we use the principal branch described in (5), we may write $\log((1-z/\rho)^{-1}) = \log(-\rho) - \log(z-\rho) + L$ with $L = 0$ when $\Im(z) \geq 0$ 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

$$
\Delta = \{z : |z| < 1\} \setminus [\rho, 1]. \tag{7}
$$

The functions $\tilde{B}_1, \tilde{B}_2, \tilde{B}_3$ obtained by replacing $\log(z-\rho)$ by $\log((1-z/\rho)^{-1})$ in (6) form a basis of the solution space of (3) in a neighbourhood of ρ in Δ, 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 (3) on the same domain contained in Δ 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 $\varepsilon \geq 0$ 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 ρ without leaving the domain Δ, and, because of the relation between B_j and $\tilde{B}_j$, that arrives at ρ 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 $\lambda_1 = [-0.042 \pm 4{\cdot}10^{-5}] + [\pm 2{\cdot}10^{-14}]\,i$, $\lambda_2 = [-0.0141 \pm 4{\cdot}10^{-5}] +$

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$[0.132 \pm 2{\cdot}10^{-4}]\, i$, $\lambda_3 = [-12.5 \pm 0.05] + [26.8 \pm 0.02]\, i$ 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 γ. The expansions (6) from Example 2.5 then give the initial terms of a singular expansion

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

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

$$f(z) = C_1 (z-\rho)^{-4} + C_2 (z-\rho)^{-4} \log \frac{1}{1 - z/\rho} + \cdots \tag{8}$$

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 ρ. ◁

Corollary 5 of Flajolet and Odlyzko [FO90] gives an explicit formula for dominant asymptotics of d_n in terms of the constants in the singular expansion (8), leading to dominant asymptotic behaviour

$$\begin{aligned} d_n &= \rho^{n-4} \frac{n^3}{6} \big(C_1 + C_2(\log n - \gamma - 11/6)\big) + O\left(\rho^{-n} n^2 \log^2 n\right) \\ &= [8.07 \pm 2{\cdot}10^{-3}]\, \rho^{-n} n^3 \log n + [1.37 \pm 2{\cdot}10^{-3}]\, \rho^{-n} n^3 + O\left(\rho^{-n} n^2 \log^2 n\right), \end{aligned} \tag{9}$$

where $\gamma = [0.58 \pm 4{\cdot}10^{-3}]$ is the Euler-Mascheroni 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 *all* terms of d_n are positive, we must delve deeper. We determine a precise natural number N such that the positive leading asymptotic term dominates the error in the asymptotic approximation for $n > N$, then computationally check the finite number of remaining values.

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 Δ defined in Equation (7), 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 $n \geq 0$. 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.

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Towards our explicit asymptotic bounds, let $\ell(z)$ denote the leading term in the singular expansion (8) 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 (8). This expansion implies the existence of functions $h_0(z), h_1(z)$, and $h_2(z)$, analytic at $z = \rho$, such that

$$f(z) = \ell(z) + \underbrace{(z-\rho)^{-3}\left(h_0(z) + h_1(z)\log\frac{1}{1-z/\rho} + h_2(z)\log^2\frac{1}{1-z/\rho}\right)}_{g(z)}. \tag{10}$$

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 Ξ to ρ, the functions h_0, h_1, and h_2 appearing in (10) are analytic on the disk $|z-\rho| < \rho$. Because f and ℓ are both analytic on Δ, 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 nth power series coefficient of $\ell(z)$, is easily lower-bounded using standard generating function manipulations.

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

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

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 $n \geq 1000$,*

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

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

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

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

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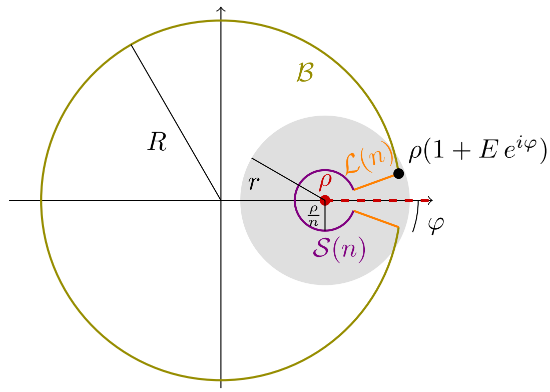

FIGURE 1. The integration path is deformed into the union of a big arc $\mathcal{B}$, a small arc $\mathcal{S}(n)$, and two line segments $\mathcal{L}(n)$. The series expansions of the basis (6) are defined on the disk $|z - \rho| < r$ with a segment removed.

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 nth term in the power series expansion of $a(z)$ centered at $z = 0$.

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

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

while the identity

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

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 nth harmonic number. Since $H_n \geq \log n + \gamma$,

$$\begin{aligned}
[z^n]\ell(z) &= [z^n]C_1(z-\rho)^{-4} + [z^n]C_2(z-\rho)^{-4}\log\frac{1}{1-z/\rho} \\
&= C_1\rho^{-n-4}[z^n](1-z)^{-4} + C_2\rho^{-n-4}[z^n](1-z)^{-4}\log\frac{1}{1-z} \\
&\geq \left(\frac{C_1 + (\gamma - 11/6)C_2}{6\rho^4}\right)n^3\rho^{-n} + \frac{C_2}{6\rho^4}n^3\rho^{-n}\log n.
\end{aligned}$$

Note that this lower bound matches the leading asymptotic behaviour (9). ∎

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

See Figure 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 φ, the paths $\mathcal{S}(n)$ 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 the punctured disk $0 < |z-\rho| < r$ does not contain any root of the leading polynomial of the differential equation (3) 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 (10) then there exist constants*

$$b_0 = [6.86 \pm 2.71{\cdot}10^{-4}], \quad b_1 = [2.85 \pm 3.20{\cdot}10^{-3}], \quad b_2 = [0.309 \pm 2.78{\cdot}10^{-4}] \tag{11}$$

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

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 ρ 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 $\log^j(w)/j!$ differ from the $\log^j(1/(1-z/\rho)) = \log(-\rho) - \log w$ appearing in the definition (8) 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 $|w^{-1}\,\tilde{u}_j(w)| \le m_0$ for $|w| \le r$.

Then, to bound the 'tails' $u_j(w) - \tilde{u}_j(w)$, we change z to $\rho + w$ in (3), 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 $|c_{j,k}| \le \hat{c}_k$ for $j = 0, 1, 2$ and $k \ge 50$ [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 $\left|w^{-1}\big(u_j(w) - \tilde{u}_j(w)\big)\right| \le m_1$ for $|w| \le r$.

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

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

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

Definition 3.6. Let B be the quadratic polynomial $B(z) = b_0 + b_1z + b_2z^2$, where the b_0, b_1, and b_2 are the constants in (11).

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

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

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

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

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

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

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

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

Proposition 3.8. *For all integers $n \geq 2$ and all small enough φ,*

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

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

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

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

$$L_+(n) = \frac{1}{2\pi}\sum_{j=0}^{2}\int_1^{E\,n}\frac{h_j\big(\rho(1+e^{i\varphi}t/n)\big)\log^j(-e^{i\varphi}n/t)}{(\rho e^{i\varphi}t/n)^3\rho^{n+1}(1+e^{i\varphi}t/n)^{n+1}}\frac{\rho e^{i\varphi}}{n}dt.$$

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

$$\int_1^\infty t^{-3}\left(1+\frac{t\cos\varphi}{n}\right)^{-n-1}dt \leq \int_1^\infty\left(1+\frac{t\cos\varphi}{n}\right)^{-n-1}dt = \frac{1}{\cos\varphi}\left(1+\frac{\cos\varphi}{n}\right)^{-n}.$$

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

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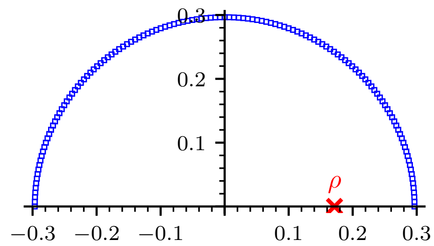

FIGURE 2. The overlapping rectangles used to establish Proposition 3.9.

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 $n \in \mathbb{N}$,*

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

Proof. Standard integral bounds imply

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

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 2, then rigorously computing bounds for $f(z)$ and $\ell(z)$ on these rectangles.

Numeric regions containing $f(z)$ on each rectangle are computed in Sage using the `numerical_solution()` method of differential operators to solve the differential equation (3) 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 [YC20] give the sequence (d_n) as a nested sequence of binomial sums. Such a sequence can be algorithmically written as the diagonal of a multivariate rational power series [BLS17], and then for sufficiently large n as an explicit multivariate saddle-point integral [PW13, Mel20]. It is theoretically possible to prove Theorem 1.4 through explicit bounds for such saddle-point integrals; this approach is less practical than going through the singularity analysis above but would give explicit constants (instead of certified intervals) for the leading asymptotic terms of d_n. A hybrid approach, using multivariate techniques to derive the leading asymptotic term with explicit coefficients then using the differential equation to bound some of the sub-dominant terms, is also possible.

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 $f(z)$ takes positive values on the real interval $z \in (0, \rho)$ [YC20, Sec. 1.3, III]. 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 of an apparent singularity $z_0 = 0.019\ldots$ of (3) in the interior of the interval 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 ρ. As a quicker alternative, we perform a *partial desingularization* of (3), yielding a new 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 ρ 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 f at the origin is bounded by 1.71 for $|z| \le r_0 = 0.0675$. As $d_0 = 72$ and $d_n > 0$ for all $n \le 1000$, 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 $|u(w) - \tilde{u}(w)| \le \hat{u}(\rho - r_0) \le m = 7.82 \cdot 10^{-9}$ for $w \le \rho - r_0$. 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 $m\left(1 - \log(\rho - z) - (1/2)\log^2(\rho - z)\right)$ 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.

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 $u_n = 2 + (-1)^n$ admits no such expansion, but the approach easily adapts to show that $u_n = [2 \pm \varepsilon] + [1 \pm \varepsilon](-1)^n \ge 0$. In the case of $v_n = 1.1 + (-1)^n + \cos(n\pi/2)$, however, additional arguments are necessary (*cf.* [vdH97]).
- The sequence $w_n = J_n(1)/n!$, where J_n is the Bessel function of the first kind, satisfies $(n+1)(n+2)w_{n+2} - 2(n+1)^2 w_{n+1} + w_n = 0$. One has $w_n \sim 1/(2^n n!^2)$, hence w_n is asymptotically positive. The minimal differential equation annihilating the generating series $f(z) = \sum_{n \ge 0} w_n z^n$

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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 $w_n=[0\pm\varepsilon]\,t_n$ for some explicit t_n with $t_n=2^n\,n^{O(1)}$ and any given $\varepsilon>0$. This is related to the fact that (w_n) is a *minimal* solution of the corresponding recurrence; the enclosure would have the correct order of magnitude for any solution not colinear with w_n.

- The crucial open case for decidability of zero checking in C-finite sequences concerns order 5 sequences (u_n) of the form $u_n=a(\lambda_1^n+\overline{\lambda_1^n})+b(\lambda_2^n+\overline{\lambda_2^n})+c\rho^n$ where $|\lambda_1|=|\lambda_2|>|\rho|$ with a,b,c real algebraic numbers and $|a|\neq|b|$. One example of such a sequence, discussed in Kenison et al. [KLOW20], is (u_n) defined by $u_{n+5}=-41u_{n+4}+952u_{n+3}-178360u_{n+2}-17673175u_{n+1}+17850625u_n$ with initial conditions $u_0=9,\ u_1=-281,\ u_2=15485,\ u_3=-1135097,\ u_4=-30999543$. Kenison et al. prove that $u_n\neq 0$ when n is a prime power. Of course, proving that the C-finite sequence (u_n^2) contains only positive terms is equivalent to proving $u_n\neq 0$ for all n.

Although there are major decidability issues related to the positivity of C-finite sequences, in naturally occuring combinatorial examples[7] these pathological issues do not arise and 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.

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[7] 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 key point for this discussion is that the singularities of an $\mathbb{N}$-rational function that are closest to the origin differ by multiples of roots of unity [Ber71]. Thus, assuming this meta-principle of Bousquet-Mélou, for any C-finite sequence c_n arising naturally from a combinatorial application there exists a positive integer $p>0$ such that $c_n\sim C_n n^{\alpha_n}\rho^n$ where ρ is a fixed algebraic number and C_n and α_n depend on n only through its value modulo p.

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Appendix: The Recurrence and Differential Equation Coefficients

The sequence (d_n) satisfies the recurrence (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

$$\begin{pmatrix}
-13041659232 & -12704294700 & -5284701480 & -1216898711 & -167529251 & -13789578 & -628408 & -12232 \\
145756088208 & 149564708370 & 65315724828 & 15735207287 & 2258693435 & 193221622 & 9123400 & 183480 \\
-647595717744 & -677411701022 & -301814933466 & -74228837833 & -10882115811 & -950915746 & -45861816 & -941864 \\
1390493835900 & 1451619424860 & 645518710454 & 158457515673 & 23184921987 & 2021855198 & 97303624 & 1993816 \\
-1472211879228 & -1524577250976 & -672459054524 & -163720428321 & -23758375953 & -2054897438 & -98090344 & -1993816 \\
709311266388 & 732023855346 & 321841622840 & 78121412337 & 11304865929 & 975235426 & 46440856 & 941864 \\
-119236161300 & -125550276502 & -56351691266 & -13970430847 & -2065443305 & -182059702 & -8857640 & -183480 \\
6546653568 & 7041743904 & 3234766134 & 822460415 & 124982969 & 11350218 & 570328 & 12232
\end{pmatrix}$$

and its generating function $f(z)$ satisfies the differential equation (3) where

$$c_3(z) = 8388593z^2(3z^4 - 164z^3 + 370z^2 - 164z + 3)(z+1)^2(z^2 - 6z + 1)^2(z-1)^3$$

$$\begin{aligned}
c_2(z) = {} & 8388593z(z+1)(z^2 - 6z + 1)(66z^8 - 3943z^7 + 18981z^6 - 16759z^5 - 30383z^4 + 47123z^3 \\
& - 17577z^2 + 971z - 15)(z-1)^2
\end{aligned}$$

$$\begin{aligned}
c_1(z) = {} & 16777186(z-1)(210z^{12} - 13761z^{11} + 101088z^{10} - 178437z^9 - 248334z^8 \\
& + 930590z^7 - 446064z^6 - 694834z^5 + 794998z^4 - 267421z^3 + 24144z^2 - 649z + 6)
\end{aligned}$$

$$\begin{aligned}
c_0(z) = {} & 6341776308z^{12} - 427012938072z^{11} + 2435594423178z^{10} - 2400915979716z^9 \\
& - 10724094731502z^8 + 26272536406048z^7 - 8496738740956z^6 - 30570113263064z^5 \\
& + 39394376229112z^4 - 19173572139496z^3 + 3825886272626z^2 - 170758199108z + 2701126946.
\end{aligned}$$