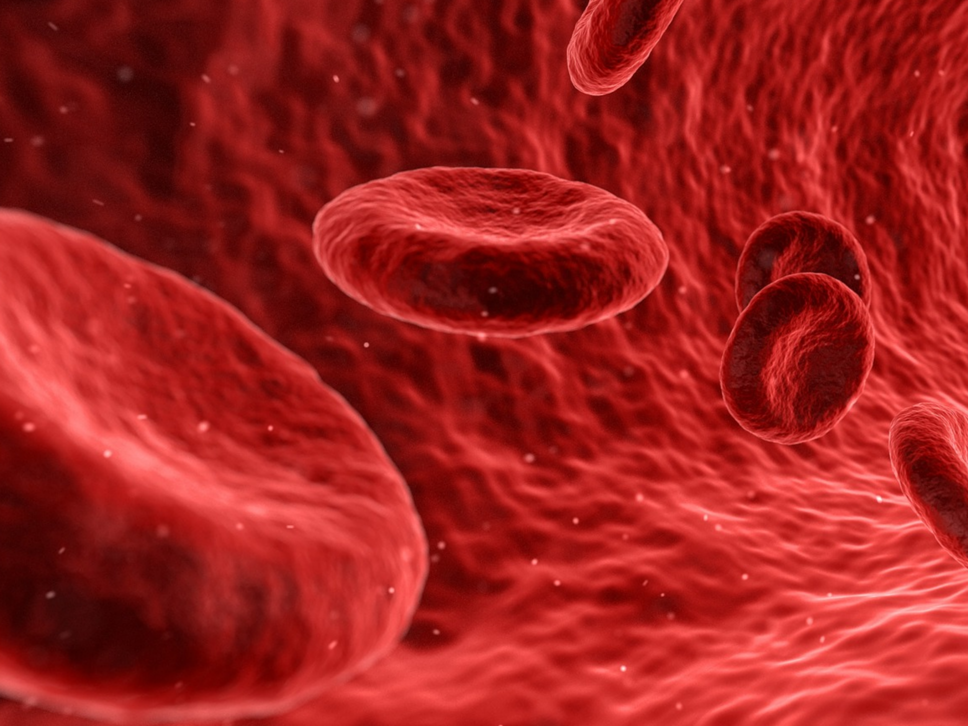
Asymptotic Expansions with Error Bounds for Solutions of Linear Recurrences

Marc Mezzarobba

CNRS, LIX, MAX

Based on joint work with **Ruiwen Dong** (Oxford) and **Stephen Melczer** (Waterloo, ON)

MAX Seminar, May 24, 2022



From Blood Cells to Minimal Surfaces

J. Theoret. Biol. (1970) **26,** 61–81

The Minimum Energy of Bending as a Possible Explanation of the Biconcave Shape of the Human Red Blood Cell

P. B. CANHAM

Department of Biophysics,
University of Western Ontario, London, Ontario, Canada

Lindström (1963) reported that cells resumed their equilibrium form within a fraction of a second after emerging from very small blood vessels. Rand (1964*b*) showed that a cell released from a micropipette returned to the biconcave shape within a few seconds. These observations imply that the biconcave form requires the least energy to be maintained. We believe the energy minimized is the bending energy of the membrane, and that the membrane is solely responsible for the cell's shape.

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Universi… Canada

Willmore Energy

$$\underbrace{\frac{1}{4}\int_S (\kappa_1 + \kappa_2)^2}_{W(S)} \quad + \quad \mathrm{cst}_g$$

Canham Model:

Min. W given g, area, volume

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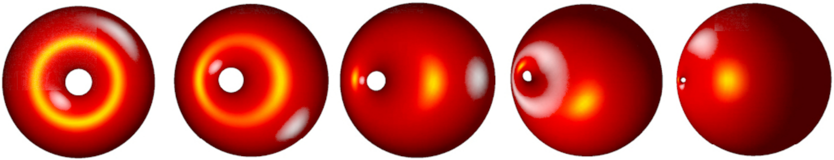
Willmore problem: minimize $W(S)$ for a surface S of given genus smoothly immersed in $\mathbb{R}^3$

- **Marques & Neves** (2012) [Willmore conjecture, 1965]
  In genus one, the unconstrained minimizers are the stereographic projections of the *Clifford torus* $\mathbb{T}_C = \mathbb{S}^1_{1/\sqrt{2}} \times \mathbb{S}^1_{1/\sqrt{2}} \subset \mathbb{S}^3$



(Yu & Chen 2022)

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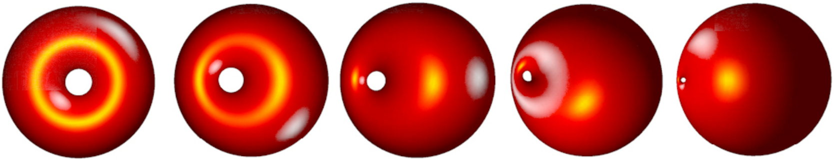
  Unique minimizer (up to scale) of given *isoperimetric ratio* $\pi^{1/6}\,(6\,V)^{1/3}\,A^{-1/2} \in [\tau_0, 1)$ (→ Canham problem)



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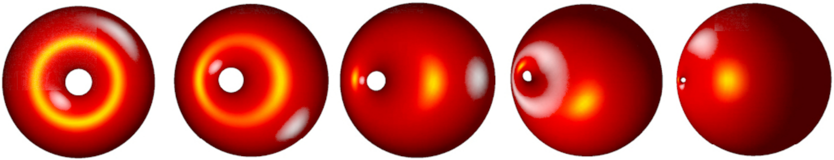
  …provided that a certain explicit sequence (d_n) is >0



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Yu and Chen's Sequence

$$(d_n) = (72, 1932, 31248, 790101/2, 17208645/4, 338898609/8, 1551478257/4, \ldots)$$

$$\begin{aligned}
&-(n+8)(n+7)(12232\,n^3+298144\,n^2+2412586\,n+6469077)(n+6)^2\ d_n \\
&+(n+8)(183480\,n^6+7655560\,n^5+131977142\,n^4+1202876299\,n^3+6112196895\,n^2 \\
&\qquad +16418149668\,n+18219511026)\ d_{n+1} \\
&-(n+8)(941864\,n^6+38326904\,n^5+644300514\,n^4+5727711699\,n^3+28407144241\,n^2 \\
&\qquad +74557779538\,n+80949464718)\ d_{n+2} \\
&+(1993816\,n^7+97303624\,n^6+2021855198\,n^5+23184921987\,n^4+158457515673\,n^3 \\
&\qquad +645518710454\,n^2+1451619424860\,n+1390493835900)\ d_{n+3} \\
&+(-1993816\,n^7-98090344\,n^6-2054897438\,n^5-23758375953\,n^4-163720428321\,n^3 \\
&\qquad -672459054524\,n^2-1524577250976\,n-1472211879228)\ d_{n+4} \\
&+(n+6)(941864\,n^6+40789672\,n^5+730497394\,n^4+6921881565\,n^3+36590122947\,n^2 \\
&\qquad +102300885158\,n+118218544398)\ d_{n+5} \\
&+(n+6)(183480\,n^6+7756760\,n^5+135519142\,n^4+1252328453\,n^3+6456460129\,n^2 \\
&\qquad +17612930492\,n+19872693550)\ d_{n+6} \\
&+(n+7)(n+6)(12232\,n^3+215600\,n^2+1256970\,n+2435511)(n+8)^2\ d_{n+7} = 0
\end{aligned}$$

Asymptotic behavior

Eventual Positivity

$$(\cdots)\, d_{n+6} + \cdots + (\cdots)\, d_{n+1} + (\cdots)\, d_n = 0$$

Routine Calculation

$$d_n = \mathbf{c} \cdot \rho^{-n} n^3 \ln(n) + O(\rho^{-n} n^3) \qquad \rho^{-1} = (\sqrt{2} + 1)^2 \approx 5.8$$

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Corollary

The sequence (d_n) is **eventually** positive.

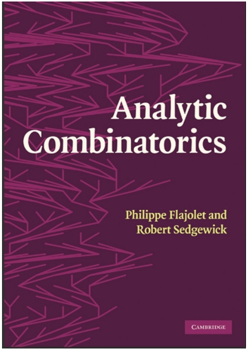
Question

Replace the $O(\cdot)$ by an explicitly bounded error term?

Positivity

Proposition [Melczer-M. 2020]

$d_n \geqslant \rho^{-n} (8.07\, n^3 \ln n + 1.37\, n^3 - 1196\, n^2 \ln^2 n)$



Corollary

$d_n > 0$ for all $n \geqslant 1000$

Real point: We now have the technology to prove bounds of this type

Next: **"General" sequences**
Algorithm + Code

[**Ruiwen Dong**'s M2 (2021) / Dong, Melczer & M. (in preparation)]

- Bostan & Yurkevich (2021) — More direct proof of Y&C's result
- van der Hoeven (2021) — Complexity of sequence evaluation

General Recurrences

$\square\, d_{n+6} + \cdots + \square\, d_{n+1} + \square\, d_n = 0$

$\Downarrow$ $d(z) = \sum_n d_n z^n$

$$\left[\begin{array}{l} z^2 (z+1)^2 (z-1)^3 (z^2 - 6z + 1)^2 \\ \quad \cdot (3z^4 - 164z^3 + 370z^2 - 164z + 3) \end{array}\right] d^{(3)}(z) + \square\, d''(z) + \square\, d'(z) + \square\, d(z) = 0$$

Assumptions

- The differential equation has **singular points** $\not\subseteq \{0, \infty\}$
- The singular points (at least, the ones we need to work with) are **regular**

Regular: $z^{i\sqrt{3}} \log^2 z + \cdots$ convergent

Irregular: $e^{\sqrt{z}+2z} z^{3/2} \log z + \cdots$ divergent

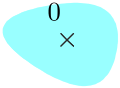
Error bounds

A Cauchy Integral

[Flajolet & Puech 1986, Flajolet & Odlyzko 1990, …]

$$z^2\,(z+1)^2\,(z-1)^3\,(z^2-6\,z+1)^2\,(3\,z^4-164\,z^3+370\,z^2-164\,z+3)\;\mathrm{d}^{(3)}(z)+\cdots=0$$

$$\mathrm{d}(z)=72+1932\,z+31248\,z^2+\cdots$$



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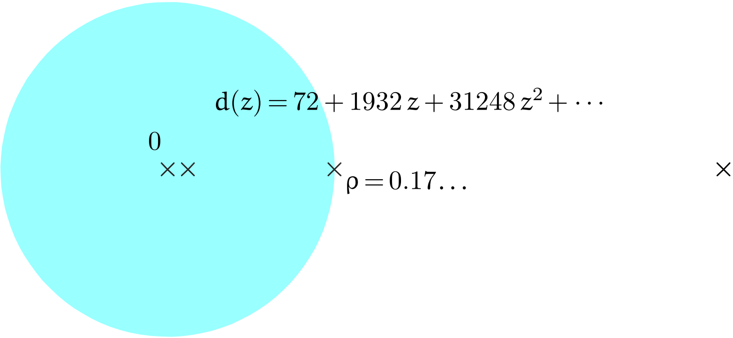

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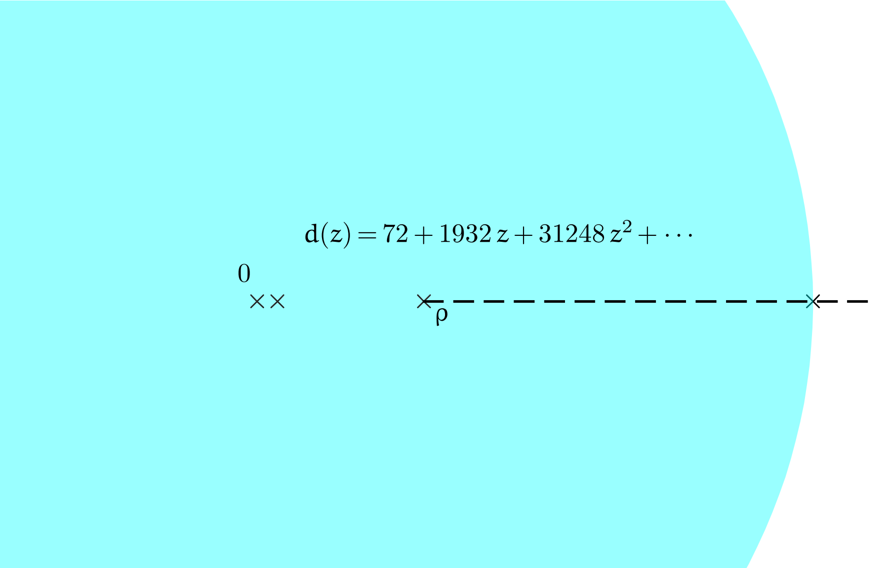

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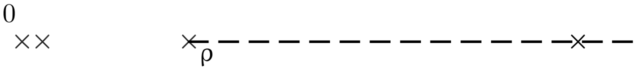

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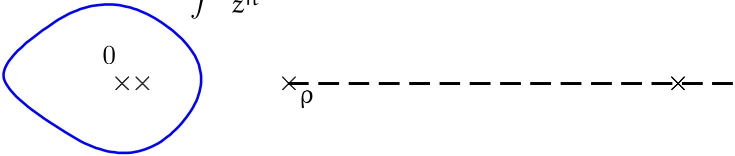

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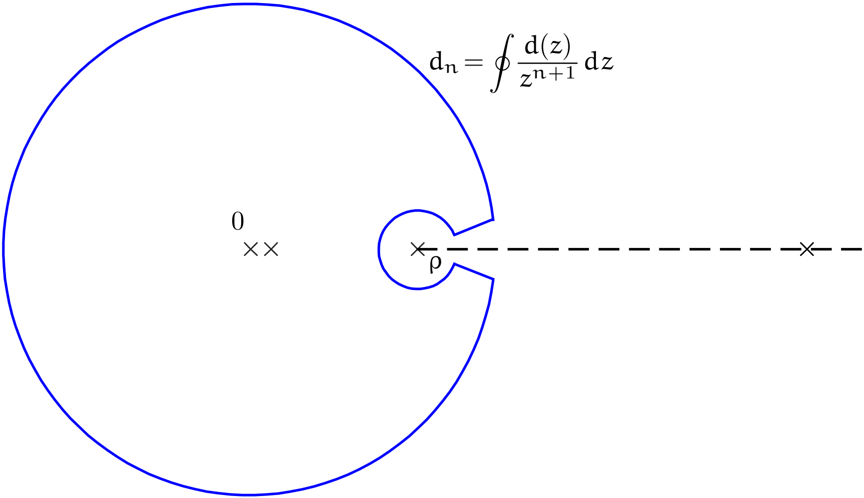

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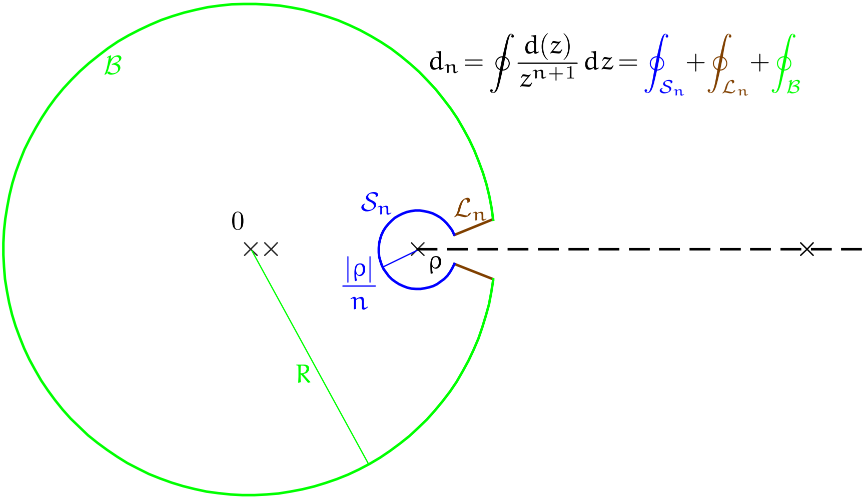

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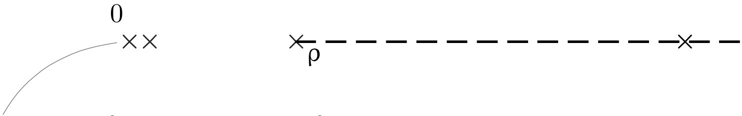

$$\left|\begin{aligned} A_1(z) &= z^{-1}\log z - 9\log^2 z + 141\log z + O(z\log^3 z)\\ A_2(z) &= z^{-1} - 18\log z \qquad\qquad\qquad\;\; + O(z\log^3 z)\\ A_3(z) &= 1 + \tfrac{161}{6}\,z \qquad\qquad\qquad\qquad\; + O(z\log^3 z)\end{aligned}\right.$$

$$\mathrm{d}(z) = 0\cdot A_1(z) + 0\cdot A_2(z) + 72\,A_3(z)$$

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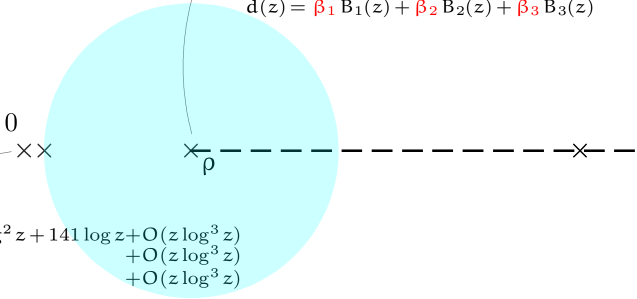

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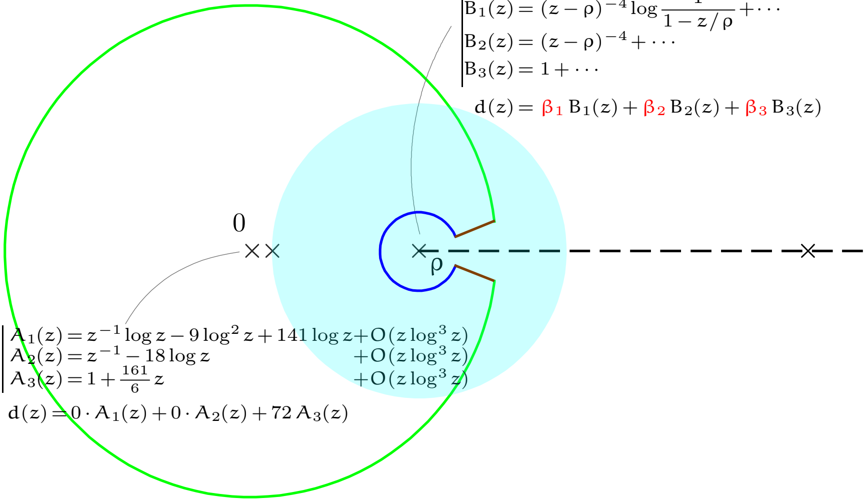

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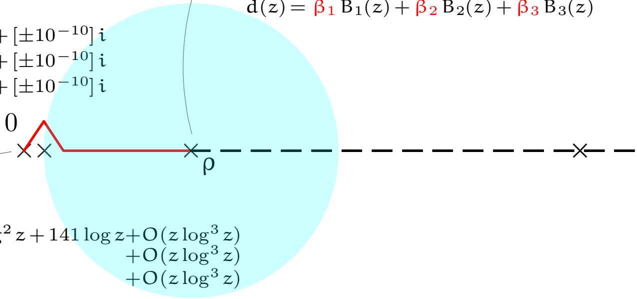
$$\begin{aligned} \beta_1 &= [0.0420\pm10^{-4}]+[\pm10^{-10}]\,i \\ \beta_2 &= [0.0598\pm10^{-4}]+[\pm10^{-10}]\,i \\ \beta_3 &= [0.7302\pm10^{-4}]+[\pm10^{-10}]\,i \end{aligned}$$



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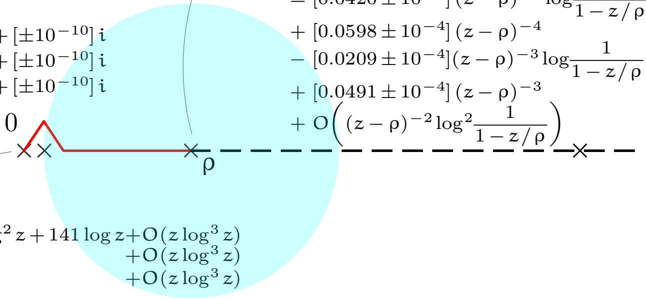

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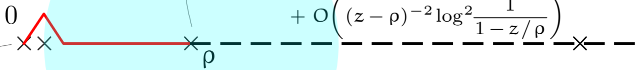

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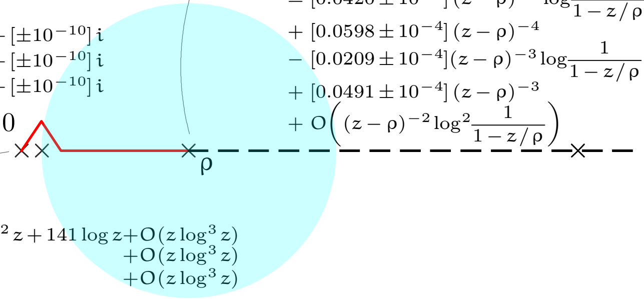
$$\begin{aligned}d(z)&=\beta_1 B_1(z)+\beta_2 B_2(z)+\beta_3 B_3(z)\\ &=[0.0420\pm10^{-4}]\,(z-\rho)^{-4}\log\frac{1}{1-z/\rho}\\ &+[0.0598\pm10^{-4}]\,(z-\rho)^{-4}\\ &-[0.0209\pm10^{-4}](z-\rho)^{-3}\log\frac{1}{1-z/\rho}\\ &+[0.0491\pm10^{-4}]\,(z-\rho)^{-3}\\ &+O\left((z-\rho)^{-2}\log^2\frac{1}{1-z/\rho}\right)\end{aligned}$$

$$\begin{aligned}\beta_1&=[0.0420\pm10^{-4}]+[\pm10^{-10}]\,i\\ \beta_2&=[0.0598\pm10^{-4}]+[\pm10^{-10}]\,i\\ \beta_3&=[0.7302\pm10^{-4}]+[\pm10^{-10}]\,i\end{aligned}$$



$$\begin{aligned}A_1(z)&=z^{-1}\log z-9\log^2 z+141\log z+O(z\log^3 z)\\ A_2(z)&=z^{-1}-18\log z+O(z\log^3 z)\\ A_3(z)&=1+\tfrac{161}{6}z+O(z\log^3 z)\end{aligned}$$

$$d(z)=0\cdot A_1(z)+0\cdot A_2(z)+72\,A_3(z)$$

A Cauchy Integral

[Flajolet & Puech 1986, Flajolet & Odlyzko 1990, …]

$$z^2(z+1)^2(z-1)^3(z^2-6z+1)^2(3z^4-164z^3+370z^2-164z+3)\,d^{(3)}(z)+\cdots=0$$

$$\begin{aligned}B_1(z)&=(z-\rho)^{-4}\log\frac{1}{1-z/\rho}+\cdots\\ B_2(z)&=(z-\rho)^{-4}+\cdots\\ B_3(z)&=1+\cdots\end{aligned}$$

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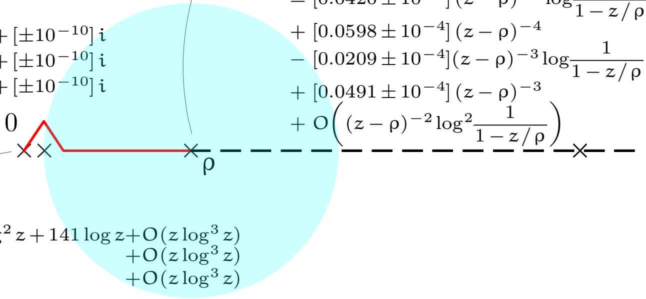

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$$d(z)=0\cdot A_1(z)+0\cdot A_2(z)+72\,A_3(z)$$

Key Numeric Tools

[van der Hoeven 2001; M. 2011, 2019; …]

z_0, z_1 — ordinary or regular singular points, with fixed associated sol bases

Rigorous Integration of Singular LODEs

Given the coordinates of a solution f in the basis at z_0:

- one can compute boxes containing the coordinates of f at z_1
- for a small enough $\boxed{z} \subset \mathbb{C}$ containing no singular points,
  one can compute a box containing $\{f(z) : z \in \boxed{z}\}$

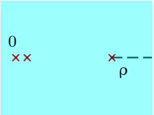
Bounds on Tails of Logarithmic Series

Given $N \in \mathbb{N}$ and $0 \leqslant \boldsymbol{\delta} < \operatorname{dist}(z_0, \{\text{singular points} \neq z_0\})$,
for each $A \in$ local basis at z_0, one can compute $\mathbf{M}_0, \ldots, \mathbf{M}_K$ such that

$$A(z) = (z-\rho)^\nu \sum_{k=0}^{K} \left(\sum_{n=0}^{N-1} u_{n,k}\,(z-\rho)^n + \underbrace{\sum_{n=N}^{\infty} u_{n,k}\,(z-\rho)^n}_{|\cdot| \leqslant \mathbf{M}_k |z-\rho|^N \text{ for } |z-\rho| \leqslant \boldsymbol{\delta}} \right) \log^k \frac{1}{1-z/\rho}$$

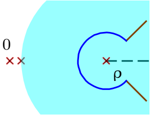
Singular Expansion

$$d(z) = \underbrace{[0.0420 \pm 10^{-4}]\,(z-\rho)^{-4}\log\frac{1}{z-\rho} + \cdots + [0.0491 \pm 10^{-4}]\,(z-\rho)^{-3}}_{\ell(z)\ \text{(more terms than needed} \Rightarrow \text{better bounds)}}$$



$$+ \underbrace{\sum_{n=\nu+r}^{\infty}\left[c_{n,0} + c_{n,1}\log\frac{1}{z-\rho} + c_{n,2}\log^2\frac{1}{z-\rho}\right](z-\rho)^n}_{g(z)}$$

$(\nu = -4, r = 2)$



$$d_n = \oint \frac{d(z)}{z^{n+1}}\,dz = \oint \frac{\ell(z)}{z^{n+1}}\,dz + \oint \frac{g(z)}{z^{n+1}}\,dz$$

$$= [z^n]\,\ell(z) + \int_{\mathcal{S}_n + \mathcal{L}_n} \frac{g(z)}{z^{n+1}}\,dz + \int_{\mathcal{B}} \frac{d(z) - \ell(z)}{z^{n+1}}\,dz$$

Bound each term for $n \geqslant n_0$

The Explicit Part (I)

[Jungen 1931, …]

$$[z^n]\,(1-z)^\alpha \log^k \frac{1}{1-z} = \frac{d^k}{d\alpha^k}\binom{n+\alpha-1}{n} \qquad (\rho = 1)$$

$$= \underbrace{\frac{\Gamma(n+\alpha)}{\Gamma(n+1)}}_{G(n)} \underbrace{\frac{1}{\Gamma(n+\alpha)}\frac{d^k}{d\alpha^k}\frac{\Gamma(n+\alpha)}{\Gamma(\alpha)}}_{H(n,k)}$$

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Lemma (Gamma ratios) Corollary of [Frenzen 1992]

For $n > |\alpha|$,

$$G(n) = n^{\alpha-1}\left(1+\frac{\alpha}{2n}\right)^{\alpha-1}\left[\sum_{j=0}^{r-1} \cdots \left(n+\frac{\alpha}{2}\right)^{-j} + R(n)\right]$$

$$|R(n)| \leqslant C_{\alpha,r,n_0}\left|n+\frac{\alpha}{2}\right|^{-r}$$

Then plug in Taylor expansions in n^{-1} of $\left(1+\frac{\alpha}{2n}\right)^{\alpha-1}$ and $\left(n+\frac{\alpha}{2}\right)^{-j}$

$\cdots$ = explicit coefficients
in terms of generalized Bernoulli numbers

C_{α,r,n_0} = explicit constant

The Explicit Part (I)

[Jungen 1931, …]

$$[z^n]\,(1-z)^\alpha \log^k \frac{1}{1-z} = \frac{d^k}{d\alpha^k}\binom{n+\alpha-1}{n} \qquad (\rho = 1)$$

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Lemma (Gamma ratios) Corollary of [Frenzen 1992]

For $n > |\alpha|$, ← Constraint on n_0

$$G(n) = n^{\alpha-1}\left(1+\frac{\alpha}{2n}\right)^{\alpha-1}\left[\sum_{j=0}^{r-1} \cdots \left(n+\frac{\alpha}{2}\right)^{-j} + R(n)\right]$$

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$\cdots$ = explicit coefficients in terms of generalized Bernoulli numbers

C_{α,r,n_0} = explicit constant

The Explicit Part (II)

$$[z^n]\,(1-z)^\alpha \log^k \frac{1}{1-z} = \underbrace{\frac{\Gamma(n+\alpha)}{\Gamma(n+1)}}_{G(n)} \underbrace{\frac{1}{\Gamma(n+\alpha)} \frac{d^k}{d\alpha^k} \frac{\Gamma(n+\alpha)}{\Gamma(\alpha)}}_{H(n,k)} \qquad (\rho = 1)$$

Lemma

$$H(n,k) = \frac{k!}{\Gamma(\alpha)} [\varepsilon^k] \exp\left(\sum_{m=0}^{k-1} \frac{\psi^{(m)}(n+\alpha) - \psi^{(m)}(\alpha)}{(m+1)!} \varepsilon^{m+1} \right) \qquad (1)$$

+ similar formula for $\alpha \in \mathbb{Z}_{\leqslant 0}$

Theorem [Nemes 2017]

For $|\arg z| \leqslant \pi/4$ and $m \geqslant 1$

$$\psi^{(0)}(z) = \log z - \sum_{j=0}^{r-1} \frac{\cdots}{z^j} + R(z), \qquad |R(z)| \leqslant C_{0,r}\, |z|^{-r}$$

+ similar formula for $m \geqslant 1$

Algorithm: plug Nemes' bounds into (1),
compose multivariate polynomials with interval coefficients

The Explicit Part: Summary

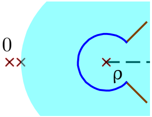
$$\ell(z) = [0.0420 \pm 10^{-4}]\,(z-\rho)^{-4}\log\frac{1}{z-\rho} + \cdots + [0.0491 \pm 10^{-4}]\,(z-\rho)^{-3}$$

$$[z^n]\,(z-\rho)^{-\alpha}\log^k\frac{1}{z-\rho}$$
$$= \rho^{-n}\,n^{\alpha-1}\Big(\square\log^k n + \square\log^{k-1} n + \cdots + \square$$
$$+ \square\,\frac{\log^k n}{n} + \cdots + \square\,\frac{1}{n}$$
$$+ \cdots$$
$$+ R(n)\Big)$$

$$[z^n]\,\ell(z) = \rho^{-n}\Big([8.07 \pm 10^{-3}]\,n^3\ln n + [1.37 \pm 10^{-3}]\,n^3$$
$$+[50.5 \pm 10^{-1}]\,n^2\ln n + [29.7 \pm 10^{-1}]\,n^2$$
$$+ [\pm 1.5\cdot 10^3]\,n\ln^2 n\Big)$$

for all $n \geqslant 50$

The Local Error Term



$$g(z) = (z-\rho)^{\nu+r}\Big(\underbrace{h_0(z)}_{|\cdot|\leqslant B_0} + \underbrace{h_1(z)}_{|\cdot|\leqslant B_1} \log\frac{1}{z-\rho} + \underbrace{h_2(z)}_{|\cdot|\leqslant B_2} \log^2\frac{1}{z-\rho}\Big)$$

$$B(z) = B_0 + B_1 z + B_2 z^2 \qquad\qquad \left|\log\frac{1}{1-z/\rho}\right| \leqslant \pi + \log n \quad \text{on} \quad \mathcal{S}_n$$

Lemma (Error term on the small arc)

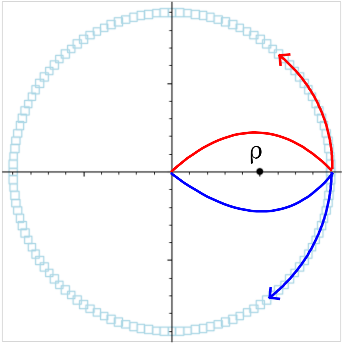
$$\left|\frac{1}{2\pi i}\int_{\mathcal{S}_n}\frac{g(z)}{z^{n+1}}\,dz\right| \leqslant \frac{C_{\rho,\nu,\mathbf{r}}}{(1-1/n_0)^{n_0+1}}\,|\rho|^{-n}\,n^{-\mathrm{Re}(\nu)-1-\mathbf{r}}\,B(\pi+\log n)$$

Lemma (Error term on the line segments)

$$\lim_{\varphi\to 0}\left|\frac{1}{2\pi i}\int_{\mathcal{L}_n}\frac{g(z)}{z^{n+1}}\,dz\right| \leqslant C'_{\rho,\nu,\mathbf{r}}\,|\rho|^{-n}\,n^{-\mathrm{Re}(\nu)-1-\mathbf{r}}\,B(\pi+\log n)$$

The Global Error Term

$$\left|\frac{1}{2\pi i}\int_{\mathcal{B}}\frac{d(z)-\ell(z)}{z^{n+1}}\,dz\right| \leqslant R^{-n}\max_{|z|=R}|d(z)-\ell(z)|$$
$$\leqslant C_{n_0}\,|\rho|^{-n}\,n^{\beta}\log^{k}n$$



compute $d(z)$ using the diff. eq.

(staying in the analyticity domain of $d(z)$!)

Conclusion

"Generic Case"

$$\rho^{-n}\,n^3\Big(\underbrace{[8.07{\pm}10^{-3}]\ln n+[1.37{\pm}10^{-3}]+[50.5{\pm}10^{-1}]\frac{\ln n}{n}+[29.7{\pm}10^{-1}]\frac{1}{n}}_{\text{truncated asymptotic expansion}}+\underbrace{[\pm 2\cdot 10^3]\,\frac{\ln^2 n}{n^2}}_{\text{error term}}\Big),$$

$n \geqslant 50$

What may go wrong

- Multiple dominant singularities $\quad 2^n\left(\square+\frac{\square}{n}\right)+(-2)^n\left(\square+\frac{\square}{n}\right)+[\pm M]\,\frac{1}{n^2}$
  - not an asymptotic expansion
  - still makes sense as a bound
- Failure to detect exact zeros $\quad 2^n\left([\pm 10^{-100}]+\cdots\right)+[12.3\pm 10^{-1}]+\frac{[4.56\pm 10^{-1}]}{n}$
  - useless bound
  - …except with an oracle
- Overestimation $\quad 2^n\left([\pm 10^{1000}]+\cdots+\right)$
  - rare in practice on "small" examples, full analysis???
- Irregular singular points

Image Credits

- Red blood cells

  https://pixabay.com/illustrations/blood-cells-red-medical-medicine-1813410/

